MODELLING APPROACHES AND MEASUREMENTS TO STUDY THE EFFECT OF NUTRIENT MANAGEMENT ON THE SUSTAINABILITY OF A DAIRY FARM

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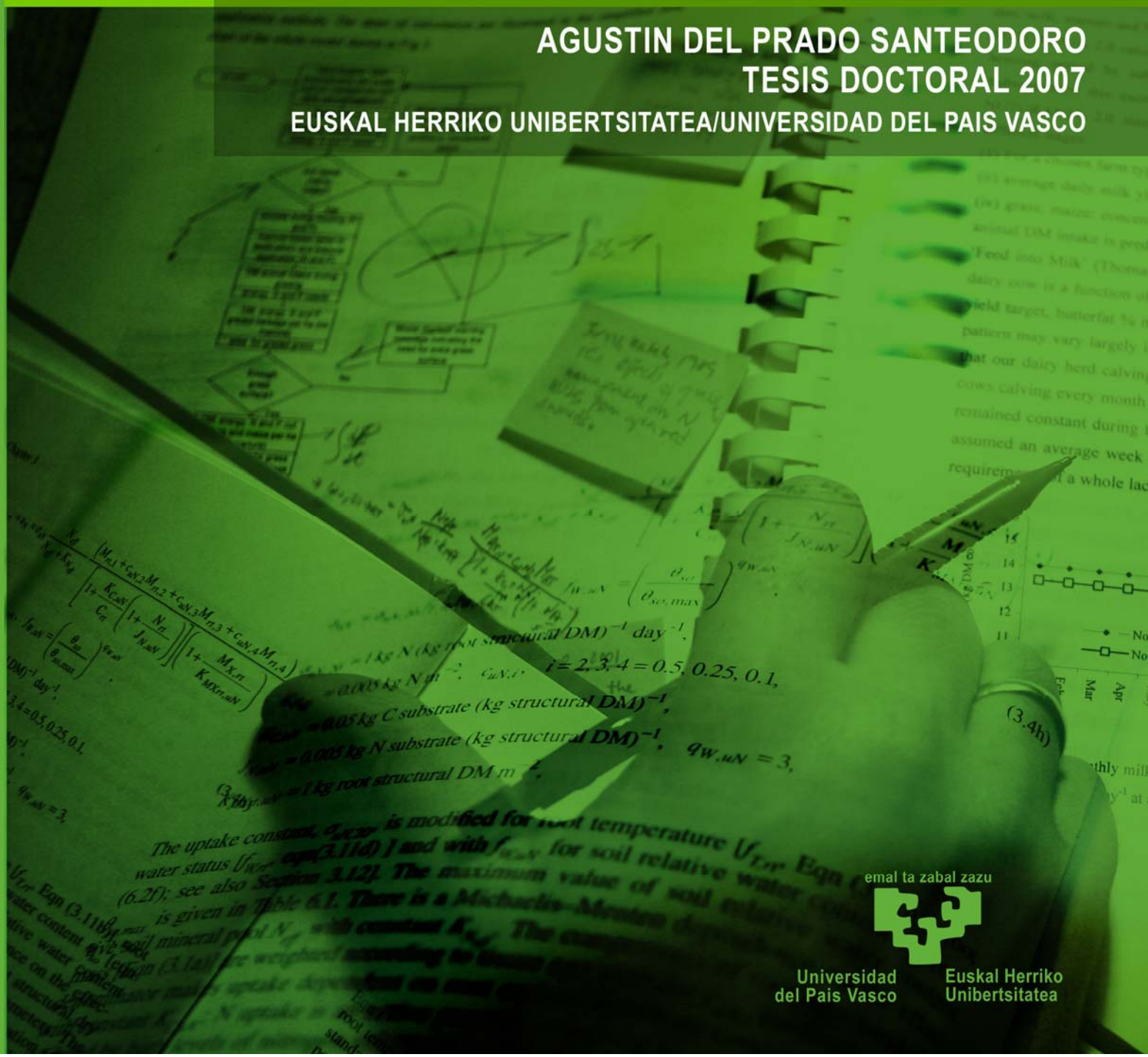
TESIS DOCTORAL 2007

EUSKAL HERRIKO UNIBERTSITATEA/UNIVERSIDAD DEL PAIS VASCO



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Universidad del Pais Vasco

Euskal Herriko Unibertsitatea

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Leioa, Marzo 2007

A mis padres, los verdaderos sufridores en casa

Agradecimientos/Acknowledgements

A la Dra. Pilar Merino. Mi directora, mentora, compañera y amiga. Empecé con ella como monitorizador, pintxe de su tesis, acolito de grado-tesina y en los últimos tiempos y a pesar de la distancia no se ha conseguido librar de mí como tesis-maker. Pilar ha sido en todo momento una pieza muy importante en esta tesis ya que ha puesto en su lugar cada cosa y ha sido una gran ayuda a la hora de atemperar mis ánimos cuando los he perdido. Científicamente, siempre he procurado seguir su estela de rigurosidad. A pesar de todos los momentos serios y llenos de ciencia, en algunos casos ficción, mis mejores recuerdos no son sino aquellos en los que me ha hecho desternillarme de risa, especialmente en aquellas interminables y divertidas sesiones de mediciones de N_2O, las campañas del COGANOG o algún que otro gran momento en congresos. Espero que en el futuro, estemos donde estemos, continuemos nuestra fructífera colaboración.

To Pfr. Dr. David Scholefield. My supervisor in Devonian territory. Thank you for putting up with this non-so-conventional thesis and my Spanglish. Most of my modelling inspiration is due to our formal/informal chatting through your visits in my office and through some binge drinking in our visits overseas. Our scientific relationship has been quite fruitful in this almost 5 years. Personally, you have also been great support. I am aware that I may be your last PhD supervision before you plan to buy some villas in Gibraltar or even in Bilbao.

A la Catedrática Carmen González-Murua. Ella fue quien me convenció para que no me fuera al extranjero con una beca “Leonardo” allá por 1997 y aceptara mejor una del INIA para estar en casita. Gracias por tu optimismo y apoyo en los momentos difíciles.

Al Dr. Txema Estavillo. Con él inicié mi andadura científica en el 1997. Sus historias de sobre lo fácil que era ser un “squatter” en Inglaterra me ayudaron finalmente a decidirme emigrar. Suyos (junto con Pilar y Miriam) son los momentos más hilarantes de las campañas del COGANOG y alguna que otra de congresos. Gracias por la ayuda en los últimos tiempos en los trámites de la tesis. Nos vemos en Comarruga. Eso sí, si me reconoces esta vez.

A la Dra. Miriam Pinto. Ella fue una gran ayuda en mis años en NEIKER. Gracias por tus consejos, tu apoyo y sobre todo ese gran humor que nos inundaba las campañas del COGANOG y congresos

varios. Creo que es el momento de que alguien exprese públicamente el temor que nos hiciste pasar en el viaje a Bayreuth. Afortunadamente eran otros tiempos donde no había carné por puntos.

To Pfr. Dr. Oene Oenema. Thank you for being such a good host in Wageningen. Thank you for introducing me to the world of modelling without having to lose weight. Thank you for your scientific conversations and visits to the local Wageningen bars. Dank u wel!

To Dr. Wim Corré. Thank you for your time in Wageningen to develop NUTGRANJA.

A Oscar del Hierro. Gracias por tu inestimable ayuda, apoyo y buen hacer en todo lo relacionado con Behi-alde. Gracias por los momentos "jumpy", las comidas, las pipas, "momento contratote", gracias por enseñarme todo sobre los mapas y el P. Siempre nos quedara Castro para largarnos con la pasta de la Cándida.

A Laura Cárdenas. Gracias por tus consejos, tu amistad, tu apoyo fuera y dentro del trabajo. Probablemente sin tu ayuda no habría sobrevivido al primer invierno en Okehampton.

A Dolores Báez. Gracias por tus inestimables consejos y esos buenos ratos de nitrógeno.

A Ainara Artetxe. Gracias por tu ayuda en Behi-alde y por aguantarnos en el salón becarios a todos los energúmenos que por élla hemos pasado.

To Lorna Brown. Thank you for guiding me in my first years at IGER. Thank you for your scientific help and friendship. By the way, apologies for not keeping in good shape your washing machine and tumble drier.

To Elaine Jewkes, David Hogan, Christopher Macleod and Phil Nightingale. Thank you for your useful comments and English corrections. Without you I would have probably crashed the "spelling and grammar" word tool.

A Antonio Vallejo. Gracias por ser un buen "mate". Gracias por tus consejos y por tu hospitalidad en Madrid y en South Zeal. Espero que nuestra colaboración conjunta en un futuro cercano vaya más allá del Macrote-vil-DNDC.

A Javier Hernández. Gracias por los momentos pipas y por tus peroratas sin fin. Gracias por los momentos cool-Harpenden, momentos chollu…

A todos aquellos que han hecho mi existencia más feliz o al menos mas entretenida en Derio, Wageningen y North Wyke: Fernando, Isma, Maria, Howard, Blanca, Sergio, David, Ana, Marta, Michael, Fabrice, Noelia, Guillermo, Emma, Joao, Martina, Pilar, Goio, Aritz(s), Maika, Susana, Leyre, Arrate, Laurita…

To those who have contributed as co-authors in the published papers appearing in this thesis:
Brown L. (chapters 3, 7 and 9), Scholefield D. (chapter 3, 7 and 9), Jewkes E.C. (chapter 7), Lockyer D.R (chapter 7), Theobald M.R. (chapter 9), Dragosits U. (chapter 9), Place C.J. (chapter 9), Smith J.U. (chapter 9), Webb J. (chapter 9), Whitehead P.G. (chapter 9), Angus A. (chapter 9), Hodge I.D. (chapter 9), Fowler D. (chapter 9), Sutton M.A. (chapter 9), Ryan M. (chapter 3), Schulte R (chapter 3), Merino P. (chapter 5), Estavillo J.M. (chapter 5), Pinto M. (chapter 5) and González-Murua C (chapter 5).

A aquellas entidades que han contribuido con financiación: DEFRA, BBSRC, NERC, EPA, CYCYT, INIA, FAIR, Departamento Vasco de Agricultura y Pesca y Fundación Cándido de Iturriaga y María de Dañobeitia.

A mi hermana Mari, Javi-cuñao y Mario. Gracias por vuestro apoyo a la hora de tomar decisiones y vuestra ayuda en todo lo que ha estado en vuestra mano.

Моей жен: Аленушке. Спасибо тебе за то, что ты нашла меня в этом мире, спасибо за то, что ты была всегда рядом, за твою поддержку и постоянную заботу обо мне, особенно в те моменты, когда я наиболее нуждался в них, я глубоко признателен тебе за энтузиазм и неоценимую помощь в обсуждении тезисов моей диссертации, переводе и ее оформлении, спасибо за то, что всегда терпеливо выслушивала меня и мирилась со мной. Теперь пришло время, когда мы будем проводить наши вечера и уикэнды, наслаждаясь общением. Я люблю тебя больше всего на свете!

A mis padres. Sin vosotros no habría sido capaz de casi nada. Gracias por alimentarme cuando estaba en casa (algunas veces de más). Gracias por vuestra comprensión y ayuda en los momentos más

difíciles y sobre todo gracias por el apoyo en todo momento en lo que habéis podido en casa y cuando he estado lejos.

Abstract

European dairy farming has evolved mainly in response to economic drivers but additionally is now being given sociological and ecological goals. There is a need to balance these socio-economic and ecological pressures in the form of more sustainable systems. Farm management has been identified as the single most important factor determining the economic and environmental performance of farming systems and has also been shown to strongly affect many sociological aspects (e.g. animal welfare). Although linking these multiple interactions that occur in these systems to practical actions and decisions is not easy; mathematical models offer this capability.

So far, existing modelling approaches have generally been either too biased on single specific issues and/or too soft-science based and/or insensitive to the main controls, hence only partially capturing the key factors and key processes and showing a partial reflection of the complex chain of causes and effects. Therefore, there is a need for modelling approaches that can overcome these shortcomings.

This thesis is centred on the development of different mass-balance empirical modelling approaches and their application to study the effect of dairy farm nutrient management and edapho-climatic conditions on: (i) environmental losses contributing to climate change (N_2O and CH_4), acid rain (NH_3 and NO_x) and water eutrophication (NO_3^- and P), (ii) farm economic variables (e.g. herbage production) and (iii) other attributes affecting farm sustainability (e.g. milk quality).

The annual N mass-balance empirical modelling approach, originally developed to simulate the N fluxes in UK grazed grasslands (NCYCLE), is successfully modified and applied to other countries (Ireland and Basque Country), using various scales (farm and landscape) and at shorter calculation time-steps (monthly). The scope of application of these approaches range from a simple simulation of N use efficiency in a grassland at an annual time-step (NCYCLE_IRL) to a complex optimisation for optimal balance between socio-economic and ecological farm variables at a monthly time-step ($SIMS_{DAIRY}$).

It is demonstrated that the simple models (e.g. NCYCLE_IRL and NUTGRANJA 2.0), by matching the available data with the suitable complexity to represent the functional

relationships among the components of the grassland-based system, are capable of: (i) integrating the key processes of nutrient cycling of N and P in grassland-based systems and (ii) simulate the effect of management and edapho-climatic conditions on the N use efficiency of grassland-based systems.

The reliability of the approaches at field scale is demonstrated by validation exercises, by which predictions of N losses and yields prove to agree reasonably well within the expected and measured ranges. However, it is highlighted the need for more and larger reliable data-sets in order to validate approaches at broader scales and also to transform deterministic into stochastic models. Sensitivity analyses are also carried out to get a good overview of the most sensitive components of the modelling approaches.

The applicability of the approaches is shown to be especially relevant for policy making (e.g. in NVZ action plan), to find existing (e.g. through balancing intensification/ extensification) or new (e.g. through new plant traits) sustainable systems and, although specifically built for current dairy farming systems in the UK, Basque Country and Ireland, they could be modified to simulate other systems (e.g. non-dairy animals), in other countries and under different future climatic conditions.

The effect of some management (e.g. fertiliser type and amount) and edapho-climatic variables on N_2O and NO emissions was also evaluated through 2 experiments and relationships between soil variables (e.g. water content, temperature and mineral N) and N_2O and NO were established for predictive purposes.

Resumen

El sector lechero europeo se ha desarrollado principalmente en respuesta a incentivos económicos. En la actualidad, además, ha de atender a demandas sociales y ecológicas. Es necesario por tanto encontrar sistemas más sostenibles que puedan equilibrar tanto las presiones socio-económicas como las ecológicas. El manejo no sólo se ha visto que es el factor más importante a la hora de determinar el comportamiento económico y medioambiental de las explotaciones, sino que además condiciona en gran medida otros aspectos sociológicos (p. ej. el bienestar animal). Aunque en la práctica ligar la infinidad de interacciones que ocurren entre estos sistemas con acciones y decisiones no es fácil, los modelos matemáticos nos permiten hacerlo.

Hasta ahora, los enfoques de modelización existentes se han centrado sólo en uno o unos pocos componentes del sistema y/o no tienen una fuerte base científica y/o son insensibles a la mayor parte de los controles importantes del sistema. De este modo, estos tipos de enfoques sólo pueden simular estos sistemas de forma parcial y sólo pueden reflejar una pequeña parte de las complejas interacciones de causas y de efectos del sistema. Por lo tanto, hay una necesidad de desarrollar modelos que puedan superar estas limitaciones.

Esta tesis se centra, por tanto, en el desarrollo de nuevos modelos matemáticos empíricos y basados en el balance de masas para sistemas de ganado vacuno lechero. Estos modelos son capaces de estudiar el efecto del manejo de los nutrientes y las condiciones edafo-climáticas de la explotación sobre: (i) las pérdidas medioambientales que contribuyen al cambio climático (N_2O y CH_4), la lluvia ácida (NH_3 y NO_x) y la eutrofización de sistemas acuáticos (NO_3^- y P), (ii) las variables económicas de la explotación y (iii) otros atributos importantes que afectan a la sostenibilidad global de la explotación (p. ej. calidad de la leche).

El modelo anual empírico de balance de masas que originalmente se desarrolló para simular el flujo de N en praderas pastadas del Reino Unido (NCYCLE) se ha usado como base para el desarrollo de los modelos de esta tesis. NCYCLE se ha modificado con éxito para ser aplicado a otros países (Irlanda y País Vasco), a diferentes escalas espaciales (escala explotación y paisaje) y con pasos de tiempo (*time-steps*) más cortos (mensuales). El alcance en la utilidad de los modelos desarrollados en esta tesis varía desde aquellos más sencillos

que permiten una simulación de la eficiencia del uso del N en una pradera y usando unos pasos de tiempo anuales (NCYCLE_IRL) a aquellos más complejos, con pasos de tiempo mensuales y que permiten optimizar las explotaciones con el fin de encontrar un óptimo balance entre las variables socio-económicas y ecológicas de la explotación ($SIMS_{DAIRY}$).

En este trabajo se demuestra que modelos sencillos (p. ej. NCYCLE_IRL y NUTGRANJA 2.0) construidos compaginando la información y datos disponibles con una adecuada complejidad del sistema pueden representar las relaciones funcionales entre los principales componentes de los sistemas de praderas. De este modo estos modelos son capaces de integrar los procesos claves del ciclo de N y P y además pueden simular adecuadamente el efecto del manejo y las condiciones edafo-climáticas sobre el uso eficiente del N en sistemas de praderas.

En este estudio se demuestra el nivel de confianza de los modelos a escala de parcela a través de ejercicios de validación, por los cuales se ve que las predicciones y las mediciones de pérdidas de N y producción en hierba coinciden razonablemente bien. Sin embargo, se destaca la necesidad de producir mayores y más fiables bases de datos para validar no sólo modelos a escalas mayores, sino también para transformar modelos determinísticos en estocásticos. Los análisis de sensibilidad de los modelos en esta tesis proporcionan a su vez una buena descripción de los componentes más sensibles del sistema.

La aplicabilidad de los modelos de esta tesis es especialmente relevante para el desarrollo de legislaciones (p. ej. el plan de acción de las zonas vulnerables a nitratos) y para encontrar sistemas sostenibles en la actualidad (p. ej. buscando el equilibrio entre extensification e intensificación de dichos sistemas) o en el futuro (p. ej. a través de mejoras genéticas en las plantas). Así mismo, aunque estos modelos se han construido específicamente para sistemas actuales de ganado vacuno lechero del Reino Unido, País Vasco y de Irlanda, estos podrían ser modificados para simular otros sistemas (p. ej. animales no lecheros), en otros países y bajo condiciones climáticas futuras.

En esta tesis también se evalúa la influencia de ciertos manejos (p. ej. el tipo y cantidad de fertilizante) y de ciertas variables edafo-climáticas en las emisiones de N_2O y NO en dos ensayos. Los datos de dichos ensayos sirven para establecer relaciones predictivas entre variables del suelo (p. ej. el contenido hídrico, la temperatura y el N mineral) y los flujos de N_2O y NO.

Laburpena

Europako esne sektorea ekonomi-pizgarriei jarraikiz garatu da batez ere. Gaur egun, horrez gain, gizarte eta ekologi mailako eskaerei ere erantzun behar die. Hortaz, beharrezkoa da nola presio sozioekonomikoak hala presio ekologikoak orekatuko dituzten sistema iraunkorragoak aurkitzea. Maneiua, ikusi da, ustiategien ekonomi eta ingurugiro mailako portaerak baldintzatzen dituen faktorerik garrantzitsuena ez eze, hein handi batean bestelako aspektu sozioekologiko batzuk ere (animalien ongizatea, esaterako) baldintzatzen dituen faktorea ere badela. Errealitatean sistema hauetan gertatzen diren interakzio anitzak ekintzekin eta erabakiekin uztartzea erraza ez den arren, modelo matematikoek posible egiten dute.

Orain arte modeloek sistemaren osagarri batean edo gutxi batzuetan besterik ez dute jarri arreta edo/eta ez dute izan oinarri zientifiko sendorik edo/eta sistemaren kontrol importante gehienekiko ez dira sentikorrak izan. Beraz, gisa honetako modeloek modu partzialean besterik ezin dituzte simulatu sistema hauek eta sistemaren kausen eta ondorioen katea konplexuen zati txiki bat bakarrik isla dezakete. Hau dela eta, muga hauek gaindituko dituzten modeloak garatzeko beharrizana dago.

Tesi honetan, beraz, masen balantzean oinarritutako modelo matematiko enpiriko berrien garapenean jartzen da arreta eta berauen aplikazioan esne-behi sistemetan, elikagaien maneiuaren eta baldintza edafo-klimatikoen eragina aztertzeko: (i) ingurugiro galeretan, zeintzuek aldaketa klimatikoan (N_2O eta CH_4), euri azidoan (NH_3 eta NO_x) eta sistema akuatikoen eutrofizazioan (NO_3^- eta P) eragiten baitute, (ii) ustiategiko ekonomi aldagaietan eta (iii) ustiategiaren iraunkortasun orokorrean eragiten duten bestelako ezaugarri garrantzizko batzuetan (hala nola, esnearen kalitatean).

Tesi honetako modeloak garatzeko, masen balantzean oinarritutako modelo enpiriko bat (NCYCLE) hartu da abiapuntu; modelo hau Erresuma Batuko bazkatutako larreetako N fluxuak simulatzeko garatu zen. NCYCLE modeloan aldaketak egin izan dira beste herrialde batzuetara (Irlanda eta Euskal Herria), espazio-eskala desberdinetara (paisaia eta ustiategi eskala) eta denbora-epe laburragoetara (urtetik hilabetera) egokitzeko; era arrakastatsuan egokitu ere. Tesi honetan garatutako modeloen erabilerari dagokionez, denetarikoak daude: urteko denbora-epea erabiliz, belardi batean nitrogenoaren erabileraren eraginkortasuna

simulatzea ahalbidetzen duten modelo sinpleetatik hasita (NCYCLE_IRL), hilabeteko denbora-epeak erabiliz ustiategiko baldintza sozioekonomikoen eta ekologikoen arteko balantze hoberena bilatzen duten modeloetaraino ($SIMS_{DAIRY}$).

Lan honetan frogatzen da eskuragarri dagoen informazioa eta datuak sistemaren konplexutasun maila egokiarekin uztartuz sortuta diren modelo sinpleak (NCYCLE_IRL eta NUTGRANJA 2.0, esaterako) gai direla belardi-sistemen osagarri nagusien arteko erlazio funtzionalak adierazteko. Honela, modelo hauetan N eta P elikagaien zikloaren funtsezko prozesuak integra daitezke eta, gainera, era egokian simula daiteke belardi-sistemetan nitrogenoaren erabileraren eraginkortasunean maneiuak eta baldintza edafo-klimatikoek duten eragina.

Ikerketa lan honetan modeloek lursail eskalan duten fidagarritasuna frogatzen da, balidazio ariketen bidez; balidazio hauetan modeloek aurrikusitako N galera eta belar ekoizpenak benetan neurtutakoekin, zentzuzko neurri batean, bat datozela ikusten baita. Haatik, datu base handiagoak eta fidagarriagoak sortzeko beharrizana agertzen da, modeloak eskala haundiagoetan balidatzeko balio dezaten eta baita modelo deterministikoak estokastiko bihurtzeko ere. Tesi honetako modeloen sentsibilitate analisiek, bide batez, sistemaren osagarri sentsibleenen deskribapena ere ahalbidetzen dute.

Tesi honetako modeloen erabilerarik nabarmenenak legeen garapenean (adibidez, nitratoekin kutsatzeko Arriskutan dauden Inguruetako jarduteko planak) eta sistemarik iraunkorrenak bilatzean dautza, bai gaur egunean (sistema hauen estentsifikazio eta intentsifikazioaren arteko oreka bilatzeko, esaterako) bai etorkizunean (landareen hobekuntza genetikoaren bidez, esate baterako). Horrez gain, modelo hauek Erresuma Batuko, Euskal Herriko eta Irlandako egungo esne-behi sistemendako berariaz garatu badira ere, bestelako sistema batzuk (adibidez, esnetarako ez diren animaliak), herrialde ezberdinetako eta etorkizuneko baldintza klimatikoak islatzeko egoki litezke.

Tesi honetan, bi entseguren bitartez, maneiu (ongarri mota eta kantitatea, esaterako) eta aldagai edafo-klimatiko jakin batzuek N_2O eta NO emisioetan duten eragina ere aztertzen da. Entseguotako datuak lurzoruko aldagaien (adibidez, ur edukia, temperatura eta N mineral edukia) eta N_2O eta NO fluxuen arteko elkarrekintzak aurrikusteko baliagarri dira.

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Chapter 1. General introduction

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1.1. Why is there a need for sustainable agricultural systems?

Agricultural production has increased at a steep rate in the last 40 years, mainly from the increased yields resulting from greater inputs of fertiliser, water and pesticides, new crop strains, and other technologies of the 'Green Revolution' (FAO, 2001; Tilman *et al.,* 2001). This has increased the global per capita food supply but it has also resulted in sparing natural ecosystems from conversion to agriculture (Waggoner, 1995).

With increased prosperity, people are consuming more meat and dairy products every year. Global meat production is projected to more than double from 229 million tonnes in 1999/2001 to 465 million tonnes in 2050, while milk output is set to climb from 580 to 1043 million tonnes (FAO, 2006). Much of this increase is expected to come from developing countries, where demand for meat and milk is growing much faster than in the developed countries (Delgado, 2005; Sims *et al*., 2005). The extra productivity required in the developing countries will be achieved by increased inputs of nutrients to pastures and to support the growth of feed crops, increased efficiency of nutrient use and, to a lesser extent, increased area of managed agricultural land (FAO, 2003). Unfortunately though, as the inputs of nutrients to pasture and crops are increased, the efficiency with which they are used is generally decreased (Scholefield *et al*., 2007).

Doubling food production again and sustaining food production at this level, are hence major challenges (Alexandratos, 1999; Postel, 1999). Doing so in ways that do not compromise environmental integrity (Vitousek *et al*., 1997; Carpenter *et al.,* 1998), landscape characteristics, biodiversity richness, soil quality, and animal and public health (Smith *et al*., 1999; Gorback, 2001) is a greater challenge still.

Projections of world population, expected to increase from 6.5 billion in 2006 to 10 billion towards the end of the century, and the interaction between the effect of 'dangerous' climate change and land use changes, adds a more daunting forecast now than ever. There is a need hence to find agricultural systems (i.e. dairy systems), that not only can be sustainable currently but also in the nearby future.

There is no agreement as how this sustainability can be achieved. For instance, Goodland (1997) proposed as a drastic and efficient solution the improvement of diets of the rich by eating lower down in the food chain. In order to reduce food-related wastage and to improve health and food availability, a food conversion efficiency tax was proposed: high taxation to least efficient product converters (pork and beef), moderate taxes to moderate converters (poultry, eggs, dairy) and most efficient converters (ocean fish) would be taxed lowest. Grain for human food would not be taxed, while coarse grain might be modestly subsidised. Although this solution may be sensible enough to be considered, it would need a major change on the current socio-economic system and hence, it is likely to be impracticable.

The current system for dairy, for instance, in the EU, during the last 30 years, is such that milk production is regulated via milk quota and the implementation of an increasing number of environmental policies (Oenema and Berentsen, 2004). The environmental policies force farmers to use nutrients more efficiently and to decrease nutrient losses to the wider environment.

Currently, the most important environmental policy in the EU affecting nutrient management is the Nitrates Directive (Anon, 1991). However, there are many more legislations and protocols affecting dairy systems. With the implementation of the EU Water Framework Directive (EC, 2000) farmers will have to further increase the utilisation of nitrogen (N) and phosphorus (P) and to further decrease N and P losses to surface waters. The Air Quality Directive (Anon, 2000) also sets limits to the emission on ammonia (NH_3) and N oxides into the atmosphere, so as to abate acidification, eutrophication and tropospheric ozone. The increasing concentration of greenhouse gases (GHG) (Kyoto protocol: Anon, 1997) and NH_3 and nitric oxide + nitrogen dioxide (NO_x) (Gothenburg protocol: UNECE, 1999) is also an international environmental concern. Agenda 2000 and the reform of the EU common agricultural policy (CAP) changes the production-based subsidies system to a single farm payment (SFP) decoupled from production. In order to receive this SFP, farmers have to meet statutory environmental and animal welfare regulations and must maintain their land in good agricultural and environmental condition.

These payments are subject to the respect of the statutory EU environmental standards, through cross-compliance, and rules of good agricultural and environmental condition. It aims not only to improve competitiveness, but also environmentally friendly production of

quality products that the public wants, a fair standard of living and income stability for the agricultural community, diversity in agriculture and supporting rural communities, simplicity in agricultural policy and linking support to providing public services that farmers are expected to provide (Oglethorpe, 2005).

Due to all these regulations farmers are undoubtedly under a lot of pressures. Dairy farmers, in particular, have to face these pressures in a yet more challenging way mainly because of their complex management. On dairy farms grass is harvested several times per year by grazing and cutting. Usually farmers record milk production, animal performance, animal intake and concentrates daily, but yield, quality and protein content of the harvested herbage in practice are surprisingly unknown values. The relationships between N application and growth, time, yield and quality of herbage are still poorly understood. Farmers, in general, continue unaware of the impact of their farm management on the environment or other aspects that jeopardise the sustainability of their activities.

Up to now, there have been many studies (i.e. experiments) that have investigated the effect of management, environment or genetic variation (i.e. plant varieties) on the main issues that affect sustainability. However, most of these studies have considered parts of the system in isolation and hence, were unable to explain the interactions between the parts. Therefore there is a need to develop approaches that successfully view the system as a whole and to be able to interrogate the system about possible desirable targets. These approaches can be comprised within the term "*systems analysis*".

1.2. "*Systems analysis*": the way forward to study agricultural (i.e. dairy farming) sustainability

The large complexities and the need to fulfil multiple objectives in sustainable agro-ecosystems call for interdisciplinary analyses and inputs from a variety of disciplines in order to better understand the complete agronomic production system. Systems approaches have been developed to support these interdisciplinary studies. Agricultural systems have both spatial and temporal dimensions. Spatial aspects can be distinguished at plant, field, farm, catchment, regional and higher levels while processes at each spatial level have

characteristic temporal components. Systems analysis in agronomic systems implies the use of various types of knowledge, such as expert knowledge or knowledge derived from scientific experiments or simulation models (Kropff *et al*., 2001). There is a need for selection and development of proper tools to carry out systems analysis. Therefore, a comprehensive interdisciplinary analysis of agricultural production systems is needed for the development of innovative, sustainable systems for the future.

The systems analysis approach can be described as the systematic and quantitative analysis of agricultural systems, and the synthesis of comprehensive, functional concepts of them. The systems approach uses many specific techniques, such as simulation modelling, expert systems, data bases, linear programming and geographic information systems (GIS). Science-based mathematical models and computer simulation provide objective tools to determine biophysical consequences of management options at different scales. For a true systems analysis, such biophysical assessment needs to be complemented by socio-economic analyses before they will result in benefits at any scale.

In order to successfully achieve an adequate holistic analysis of these systems one must know about the parts that comprise the main components of such systems of integration. This thesis aims at studying the effect of nutrient management on the sustainability of a dairy farm. Therefore, a good understanding *a priori* of the components that comprise the dairy farm system and how these components interact with each other is needed at the different scales where a dairy farm can be studied. The main way to understand this is by understanding the nutrient cycling within this system.

1.3. Nutrient cycling within temperate grassland-based dairy systems

1.3.1. Cycling nutrients as a tool to understand grassland-based systems

The cycles of the nutrient elements within a grassland system are extremely complex and although they interact one with another in various degrees, researchers have tended to study each in isolation (Scholefield and Oenema, 1999). The manner in which the soil, climate and management of the dairy farm system interacts with nutrient flows can be quite complex. It is hence important not only to know about the individual components, and the implications

of farm management decisions, but also the need for a holistic view of the way the total system is operating and influencing nutrient inputs and outputs.

Currently, our greatest knowledge is of the N cycle, because herbage production is N limited (Wedin, 1996), because of the great importance of N fixation in legume-based systems (Rochon *et al*., 2004) and because of the growing concerns about the environmental impact of N losses (i.e. EU Nitrate directive).

Progress towards better understanding and quantification of the cycles of other macronutrients has been less rapid compared to that with N. With P, for example, while there is general concern about its contribution to the eutrophication of surface waters (Vollenweider, 1987), there is yet a rather poor understanding of the mechanisms controlling either plant availability (Harrison, 1985) or transport within the soil (Haygarth and Jarvis, 1996).

The nutrient cycle in grassland-based systems comprises the nutrient transfers and transformations within and between the soil, plant and animal pools, the transfers between these pools and the gaseous and aqueous environments, and inputs to the soil of manufactured fertilisers (Fig 1).

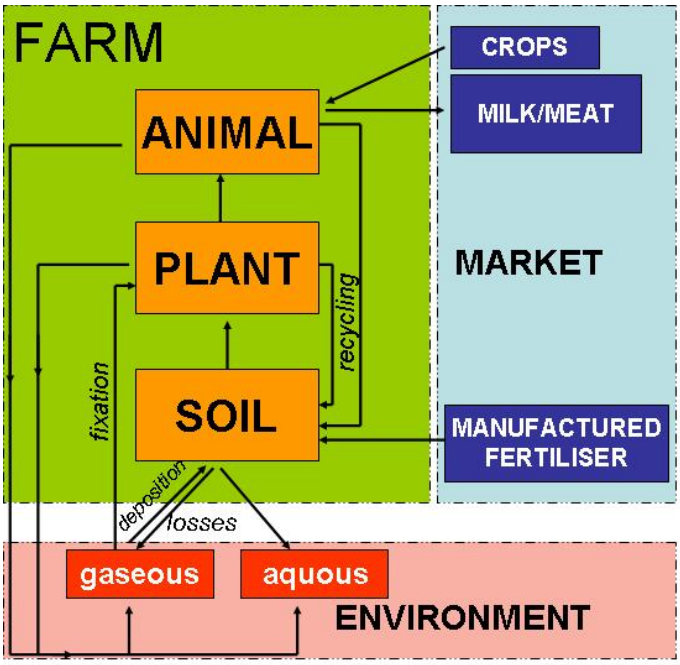


Figure 1. Nutrient fluxes in a dairy farm system.

There is sufficient knowledge of the N cycle at least, to enable all the processes and trade-offs between production and environmental impact to be quantified and studied on a systematic basis.

1.3.2. Main processes of the N cycle.

1.3.2.1. The N cycle in the soil-plant system

The soil N cycle and its processes play a major role on the sustainability of the N management at any given scale. Fig 2 shows the main flows of N in a soil-plant system. Much N is contained within soils, a majority of which is held within the organic materials that accumulate over time. Unlike arable systems which, depending on the cultivation practice, more or less attain an equilibrium in soil organic matter (SOM) content and hence background N contents, grassland soil are rarely at equilibrium with respect to SOM and N contents. This makes prediction of the impact of SOM on N behaviour difficult.

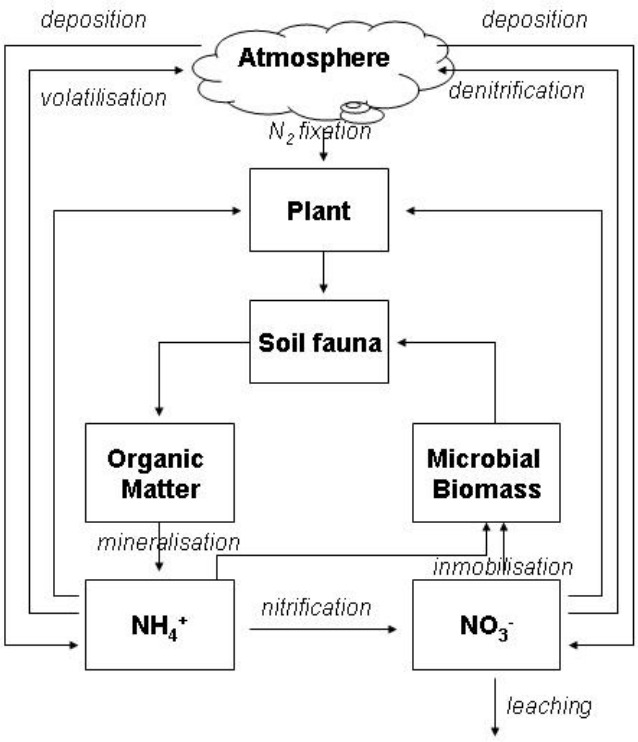


Figure 2. N cycle at the soil level (adapted from Jarvis *et al*., 1996a).

The other major difference is the amount of N present: typically an old pasture soil contains 3-10 t N ha^{-1} compared to 1-4 t N ha^{-1} in an arable soil (Archer, 1988). Nitrogen in SOM can

be categorised into many categories (Haynes, 1986), and ranges from materials which have been recently returned or added (i.e. manure, dung, plant residues) to those which may be up to thousands of years old, with a range of recalcitrance/degradation capacities. The relative proportions of these materials are a reflection of past managements and soil environmental conditions.

The current environmental, soil and management conditions determines in great manner the rate of delivery by the actions of the soil organisms of N into the soil mineral N pool (mineralisation). Studies have shown that, depending on previous managements, long term grasslands can release more than 300 kg N ha^{-1} during an annual cycle as net mineralisation (Hatch *et al*., 1991; Clough *et al*., 1998).

An important component of the SOM pool is the soil microbial biomass (SMB). Nitrogen moving into from this pool provides the biological mechanism by which mineral N is removed from, in competition with other removal processes, or as the biomass turns over, added to the available pool in the soil. The soil mineral N pool contains ammonium (NH_4^+) and nitrate (NO_3^-). Nitrogen can enter as NH_4^+ from degraded organic matter including dead SMB and plant residues, urine, manures or directly from some forms of fertilisers. Nitrate N enters either directly from fertiliser addition or after the microbial process of nitrification. It is an important controlling process in most grassland soils because of the large amounts of NH_4^+ added from urine and manure as well as from mineral fertiliser.

The main pool of plant available N is the aqueous phase of the soil. Plants can utilise both form of N although the predominant form of N available to plants is NO_3^- since under most soil conditions NH_4^+ is rapidly nitrified to NO_3^-. The utilisation of NO_3^- by plants involves several processes, including uptake into the plant, storage into vacuole, translocation to the shoot, reduction into NH_4^+ and incorporation of N into organic forms. Some species reduce great quantities of NO_3^- in their roots whereas others translocate most of it to the shoot where it is reduced. Ammonium is the major form of N available to plants under conditions that are unfavourable for nitrification (i.e. poor aeration, soil acidity or cold temperatures). Ammonium can not accumulate in cells as it is toxic to the plant and it is normally converted to amino acids or amides in the root and translocated to the shoots in these organic forms.

Nitrate uptake seems to be repressed by NH_4^+ in some cases and species. In the majority of cases, NH_4^+ appears to have an inhibitory effect on NO_3^- uptake that is independent of any

such effect on NO_3^- reductase enzyme activity. Temperature also appears to exert a great influence on some species and under some conditions on preferential NH_4^+ uptake. The effect of root temperature on the uptake of N and the size of the root system has been investigated thoroughly by Clement *et al.* (1978), Clarkson and Warner (1979), Clarkson *et al.* (1986), Watson (1986) and Macduff and Jackson (1991). The rate of supply of nutrients into this pool and the plant's effectiveness in competing with other soil processes for them determine plant uptake, in relation to the plant's potential and the ambient conditions of light, temperature and soil water content. The competing soil processes are those resulting in loss (volatilisation, leaching, nitrification and denitrification), and those resulting in immobilisation, either by microbial activity or by adsorption to soil colloids. Ammonium ions or organic N are not usually mobile, however, some movement of NH_4^+ (Herrmann *et al*., 2005) and organic N (Vinther *et al*., 2006) can also take place. There can also be large losses from the soil through volatilisation when urea in either fertiliser or urine or manure is added before NH_3 is transformed into ionic form and bonds with exchange surfaces on soil particles.

Nitrate is also removed into gaseous forms by the denitrification process. In this process, NO_3^- is sequentially transformed into NO_x, nitrous oxide (N_2O) and dinitrogen (N_2) gases, either of which can be emitted to the atmosphere. It has also been found that NO_x and N_2O can be produced through nitrification processes (Firestone and Davidson 1989; Williams *et al*., 1992; Conrad, 1996a). Other exchanges that may influence directly the pool of inorganic N in the soil are the deposition of atmospheric NH_3, NO_x and NH_4^+.

1.3.2.1. a. The mineralisation process.

Mineralisation is the transformation process whereby NH_4^+or NH_3 is released by soil microorganisms as they utilise organic N compounds as an energy source (Janssson and Persson, 1982). The process is complex and depends upon the activities of non-specific heterotrophic microorganisms under both aerobic and anaerobic conditions. Mineralisation occurs, to different extents, with both newly added residues and existing, already degraded organic materials of various ages and degrees of recalcitrance. Much of any NH_4^+, NO_3^- or simple organic N compounds that are released are assimilated rapidly by the SMB

population and transformed into the organic N constituents of their cells during the oxidation of suitable C substrates. However, immobilised N is likely to be available subsequently for mineralisation as the microbial population turns over. Gross mineralisation is the total release of NH_4^+ through microbial activities. The difference between gross rates of mineralisation and immobilisation is net mineralisation or, in some circumstances, net immobilisation.

Recent additions of organic materials have the potential to mineralise at the greatest rates. Roots and root exudates offer a source of organic matter for mineralisation during the growing season. A large pulse is made available when the soil is cultivated. In grasslands after either cutting or grazing, much plant material remains in the stubble and roots and there is a continuous turnover of N through the leaf litter and roots (Parsons *et al*., 1991). The quantities of roots and macro-organic matter in the soil increase with the age of the sward (Garwood, 1967).

Process controls of mineralisation can be summarized as: (i) resource quality, (ii) environmental controls, (iii) effects of cultivation and (iv) soil architecture (Jarvis *et al*., 1996a).

(i) Resource quality: the nature of returned organic materials is very variable. Crop residues, for instance, can be described as any of the following 3 groups: cell wall and structural material (i.e. cellulose), reserve substrates (i.e. starches, fats and proteins) and cell contents (i.e. proteins, sugars). Once in the soil, the simpler N compounds mineralise more quickly than complex materials. Lignin, for example, it is resilient to attack. Biologically fixed N may also increase the N content of the residues and, thus, potential mineralisation rates. There has been some evidence that white clover increases mineralisation perhaps because of high N contents in roots and nodules, but also because soil structure may be improved in the presence of the clover which could increase mineralisation (Mytton *et al*., 1993).

The C: N ratio of materials provides an indication of the likely balance between mineralisation and immobilisation processes. However, there is little evidence to suggest that these ratios can be used for predictive purposes (Haynes, 1986). In general, as substrate C: N increases, mineralisation decreases until some critical point is reached (Kirchmann and Marstorp, 1991). The C: N of manures has also been suggested to have a major influence on

subsequent mineralisation in soils. Kirchmann (1985) suggested that C: N of 15 was critical, with N immobilisation occurring above and mineralisation below this value.

(ii) Environmental controls: those factors influencing soil aerobicity are very important. Aeration status is dependent upon soil texture, structure and moisture, the management of the system and the returns of organic material. Soil temperature and moisture then further interact by influencing microbial activity. Significant proportions of SOM are associated intimately with clay and other inorganic components of the soil matrix which restricts the potential for mineralisation. Net mineralisation rates increase with temperature and tend to become less variable at higher temperatures (Stanford *et al*., 1973). At optimum soil water content, an Arrhenius function with a Q_{10} of approximately 2 described the relationship between net N mineralisation and temperature (Kladivko and Keeney, 1987).

Changes in the availability of soil water can limit biological activities and hence mineralisation, limit solute diffusion and mass distribution of microbial activity products and cycles of wetting/drying may increase the availability of substrates (Cabrera, 1993; Fierer and Schimel, 2002). Drainage of permanent grassland soils increased the amounts of NO_3^- leached because of an enhanced mineralisation capacity where aerobicity was increased (Scholefield *et al*., 1993).

Maximum net mineralisation rates have been achieved at between -0.33 and -0.1 bar where water occupied 80-90% of the pore space; the rates fell as soil moisture fell below -0.33 bar (Stanford and Epstein, 1974).

There have been suggestions that adding immediately available N stimulates mineralisation, a so-called priming effect. Priming effects are strong, generally short-term changes in the turnover of native soil organic matter induced by comparatively moderate treatments of the soil (Kuzyakov *et al*., 2000). Such treatments might be, e.g. inputs of organic or mineral fertiliser to the soil (Bol *et al*., 1999; Clough *et al*., 2003), exudation of organic substances by roots (Mary *et al.,* 1993) or remaining plant residues (Liang *et al*., 1999). The mechanisms and specific sources of priming effects, however, are still not fully understood due to method related factors (Kuzyakov and Bol, 2006).

Soil texture exerts an important control over mineralisation by influencing aeration/moisture status, affecting the physical distribution of organic materials and

conferring some degree of protection through an association of organic material with clay particles (Hassink *et al*., 1993).

Other soil factors that are also important are pH and contamination of soil. For instance, heavy metals have immediate impact in reducing mineralisation rates (Chang and Broadbent, 1982; Gibbs *et al.,* 2006).

(iii) Effects of cultivation: cultivation, its timing and methodology, is an important tool for modifying mineralisation of old organic matter as well as recent additions. Mechanical disruption of the soil structure makes previously protected SOM available for degradation and increased rates of mineralisation have been observed in disturbed soils (Hamza and Anderson, 2005). The cultivation method, type of machinery used, and the energy input affect the amount of N mineralised. For example, ploughing is thought to cause more mineralisation than establishing crops with direct drilling by some authors (i.e. Goss *et al*., 1993). However, other authors showed otherwise (Angus *et al*., 2006).

It is also important to consider the effect of adverse soil conditions on mineralisation. Compaction caused by for example heavy machinery or cultivating the soil at the wrong time, reduces soil porosity, which modifies and reduces net mineralisation.

(iv) Soil architecture: there are substantial diffusional constraints to the movement of ions in soils. These constraints may influence further transformation of transfer of N. Restricted diffusion of NH_4^+ may result in preferential immobilisation by SMB and only the N in excess of microbial requirements enters the NH_4^+ pool (Drury *et al*., 1991).

1.3.2.1. b. The plant N uptake.

Plant uptake response to increasing supply of applied fertiliser N follows a characteristic relationship, which is usually linear from zero to between 250 and 700 kg N ha^{-1} yr^{-1} in north Western Europe (Mannetje and Jarvis, 1990). The yield response per increment of N then gradually diminishes to zero, at which point N is no longer a limitation to yield (Fig 3). The economic optimum yield has been defined, however, as the level of fertiliser N above which the yield return on unit of added N per ha falls below a certain value (for instance less than 7.5 kg dry matter (DM) yield and N-yield, respectively for the RB209 England and Wales fertiliser recommendations).

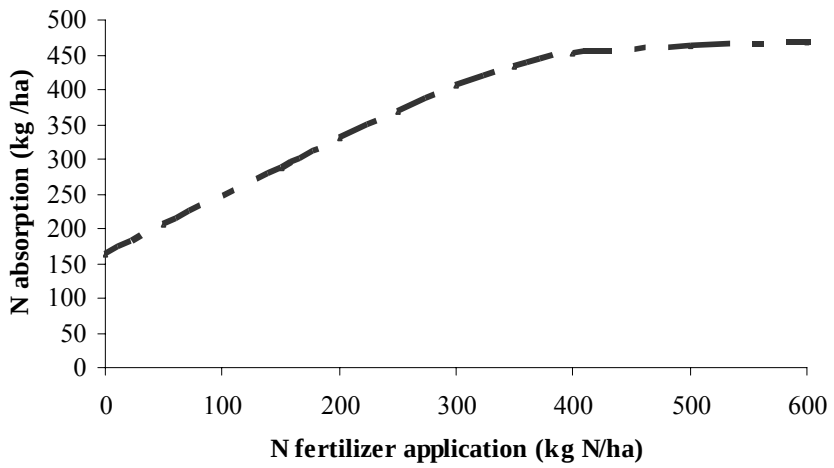


Figure 3. Typical representation of the relationship between N absorption by grass and fertiliser N application.

Whitehead (1995) has calculated that grass harvested either by cutting or grazing in a temperate environment and producing 8-15 t DM usually contains between 200 and 350 kg N ha^{-1}. If the stubbles and roots are also taken into account, then the total plant pool increases to 300-800 kg N ha^{-1}.

In general, the more N is applied to the soil, the more N there is in the plant. This is not only fundamental from the plant response and herbage quality point of view, but any resultant changes in the C: N balance of cow's dietary intake may, in turn, influence the retention of N and the extent and mode of excretion by the animal. Plant contents can range between 1% and 5% (Whitehead, 1995) on a dry weight basis, with distinct annual patterns of decreasing contents with maturity of the sward. Management influence on the utilisation of herbage has substantial effect on the herbage N concentration (Frame, 1992). Grazing pattern also has a considerable influence on the manner of N utilisation.

Management of the interaction between plant response and N utilisation demands a balance of a number of factors. These may include: the determination of a realistic yield under the prevailing soil type, environmental, climatic conditions and botanical composition. The pattern of nutrient uptake and herbage production through the growing season is determined by the physiology of the plant, its frequency of defoliation and the ambient conditions of temperature, light and soil water content. For the most efficient use of nutrient from fertiliser the pattern of application should be the same one as the pattern for uptake.

However, this may not be the most efficient for the farmer as animal requirements at grazing may not match the herbage on offer. Under conditions of no constraints, uptake capacity by plants from the soil solution is high even only when only low concentrations are present.

Species with C_4 metabolism, like maize, a plant very relevant in dairy systems, are usually more efficient in N utilisation than C_3 plants. Incorporation of maize into dairy farming managements as an energy rich forage source is an important feature in many environments and the geographic range under which it can grow is continually expanding due to mainly plant breeding advances, but also in the long term to climate change.

1.3.2.1. c. Plant biological N fixation.

The process by which N_2 is reduced to NH_4^+ is called N fixation. In dairy systems, biological N fixation, especially the symbiotic association between legumes and rhizobia, can provide substantial amounts of N to plants and soil, which reduces the need for industrial fertilisers (Ledgard and Steele, 1992). In temperate grasslands, perennial forage legumes are very important for the biological supply of N. The efficiency of N_2 fixing symbioses is a function of host genotype, *Rhyzobium* genotype, and environmental factors (Unkovich and Pate, 2000). Field management practices that ensure favourable conditions for plant growth and bacterial activity are associated with high rates of N_2 fixation (Whitehead, 1995). White clover (*Trifolium repens L.*) and red clover (*Trifolium pratense L.*) are the most important legumes in temperate pastures.

White clover, in particular, is the most widespread grazing legume for dairy farming systems in temperate areas. White clover is generally grown in combination with perennial ryegrass (*Lolium perenne L.*) and is grazed by cattle or sheep. The productivity and fixation of atmospheric N_2 by white clover in mixed pastures is dependent on the extent of competition with the associated grass, as controlled by a range of factors of which a primary factor is soil inorganic N status (Ledgard and Steele, 1992). White clover has a large potential for N_2 fixation, which has been estimated at up to 680 kg N ha^{-1} yr^{-1} (Sears *et al.*, 1965) in a soil of very low N status and under mowing, thereby avoiding the recycling of excreta N which occurs under grazing.

Application of fertiliser N and or excreta N by grazing animals decreases N_2 fixation (Vinther, 1998) due to an increased competition by the associated grass and to substitution of uptake of added N for N_2 fixation (Mallarino and Wedin, 1990).

1.3.2.1. d. Environmental losses of N

Nitrous oxide (N_2O)

Nitrous oxide is formed in the soil through nitrification and denitrification and is controlled by a number of soil factors, including moisture content (del Prado *et al*., 2006b), temperature (Hatch *et al*., 2005), fertiliser additions (del Prado *et al.,* 2006b), pH (Merino *et al*., 2000), organic matter content (Smith *et al.,* 1997; Chadwick *et al.,* 2000b; Estavillo *et al*., 2002), NO_3^- and NH_4^+ (Tiedje, 1988; Granli and Bockman, 1994).

Nitrate and NH_4^+ in the soil are subject to the following process dynamics. Nitrate may: (1) undergo denitrification to gaseous oxides of N and to N_2; (2) be taken up by organisms (assimilatory reduction); (3) be used by micro-organisms as an electron acceptor and become reduced to NH_4^+ (dissimilatory reduction); (4) be leached or removed in run off; or (5) accumulate in the soil. Ammonium may: (1) be taken up by plants; (2) be immobilized in microbial biomass; (3) nitrify to NO_3^- and be partially lost as gaseous oxides of N (4); be leached; (5) accumulate in the soil (Paul and Clark, 1996); or (6) be volatilised as NH_3.

The regulation of trace N-gas production via nitrification and denitrification has been described by the 'hole-in-the-pipe' conceptual model (Firestone and Davidson, 1989). The rate of the processes (denitrification and nitrification) and the relative proportions of end products are controlled at two different levels. First-level factors control the movement of N through the 'pipe'. Second-level factors control the partitioning of the reacting N species to N_2, N_2O, NO, etc. and therefore control the size of the 'holes' in the pipe through which the gases 'leak' (Fig 4).

In general, N_2O emissions can be reduced by implementing practices aimed at enhancing the ability of the crop to compete with processes that lead to the escape of N from the soil-plant system (Freney, 1997). For instance, there are several methods for increasing the efficiency of the crop to remove mineral N from the soil. These include improving fertiliser efficiency (Brown *et al*., 2005), optimising methods and timing of applications (Dosch and Gutser, 1996), using NH_4^+-based fertilisers rather than nitrate-based ones (Eichner, 1990;

Dobbie and Smith, 2003) and employing nitrification chemical inhibitors (Dittert *et al*., 2001; Merino *et al.*, 2002; Macadam *et al*., 2003).

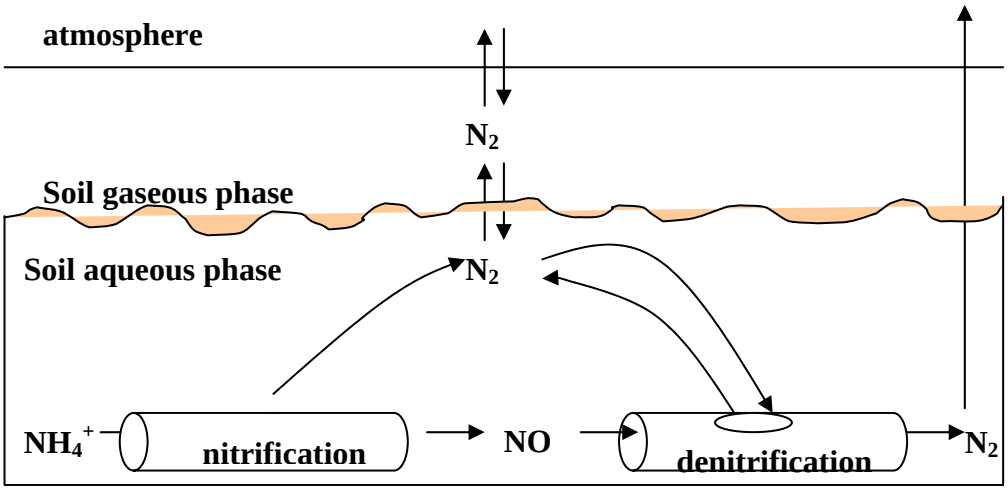


Figure 4. Conceptual model 'Hole-in-the-pipe' (adaptation from Firestone and Davidson, 1989).

Increasing the soil aeration may significantly reduce N_2O emissions. Improving drainage would be particularly beneficial on grazed grassland (Monteny *et al*. 2006). Hence, avoiding compaction by traffic, tillage (Pinto *et al*., 2004) and grazing livestock may help to reduce N_2O emissions (De Klein and Ledgard, 2005). Housing system and management will also influence N_2O emissions, e.g. straw-based manures result in greater N_2O emissions than slurry-based ones (Groenestein and Van Faassen, 1996). Minimising the grazing period is likely to reduce N_2O emissions as long as the slurry produced during the housing period is uniformly spread.

Because of the many factors that may control N_2O emissions, temporal and spatial variability of N_2O emissions from soils are often found to be large (i.e. Groffman, 1991). As an example, all of the published data from the Basque Country of the effect of %WFPS and soil temperature on N_2O emissions are plotted (Fig 5) showing the degree of variability associated with the effect of major environmental control factors on N_2O emissions from soils. This large variability strongly hampers the quantification of N_2O emissions from soils (Velthof, 1997).

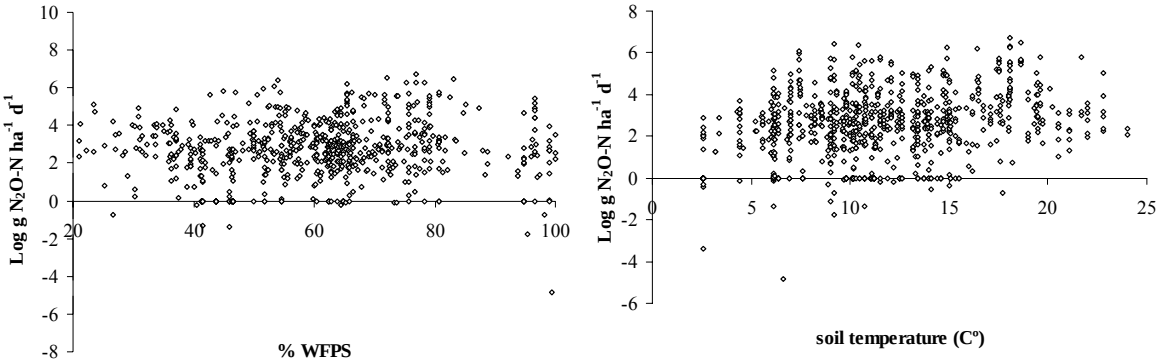


Figure 5. Example showing the enormous variability of the effect of soil moisture content (as %WFPS) and soil temperature on N_2O emissions (data from Prado *et al.* 2000b; Merino *et al*., 2001ab; Estavillo *et al*., 2002; Merino *et al.,* 2002; Macadam *et al*., 2003; Pinto *et al*., 2004; Merino *et al*., 2005 y del Prado *et al*., 2006b).

Nitric oxide (NO)

Being a highly reactive trace gas, NO plays a crucial role in tropospheric chemistry (Crutzen, 1979). For the fast chemical interconversion with nitrogen dioxide (NO_2), which typically occurs within seconds or minutes, both species are referred to as the single quantity NO_x (NO_x = NO+NO_2). Nitric oxide and NO_2 (NO_x) are precursors in the photochemical formation of nitric acid (HNO_3) and thus contribute to the acidity of clouds and precipitation (Warneck, 1988). Probably even more severe is the impact of NO_x on the oxidative capacity of the troposphere. NO_x mediates the production and destruction of ozone and influences the formation of hydroxyl radical (OH).

Several abiotic and biotic processes in soils and plants are mechanisms for production and consumption of NO (Conrad, 1996b). A number of studies have demonstrated that plants can directly absorb several nitrogen-containing trace gases including NO and NO_2 through their foliage (Hill, 1971; Neubert *et al*., 1993; Hereid and Monson, 2001; Sparks *et al*., 2001). Assimilation of gaseous NO_2 into leaf nitrate, nitrite and amino acid pools has been directly demonstrated using 15^N as a tracer (Rogers *et al*., 1979; Segschneider *et al.,* 1995). Plants also emit some nitrogenous gases into the atmosphere. The emission of NO (Dean and Harper, 1986; Wildt *et al*., 1997) and NO_2 (Rondon *et al*., 1993; Wildt *et al*., 1997; Sparks *et al*., 2001) from plants at low atmospheric mixing ratios has been reported.

Both nitrification (Skiba *et al*., 1993; Yamulki *et al*., 1995) and denitrification (Cárdenas *et al*., 1993; Remde *et al.,* 1993) processes have been found to contribute to the observed NO

fluxes. However, to assess the importance of nitrification vs. denitrification for the exchange of NO is a difficult task.

Up to recently, little attention has been given to the role of transport processes for soil-air exchange of NO. Commonly, molecular diffusion is regarded as the driving mechanism for gas transport in soil pores (Galbally and Johansson, 1989). Recent studies, however, have pointed out that convective transfer may not be ignored.

Among the factors influencing the NO exchange the most important are: N availability and fertilisation, soil moisture content and temperature. It has been shown by a large number of studies that availability of soil N has a strong impact on NO emission rates. Special interest in this respect is given to the pool size of soil NH_4^+ and NO_3^-, since these compounds; serve as substrate for nitrifying and denitrifying bacteria. It is widely accepted that soil moisture content strongly affects the exchange of NO. Addition of water to very dry soils, for example, typically produces a distinct increase of NO emission rates (pulsing). Soil temperature also exerts an important influence on NO exchange. The bulk of existing studies has shown an increase of NO emissions with increasing soil temperatures.

Ammonia losses from fertiliser application

Animal waste is the main source of NH_3 emissions in animal husbandry (Buijsman *et al.,* 1987), with dairy cows as the major source (Swensson, 2003). Urea-containing fertilisers also play an important role on NH_3 emissions. Part of the animal excreted N (urine and faeces) is annually lost as NH_3. The most important source of NH_3 emission is the content of urea in the urine (Monteny and Erisman, 1998). The amount of urea in urine varies between 50-90% (Doak, 1952)

Urea in animal waste and in urea-containing fertiliser has to hydrolyse to ammonium carbonate before it becomes prone to NH_3 volatilisation.

$$CO(NH_2)_2 + 2H_2O \rightarrow (NH_4)_2CO_3 \leftrightarrow 2\ NH_4^+ + CO_3^{2-}$$

The enzyme urease acts as a catalyst in the hydrolysis. This enzyme is abundant in agricultural soils and on stable soils. Hydrolysis occurs rapidly, with complete conversion of urea N to NH_4^+ possible within a matter of hours, depending on environmental conditions (Beline *et al*., 1998). Hydrolysis is affected by not only the amount of enzymes but also

temperature, pH, soil moisture, organic matter content and cation exchange capacity (Freney *et al*., 1983). Generally it follows Michaelis-Menten kinetics; that is, the hydrolysis rate increases with increasing substrate concentration until the enzyme is saturated. Normally hydrolysis increases with increasing temperature (according to the Arrhenius equation), and has an optimum pH from 7-9. With respect to the soil water, the effect is unclear.

Apart from hydrolysis, urea can also be leached below the root system. In winter if urea hydrolysis is delayed (low organic matter, low pH and cold temperatures) and if the rainfall rate is high, urea may be transported down the soil profile and be leached as urea-form N below the root system.

The urea that has not been leached would then be adsorbed in the soil as NH_4^+ or volatilised as NH_3. But before NH_3 volatilisation takes place, the NH_4^+ has to be converted into NH_3. The NH_3 volatilisation rate is controlled by the rate of removal and dispersion of NH_3 into the atmosphere.

Generally, high temperatures, pH, windspeed and N concentration of animal wastes stimulate NH_3 emission, whereas high rainfall, CEC, infiltration rate, buffer capacity and atmospheric NH_3 concentrations reduce NH_3 emissions (Bussink, 1996).

Seasonally, the risk of NH_3 loss from manure application to soils would be greatest in summer as higher temperatures will increase hydrolysis and transport of urea into the soil would be prevented by low water content in the soil (O'Toole and Morgan, 1983). For instance, in the UK so far, although relatively large number of experiments have been carried out, the evidence only justifies discriminating between emissions of slurry applied in the three summer months [Emission Factor (EF) = 60 % of total NH_4^+-N (TAN) compared with emissions of slurry applied in the rest of the year of 15-59% TAN, depending on the slurry DM content (Defra, 2005a)].

Grazing grassland may result in N returns with urine and faeces up to 400 kg N ha^{-1} yr^{-1} (Bussink, 1996). This is obviously a high potential for NH_3 losses. There have been experiments to quantify this contribution. Buijsman *et al.* (1987), for instance, estimated that NH_3 volatilisation from the N contained in urine and faeces was 40% and 5%, respectively. However, under real conditions, the situation is more complex. With micrometeorological techniques the net NH_3 flux can be measured.

Abatement methods to decrease the magnitude of these losses after application of fertiliser include those related to application methods and dietary manipulation. For instance, replacing surface application of slurry with band-spread or deep injection can reduce up to 90 % the NH_3 emissions (Huijsmans *et al*., 1997). Poorer efficiencies have been found for shallow injection (Misselbrook *et al*., 1996). For all manures (slurry and FYM) it is also possible to incorporate them into tillage land. For instance, incorporation of cattle slurry immediately after application can reduce NH_3 emissions up to 90 % compared with surface broadcast application (Webb *et al*., 2006). Although effective, some of these measures can be expensive and can increase losses in other N forms (so-called 'pollution swapping').

Manipulation of the animal diet through reducing the crude protein (CP) content of the diet resulted in slurry with lower total N and TAN content and also a lower slurry pH from pigs (Misselbrook *et al*., 1998) and dairy cows (Broderick, 2003), respectively. For ruminants, an additional strategy to improve N utilisation by the animal is to protect a proportion of the protein in the diet of the animal from rumen degradation (Misselbrook, 2005). For instance, the inclusion in the diet of forages with significant condensed tannin content (Misselbrook *et al*., 2005c) or starch-rich diets (Kebreab *et al*., 2001) resulted in a shift in N excretion from urine to faecal N which, being less labile, resulted in lower NH_3 emissions following application of the slurries to the soil. Although effective, these dietary measures may have implications in the animal performance (i.e. milk amount and quality) and on other pollutants (i.e. methane from rumen). A wide range of additives have been also described to decrease NH_3 emission from slurry application (McCrory and Hobbs, 2001). Hendriks *et al.* (1997), for instance, found that a digestive additive applied to pig slurry reduced the mean NH_3 emission rate by up to 50%. Other additives include acidifying additives and NH_3/NH_4^+ adsorbents (McCrory and Hobbs, 2001). The effectiveness of acidifying additives, for instance, is based on the capacity of these additives to neutralize the alkaline nature of the livestock slurry (Husted *et al*., 1991). Acidifying additives can be divided into three groups: acids (sulphuric: Pain *et al*., 1990; hydrochloric: Martinez *et al*., 1997; lactic acid: Berg and Hornig, 1997), base precipitating salts (Vandre and Clemens, 1996), and substrates that induce acid production (labile C: Hendriks *et al.,* 1997).

Nitrate leaching losses.

Environmental regulations such as the Nitrates Directive are generally concerned with the concentration of NO_3^- in the water, rather than the total quantity leached. However, for a particular farm, climate and soil conditions, measures that reduce the total NO_3^- loss will generally also reduce peak concentrations.

Nitrate leaching occurs partly due to the great solubilisation of NO_3^- ion in water. Of all the others forms of N in the soil, only NO_3^- is generally leached in a large quantity. Some urea may be leached under low temperature conditions (5ºC), when the rate of conversion to NH_4^+ is low and the NH_4^+ soil concentration is large. In addition, small quantities of denitrified or nitrified N_2O may also dissolve in soil water and hence may leach.

Run-off occurs when the rainfall intensity exceeds the infiltration capacity of soil. Water at this moment moves laterally across the soil transporting soluble (NO_3^-) or particulate material. Run-off occurs in a larger way in poorly structured soils, soil with a high water table or soils with steep slopes. Run-off events are more frequent in winter or in spells with high intensity rainfalls, which generally do not coincide with mineral fertiliser applications but on the other hand may occur at the same time as slurry is spread to the soil.

Although the same principles apply to the processes that govern N leaching and run-off from grassland as those controlling arable soils, there are particular characteristics of grasslands that can have a marked effect on the amounts leached. On the one hand, grasslands can be less leaky than arable crops because of 2 factors: (i) grasslands are permanent crops with well developed root systems and therefore they are able to use the inorganic N throughout the growing season more efficiently and (ii) grasslands are also cultivated less frequently that arable crops and thus, as cultivation increases the risk of NO_3^- leaching, that from grasslands, will be affected less frequently than arable crops by cultivation. On the other hand, other characteristics of grasslands increase the risk of loss. Soils under long-term grasslands accumulate higher contents of organic matter than arable cropping. There is thus potential for considerable amounts of N to be released by mineralisation of SOM. The high organic N content of grassland soils may also increase the likelihood of leaching of organic forms of N from fine textured soils (Hawkins and Scholefield, 2000).

The major factor, however, contributing to N leaching from grassland is the presence of grazing animal. Where grass swards are grazed, much of the N that is consumed is excreted back onto the pasture. Therefore, much of the season's N input will remain in the soil in autumn, concentrated into urine and dung patches.

In a review study, Cuttle *et al.* (2004) described a set of potential abatement measures to control NO_3^- leaching losses. Those measures included measures such as: (i) avoiding grazing on soils with a high risk of NO_3^- leaching, (ii) reduce the effects of soil compaction, (iii) avoid drainage of grassland, (iv) management choices that reduce leaching after reseeding of grassland, (v) irrigate grassland in drought season, (vi) weather forecasting, (vii) selecting the most suitable grasses to maximise N uptake, (vii) select grasses with different decomposition or improved nutritional properties, (viii) replace N fertiliser with fixed N from grass/clover swards, (ix) grow other legumes for forage production, (x) optimising fertiliser use, (xi) reduce the rate of N applied, select the most suitable fertiliser type, (xii) reduce stocking rates, (xiii) reduce the length of the grazing season or day, (xiv) reduce the replacement rate for dairy herds, (xv) manipulate cattle diet to reduce the amount of N excreted, (xvi) apply manure at the most suitable time, (xvii) use types of manures with a lower risk of N leaching, (xviii) use nitrification inhibitors and (xix) export manures for off-farm disposal.

The degree of efficacy of these measures are still to be fully proved in most cases and moreover, the impact of these measures on other forms of pollution or other issues that affect the sustainability of the farm need to be thoroughfully studied.

1.3.2.2. The N cycle in the soil-plant-animal system (the farm)

A typical N cycle in a dairy farm comprises 4 main compartments (Fig 6): soil, plant (grass and grass/clover swards and typical arable fodder crops), animal (dairy cattle and followers) and excreta (grazed excreta and slurry or straw-based manure). Manufactured fertilisers and purchased feeds are generally the main inputs in a non-legume grassland-based dairy system.

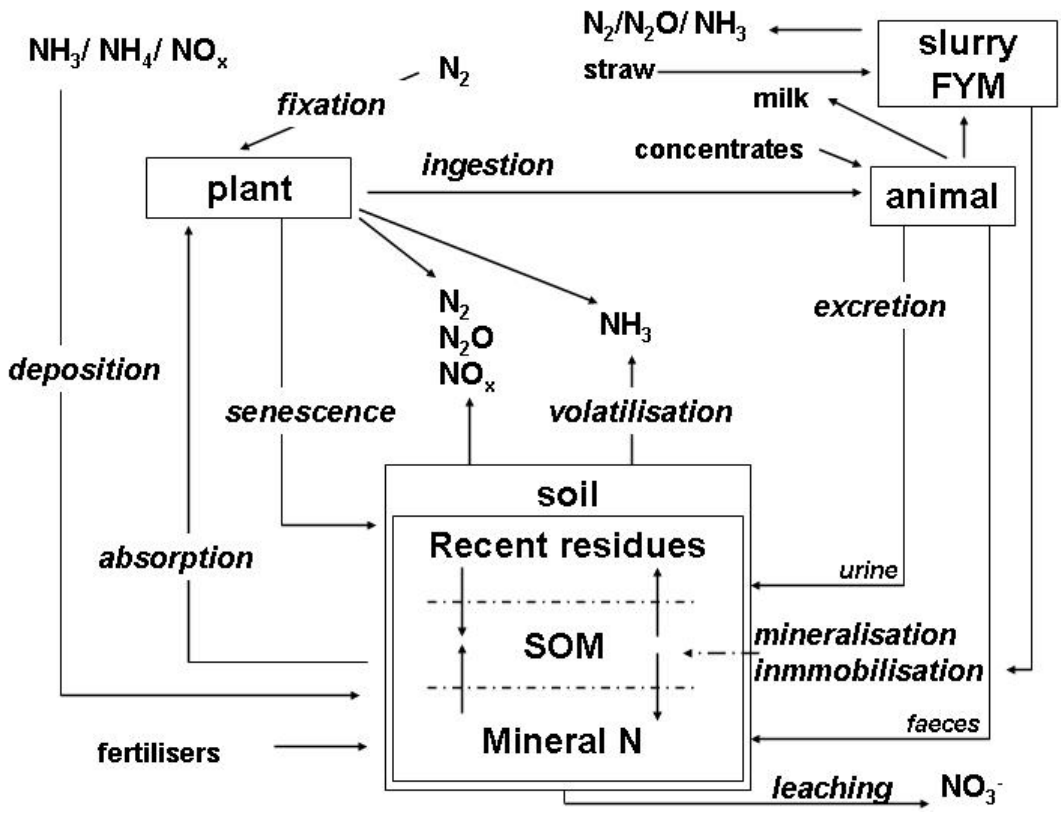


Figure 6. Nitrogen cycle in dairy farming systems.

The N pool in the plant component comprises that plant N which is grazed by the animal and that plant N harvested from grass and grass/clover swards and typical arable fodder crops. A proportion of the plant N that is neither harvested nor grazed is subject to decay/senescence and may join the pool of available N in the soil. The harvested grass or grass/clover generally undergoes the processes of ensiling, whereby a proportion of the N can be lost to the atmosphere. This silage together with feed from outside the farm (concentrates) is subsequently fed to the animals in the stable. The animals will partition some of this ingested N into milk production and weight-gain. The remaining N is excreted as urine and dung. These excreted N materials will be further transformed if produced during housing (mixture with bedding straw and water, storage, volatilisation losses and application to the soil) or be excreted in patches if produced during the grazing activity. After application of housed manure or deposition of urine and dung by the animals themselves, some N will be lost as NH_3 volatilisation and some will enter the N pool in the soil. Some of this N will then be lost to the wider environment, taken up by the plants or accumulated in more recalcitrant forms.

1.3.2.2. a. The animal intake and excreta.

The major influence of the animals on the cycle of N in a dairy farm is as a consumer, processor, excreter and tranfer agent, either at grazing or during the housing phases of the production cycle (Jarvis, 1998b). Large amounts of N are excreted in dung and urine. At best the theoretical maximum efficiency of conversion of N into milk is 40-45% and most usually is less than 25% (van Vuuren and Meijs, 1987).

As well as these direct effects on N, there are other effects of the animal, which may directly or indirectly affect N transfer or utilisation:

- Removal of shoots, resulting in temporal disruption of the N plant uptake.
- Increased returns of plant residues with grazing as compared with cutting.
- Treading, compaction and poaching the soil, with effects on soil microbial activities (mineralisation, nitrification and denitrification).
- Physical transfer of N from field to field and to milking parlour and housing and waste store.
- Possible impact on sward composition through dietary selection.
- Preference and diet rejection through contamination by dung.

Nitrogen excreted outdoors represents a large internal pool of N in the grazed fields and thus in the whole farming system. The amount per hectare and per year depends on the amount of time that the cows spend grazing and the number of cows per hectare. Nitrogen excreted indoors and accumulated in manures also represents a large internal N pool within the dairy farming system. Before that stage, however, there is ample opportunity for loss from the cubicle, hard standings or storage system used as NH_3 (more details in subsequent subchapters).

Excretion during grazing: a dairy cow excretes between 10 and 40 l urine per day (Hayness and Williams, 1993). The volume depends largely on diet factors. They urinate between 8-12 occasions per day, which contains 2-20 g N l^{-1}. Although NH_3 can be lost from urine patches, much of the N from urine quickly infiltrates the soil and its urea is hydrolysed into NH_4^+ and subsequently nitrified into NO_3^- rapidly.

Typically, dung contains between 1.2 and 4% N on a DM basis and is excreted on 7-15 occasions per day to return 2.5 to 5 kg DM day^{-1}. Contents of mineral N in dung are low and there is little direct loss as NH_3. The fate of dung N in the soil is subsequently regulated by

the processes of incorporation, affected by soil moisture content and temperature conditions with soil macrofauna and earthworms, and the processes of mineralisation-immobilisation.

Manures and slurries: Depending on the management system, dung and urine from the housed animals are usually collected together as semi-liquid slurries containing more or less water depending on mixing with rain water and parlour/yard washings, or more solid manures with straw and other similar bedding materials. These materials are valuable nutrient reservoirs containing much N that could be regarded as useful source of fertiliser.

Utilisation and recovery of N supplies, effective use of organic manures still represents a considerable challenge to researcher, advisor, and regulatory bodies in order to integrate existing expertise and knowledge, legislative requirements and nutrient use efficiency. One of the major factors influencing the quality of the waste with respect to N is the opportunity for loss that occurs through varying stages from excretion to spreading. The losses are in the main, associated with the change in form from urea to NH_4^+/NH_3 and the release of N as gaseous NH_3.

1.3.2.2. b. Emissions from livestock housing, yards and storage

Dairy systems produce both solid and liquid wastes. Solid manure is generated from confined dairy facilities, whereas liquid manure is generated from a dairy parlour and in some confined dairy operations. Large dairy operations (>200 milk cows) and some medium sized farms (80-200 milk cows) tend to use liquid rather than solid (Toor *et al*., 2006). Smaller farms commonly employ traditional solid manure due to the higher costs associated with installing automatic flushing systems. In rotational grazing, for instance, manure is naturally spread on land as the animals graze.

The amount and type of bedding material not only affects manure solids contents but also alters the physical, chemical, and biological composition of the manure. The most common bedding materials are sand, sawdust and straw. Animal manure from housing is a mixture of faeces and urine, bedding material, split feed and drinking water, and water used for washing floors. In cattle housed based on slurry, excreta are collected from below the slatted house or in tied housing systems in a gutter behind the animals. The slatted floor area may cover the entire floor or be restricted to the walking alleys or the area behind tied cows. Some buildings with slurry systems are also equipped with automated scrapers. In a large part of

buildings with tied dairy cows, the excreta are separated into FYM, mainly containing faeces and straw, and liquid manure, which is a mixture of water, urine, and dissolvable faecal components.

Cattle housing can be classified as: (i) cubicle (slatted floor) and (ii) deep litter.

Release and transfer of NH_3 in cubicles: Approximately 40 % of the NH_3 in a cubicle dairy cow house with slatted floors originate from slurry stored in the pit below the slatted floor, and the remainder is produced from urea deposited on the slats (Monteny, 2000). The emission from the floor is relatively constant, whereas the pit emission fluctuates depending on the temperature difference between the air inside the pit and that above the slats (Monteny, 2000). In periods with a positive temperature gradient (e.g., relatively warm pit air), the emission from the pit may account for over 75 % of the total emission from the house, whereas pit emissions are as low as 20 % in the situation of relatively cold air in the pit. In the UK, NH_3 emission in the summer was 56 % of the emission during winter (Philips *et al*., 1998), because the animals only had access to part of the building in summer and only about 50 % of the area soiled during winter was soiled during summer.

Release and transfer of NH_3 in deep litter systems: Cattle urine will infiltrate the deep litter (straw), thus, reducing the surface area in contact with the air. Straw has also the effect of reducing the airflow over the emitting surface. Deep litter houses, are, in general, also, naturally ventilated and hence, resulting in a cooler environment (Koerkamp *et al*., 1998). Emissions may also be limited because a significant fraction of the TAN mineralised from the easily metabolisable fractions in urine and dung can be absorbed through cation exchange processes by the straw and transformed into organically bound N by microorganisms (immobilisation of NH_4^+). However, oxygen (O_2) diffuses into the porous surface layer and the O_2 is utilized by aerobic microbial activity in the deep litter, which may cause a temperature increase to about 40-50 ºC at 10 cm depth (Sommer *et al*., 2006). The increase in temperature will induce an upward current of air and, as a result, NH_3 losses will be substantial (10 % N that is excreted and collected in the straw litter).

Generally, a straw-bedded cattle house is likely to emit less NH_3 than a slurry-based. In comparisons between FYM and slurry based housing systems (Chambers *et al*., 2003), the straw-based system resulted in significantly less NH_3 emission than the slurry system (33 and 49 g NH_3 $cow^{-1}day^{-1}$, respectively).

Outdoor concrete yards represent a potentially source of NH_3 emissions to the atmosphere. In a study by Misselbrook *et al.* (2006), estimations of emissions from outdoor concrete yards to the total contribution of NH_3 represented almost 10% of total NH_3 emissions from UK agriculture. It was proposed as effective means of reducing NH_3 emissions from these yards the use of pressure washing and the use of urease inhibitor in addition to yard scraping. Emissions from manure storage can be significant from both straw-based and slurry-based systems. Ammonia emissions from open slurry stores may be substantially reduced by the fitting of rigid covers or the use of a variety of materials (i.e. straw, peat) as a floating cover, all of which have been shown to give reductions in excess of 80% (Sommer, 1997; Hornig *et al*., 1999; Bicudo *et al*., 2004) and by slurry crust formation (Sommer *et al*., 1993; Misselbrook *et al*., 2005a), which is also reported to reduce up to 80 % NH_3 emissions compared with open stores. The downside to some of these measures is that some are either expensive (rigid covers) or difficult to manage/maintain (floating covers and slurry crusting). Solid manure heaps are significant sources of NH_3 and other N pollutants (N_2O) and methane (CH_4) (Chadwick *et al*., 1999; Chadwick *et al*., 2000b). In contrast to slurry-based storage systems, no satisfactory technique has been developed so far to reduce NH_3 emissions during storage of FYM (Chadwick, 2005). Recent studies (Chadwick, 2005; Hansen *et al.,* 2006) have researched into covering the FYM heap as a potential abatement measure. Chadwick (2005) reported a potential abatement measure which consists of compacting and covering FYM heaps when the manure has relatively high NH_4^+-N contents.

This measure, however, led to increased CH_4 emissions sometimes. Hansen *et al*. (2006) covering the heap with an airtight material delayed aeration of the bulk of the stored manure, which reduced the internal heat production, degradation of organic matter, and emission of NH_3 and GHG. Emissions of NH_3, N_2O, and CH_4 were reduced by 12%, 99%, and 88%, respectively, when the manure heap was covered.

1.3.2.2. c. Losses during silage making

Williams *et al.* (1997) studied gaseous changes in silage during ensiling, storage and feeding, limiting themselves to O_2 and CO_2, however, there is little information on gaseous loss of N as NH_3 or oxides from silage.

Mayne and Gordon (1986ab) examined the effect of 3 different grass ensiling treatments (Unwilted Flail: UF, Unwilted Precision: UP and Wilted Precision: WP) on the N and DM losses occurring during silage making. Total DM losses amounted to 20.6 %, 13.4 % and 6 % of that ensiled for the UF, UP and WP ensiling treatments, respectively. Losses were classified in 3 classes: (i) surface waste, (ii) silage effluent and (iii) and invisible losses (from plant respiration, fermentation loss and from gaseous loss accompanying surface). Losses from (i) surface waste amounted to 1.3 %, 1 % and 1.2 % for the UF, UP and WP ensiling treatments, respectively. Losses from (ii) silage effluent amounted to 2.9 %, 2.5 % and 0 % for the UF, UP and WP ensiling treatments, respectively and losses from (iii) invisible losses amounted to 16.4 %, 9.9 % and 4.8 % for the UF, UP and WP ensiling treatments, respectively. Bastiman and Altman (1985) indicated that conservation losses can be as high as 30 %.

Nitrogen losses during conservation are assumed to be proportional to the loss of DM (Schils *et al.,* 2005). Nitrogen losses from conservation are a mixture of NH_3 and N oxides (Maw *et al.,* 2002). Schils *et al*. (2005), in the absence of sufficient quantitative data, assumed a 50:50 ratio between NH_3 and N oxides losses.

1.3.3. The P cycle.

Environmental concerns associated with P are based on its stimulation of biological productivity in aquatic ecosystems. In most freshwaters systems primary productivity is limited by inadequate levels of P. External inputs from urban wastewater, surface run-off or sub-surface flow can remove this limitation and stimulate the growth of aquatic organisms to ecologically undesirable levels. Total P concentrations of >100 µg P l^{-1} (ppb) are regarded as unacceptably high in most surface waters and concentrations as low as 20 µg P l^{-1} can cause environmental problems (eutrophication) in some waters. Many point and non-point sources of P have the potential to induce eutrophication in surface waters. Among the non-point sources of P, the agricultural ones in general, and those from dairy farming systems represent a large proportion.

The total quantity of P in a surface water body will be controlled by the balance between the inputs form external sources (i.e. agriculture) and the outputs as water drains from the

water body. A net raise in P increases the likelihood of eutrophication, but the cycling of P, between soluble, organic, and sediment-bound forms within any aqueous ecosystem will regulate the bioavailability of P and thus the extent of eutrophication that occurs. The importance in eutrophication, therefore, will be regulated by the chemical, biological and physical reactions that control P solubility (source control), and the transport processes that move all forms of P to and within water bodies (transport control).

A conceptual model to provide an overall representation of the mechanisms of P export from agricultural land (Heathwaite *et al.,* 2000) is shown in Fig 7.

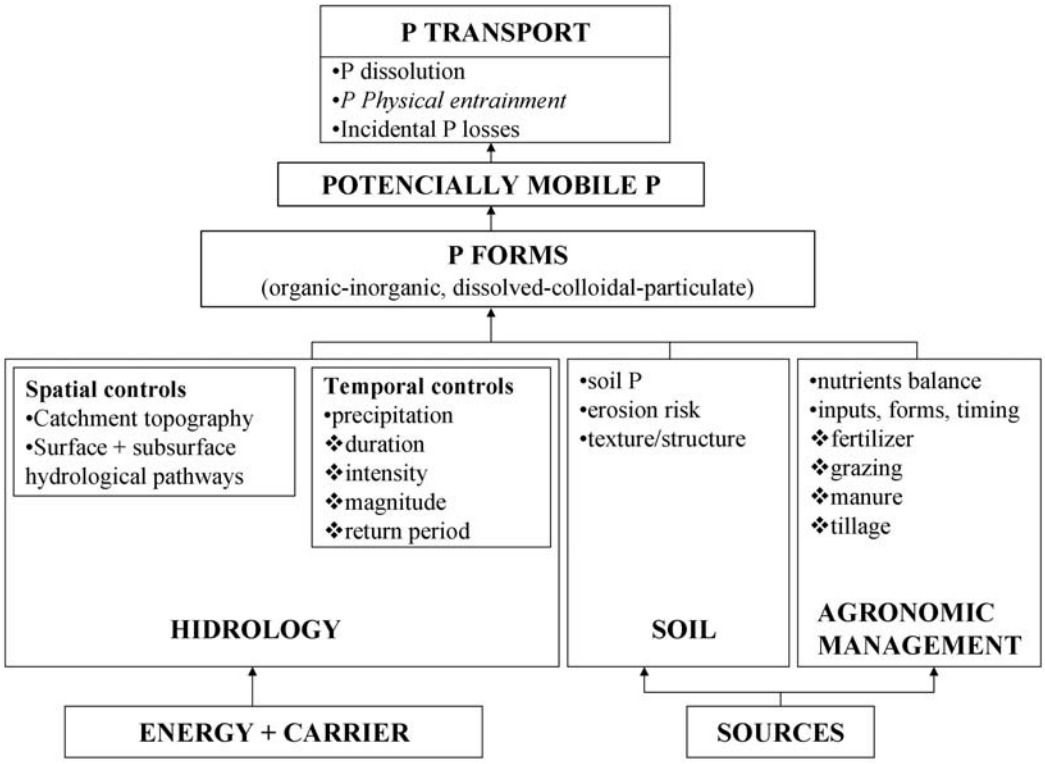


Figure 7. Conceptual model of P transport (after Heathwaite *et al*., 2000)

This model highlights the significance of hydrology as the driving mechanism of P transport. The nodes of P transfers described are dissolution, physical entrainment processes (i.e. erosion) and incidental direct losses. The latter are defined as losses occurring soon after application of fertiliser and manures when coincident with a rainstorm. While dissolution will be instigated by low discharge rates associated with base flow (high frequency/ low

magnitude rainfall), physical transfer and incidental transfer may also be affected by low frequency/high intensity rainfall events.

The concentration of total P in agricultural soil ranges from 100 to 3000 mg P kg^{-1} (Frossard *et al*., 2000). Most of this P is present in orthophosphate compounds. The concentration of dissolved inorganic P in the soil solution is generally low, but is replenished from the desorption of inorganic P held in soil particles, and through the mineralisation of organic P (Frossard *et al.,* 2000). Phosphorus forms are commonly subdivided according to their size into particulate, colloidal and dissolved fractions and according to their chemical nature as organic or inorganic. The contribution of organic P to the soil pool varies, but is generally in the range of 35-65% (Sharpley and Rekolainen, 1997). In contrast to dissolved inorganic P, which may be held in the soil matrix, dissolved organic P is more labile and susceptible to leaching.

1.3.4. Other important losses. C losses.

1.3.4.1. Losses of CH_4

Enteric fermentation in livestock is the main agricultural source of CH_4 in Europe, with emissions from livestock manures accounting for most of the rest. Methane is produced as a by-product of digestion of structural carbohydrates, principally cellulose, due to the action of microbes (bacteria, fungi and protozoa) in the rumen. During this digestion, mono-saccharides are fermented to hydrogen (H_2), carbon dioxide (CO_2) and volatile fatty acids (VFAs) such as acetate, propionate or butyrate. As part of this stage of ruminant digestion some of the microbes (called methanogens) produce CH_4 from and CO_2.

Several studies have aided the formulation of abatement strategies to mitigate CH_4 emissions. Mitigations can generally be split into two groups, (i) those aimed at enteric fermentation and (ii) those targeting manure management.

(i) <u>Enteric fermentation strategies</u>

These may be addressed at 3 different levels (Jarvis, 2001): dietary changes, direct rumen manipulation and systematic changes. The dietary changes suggested so far involve measures which enhance the efficiency of feed energy use. Even assuming a constant

percentage of CH_4 loss, this strategy will decrease CH_4 loss per unit of product and probably decrease CH_4 emissions in the long term (Johnson and Johnson, 1995). The most natural way to depress CH_4 production would be to manipulate the diet to give high rates of fermentation and/or passage through the rumen, which might increase the molar percentage of propionate and decrease that of acetate in the rumen VFAs. These changes in VFA proportions have been associated with a decrease in the fibre content of the diet (i.e. switching to high starch concentrates or maize silage). Ingestion of organic acids (aspartate, malate and fumarate) and yeast culture has been associated with reduced emissions in total CH_4 per cow and also with beneficial increases in animal product (i.e. milk yield). Their reactions in the rumen produce propionate and butyrate, which behave as electron metabolic sinks competing for the H_2 and thus minimising the chances of methanogens to produce CH_4 from H_2.

The use of some plant extracts (i.e. tannins, saponins) has also been associated with CH_4 reduction (Sliwinski *et al*., 2002; Hess *et al*., 2003; Carulla *et al*., 2005; Hu *et al*., 2005; Puchala *et al*., 2005). As yet there is no consensus on its efficacy (Newbold and Rode, 2005).

There are some drawbacks to using these dietary supplements. The organic acids are not commonly used as yet, and they may also trigger pH problems in the rumen. Wallace *et al*. (2005) showed that the pH problem may be overcome by the encapsulation of the organic acid (i.e. fumarate). Plant extracts may also have anti-nutritional effects and even be toxic (Teferedegne, 2000). For instance, in a study by Hess *et al*. (2005), extracted tannins had a positive effect on feed rates and hence a possible reduction of CH_4 per kg product, whereas the use of shrub legumes rich in tannins resulted in decreased feed rates. Yeast culture, on the other hand, although variable, may be promising as a successful mitigation option as it is already in common use.

There have been several attempts to reduce enteric CH_4 production through direct rumen manipulation; for instance, defaunation of protozoa may decrease the number of methanogenic bacteria as an important proportion of rumen methanogenic bacteria are parasitic to protozoa (Takahashi, 2005). The main drawbacks though are that protozoa defaunation may trigger some metabolic diseases.

The ingestion of ionophores acts as propionate enhancers and hence increases the ratio of propionate: acetate. Their use is very limited as they are antibiotics (i.e. monensin) and their main drawback is that they may enhance bacterial resistance to antibiotics. Some changes in the dietary fat contents of the ration have been described to reduce CH_4 emissions from ruminants (Dong *et al*., 1997; Machmuller *et al*., 1998; Johnson *et al*., 2002; Giger-Reverdin *et al.,* 2003) as some fats alter the ruminal microbial ecosystem and, in particular, the competition for metabolic H_2 between the CH_4 and propionate production pathways (Czerkawski, 1972).

Systematic changes may involve identifying animal breeds which result in a reduction of CH_4 output per animal. However, and so far, no clear evidence has been found (Münger and Kreuser, 2005). Waghorn *et al*. (2005), for instance, found that variability within animals is greater than between animals, and it is therefore difficult to come to any conclusions. Increasing productivity per head (i.e. milk yield per cow), or increasing the number of lactations for which the average cow remains economically productive, would decrease CH_4 production per unit of milk, and within the framework of production quotas would decrease total CH_4 emissions. Although more intensive forms of animal production tend to decrease total CH_4 output, they might not be compatible with other issues for water, atmosphere, soil, biodiversity, landscape or animal welfare.

(ii) Manure management

Opportunities to decrease total CH_4 outputs from farming systems are limited to either increasing the O_2 supply to restrict methanogenesis, minimising the release of CH_4 to the environment (e.g. covered lagoons) or using anaerobic digesters to produce more CH_4 in a controlled environment and hence use this CH_4 as a source of energy. This last technique could represent a future sustainable option, but currently has the drawback of high capital cost.

1.3.4.2. Losses of CO_2

Carbon dioxide is formed naturally in grassland systems through respiration (below-ground soil, shoot plants and herbivores) and is fixed into carbohydrates via photosynthesis. Grasslands are generally regarded as potential sinks for CO_2 although soil management factors such as the frequency of ploughing and reseeding might alter the potential for carbon

sequestration. Other management factors may also affect on the whole C balance of a farm, including emissions from farm machinery, and indirect CO_2 emissions associated with fertiliser manufacturing, transport of feed and other inputs to the farm. There is also the issue of the C balance of the whole farming and food supply business, including the fuel consumption issues of food chains and connectivity between the farm and the consumer (Jones, 2001).

There are a number of possible C sequestration measures that may be applied on grasslands and some present management schemes have probably helped to maintain soil-C stocks (Smith, 2004; Freibauer *et al*., 2004). These include improving efficiency of animal manure and crop residue use, reducing soil disturbance, maximising the C returns in manure, use of deeper rooting species, application of sewage sludge or compost to land, irrigation, extensification and improved management to reduce wind and water erosion. The increase in soil C content after a shift from arable to grassland is partly explained by a greater supply of C to the soil under grass, mainly from the roots, but also from the shoot litter, partly by the increased residence time of C due to the absence of tillage (Soussana *et al*., 2004). Whereas this rate of increase of soil C after conversion to grassland is slow, the rate of C disappearance from soil after returning grassland to arable is rapid. A grassland sward aged more than 20 years no longer acts as a C sink (Frank, 2002). Converting grassland to forest can lead to an accumulation or to a release of soil C, depending on the conditions (Post and Kwon, 2000). Introducing short duration leys tends to have an intermediate C sequestering potential between crops and permanent grasslands (Soussana *et al*., 2004).

In this context we can also include the growing of biofuel and other industrial crops on agricultural land, with the potential for non-food crops to further mitigate CO_2 emissions by displacement of fossil fuels.

1.4. Improving the efficiency of nutrient use within temperate grassland-based dairy systems

Most dairy systems import large amounts of nutrients in the form of artificial fertiliser and purchased feeds. It has been estimated that only about 15-30% of the N, for instance,

entering a typical dairy farm is captured in milk. To some extent losses are inevitable. However, a goal of modern agriculture is to reduce nutrient losses to the environment as much as possible within economic and social constraints (Jarvis and Aarts, 2000).

The efficiency of nutrient use can be expressed as the ratio between outputs and inputs at different spatial boundaries. For instance, while the efficiency of N use of a plant is the ratio between plant N uptake and soil available N, the efficiency of N use of a dairy farm is the ratio between milk + meat N and inputs of mineral fertiliser and purchased feeds.

The efficiency of the system within the herd and stable is mainly determined by the ability of the animals to convert nutrients in feed and bedding material into milk and meat product. Needless to say that if manure is considered a valuable output, the system can appear quite efficient.

The boundaries of the system can be widened to a farm level, including the soil and crop components and even broader to catchment, where hydrology and local climate would be the most important processes controlling the flows of nutrients and the boundaries could go even further (landscape…global) where the analysis would be even more complicated as geographical and atmospherical components would have a major influence on the nutrient flows (see figure 8).

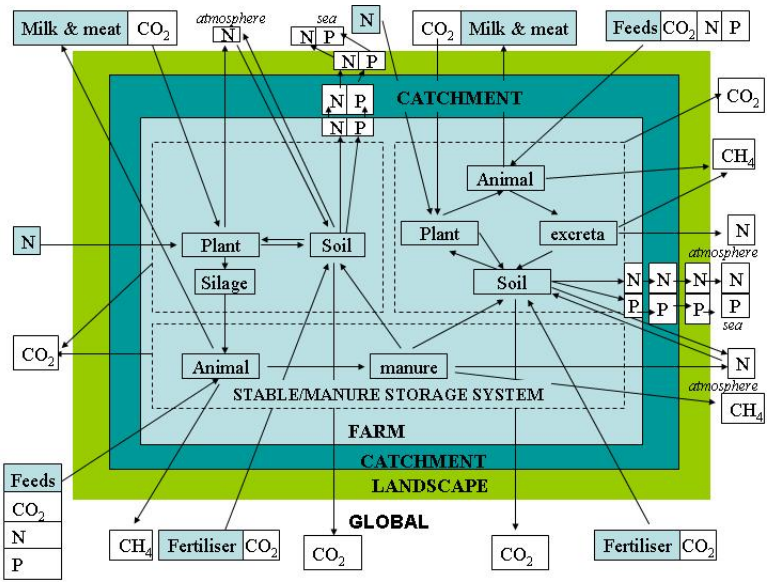


Figure 8. Nutrient fluxes at different levels (herd, field, farm, catchment, landscape and global).

The extent to which a farm relies on feed produced outside the farm has a notable impact on the loss and efficiency. Substitution of mineral fertiliser N by imported feed N reduces the

loss per unit of area and unit of product, and drastically improves the farm N use efficiency. However, from a sustainability point of view there are limits to this as this feed is likely to have produced N losses outside the boundaries of the farm and also used a substantial amount of synthetic N fertiliser (with its associated CO_2 emission). Within the farm boundaries this replacement of purchased N feed is generally associated to an amount of P in this feed, which generally exceeds the herd and crops requirements substantially and thereby, leading to accumulation of P in the soil and eventually to P losses from the soil.

In order to improve the conversion of nutrients within farms we need to know the scope for some factors to alter the nutrient use efficiency at smaller scales.

The N and P use efficiency from feed to animal product (milk and meat) and manure can be improved by increasing the level of production per animal and by better adjustment of matching N and P animal requirements with N and P supply for a given level of milk production, thereby preventing the excretion of excess N and P with urine and faeces. There are several ways to increase milk yield per cow and thereby achieve farm production level with fewer cows. These may include feed quality, genetics and technical measures such as the use of growth hormone, increasing the frequency of milking or extending the photoperiod by artificial lighting (Schröder *et al*., 2005a). Increasing milk yield per cow may be associated with a higher rate of replacement rate of lactating cows and hence a large number of young cattle which partially may compensate for the increased efficiency of nutrient utilisation.

The fact that for practical reasons in most cases young livestock are offered similar feeds as those offered to lactating cows, leads to feeding young livestock in excess and hence to larger N and P losses in urine and dung. Although increasing milk yield per cow still seems to pay off, the effect may be smaller than indicated by an analysis of milking cow production data only (Schröder *et al*., 2005a).

Increasing milk yield per cow requires a high intake of metabolisable energy. The possibilities to increase DM intake, however, are limited. Several measures can be taken to improve the efficiency of N use by the lactating cow. Diets almost completely based on fresh forage with a high N content are highly digestible, and a relatively large fraction will be excreted and not partitioned into milk. On the other hand, diets mainly composed of

concentrates of low N content (i.e. maize) may result in much more efficient N retention up to levels just below 40% (Schröder *et al*., 2005a).

A balance between rumen digestible energy and N must be met in the diet to improve N conversion to milk. A relatively high quantity of rumen degradable protein (RDP) compared to the quantity of rumen digestible energy is another main cause of large losses of NH_3 through fermentation of feed N, this NH_3 absorbed from the rumen to the blood and eliminated from the system as urea by urine production (Valk, 2002). Exchanging these diets by energy-rich compounds will capture more RDP in microbial protein which, after subsequent digestion, becomes available as microbial protein (MP). Relatively low quantities of RDP compared to rumen digestible energy strongly stimulate the reflux of urea from blood to the rumen (Dijkstra *et al*., 1992), allowing microorganisms to synthesise despite the low quantities of N delivered by the feed. Manipulation of the quantity of RDP that is not incorporated by microbial synthesis may improve N use efficiency by the lactating dairy cow. An excess supply of protein or imbalanced diet composition will lead to an increased urea concentration in the milk (Borsting *et al*., 2003).

From a viewpoint of gaseous losses, it is of considerable importance to distinguish between urine and faecal N excretion, because the former is much more susceptible to volatilisation. Nitrogen excreted as faeces is reported to be rather constant in proportion to DM intake, this being about 7.5 g/kg DM ingested or 0.6 % of the dietary DM intake. Faeces are composed of undigested feed N, undigested microbial N and endogenous N. Reduction in faecal N excretion does not appear to be a promising way to improve N use efficiency and this is due to the fact that most dairy cow rations are high in digestibility.

Nitrogen excreted as urine is more variable than faeces. Various routes contribute to urinary N output including ruminal and metabolic losses. Increases in dietary N lead to substantial increase in urinary loss. Normally, diets based on high-quality forages such as grass silage and Lucerne silage are cheaper and are the main source of N for dairy cattle (Castillo *et al*., 2000). However, one of the main problems with these forages is the reduced efficiency of N utilisation. To overcome these problem there are solutions such as supplementation with low rumen-degradable protein (not very successful as it could stimulate N excretion), increasing readily available carbohydrates (CH) in the rumen, and replacing high fertilised herbage by low-protein and high energy feeds (with maize and

concentrates). This last measure can reduce urinary N excretion, and moreover, concentrates mixtures based on digestible fibre or starch increased N output in milk, a smaller response was observed using maize.

In diets with high proportion of RDP or an excess of RUP, a substantial proportion of this N will normally be excreted in urine. A significant negative linear relationship between relative rumen degradability of protein and urinary excretion was found by Castillo (1999).

In the case of P, a high phytase activity of rumen contents ensures that almost all P will flow into the small intestine in the inorganic form. Although feed P is highly digestible in principle, the normal excretory route is through faecal excretion only. P excretion with faeces depends on P content in feed and the level of animal production. In lactating cows, the efficiency of P retention in milk ranged from 0.42 to more than 0.55 on diets ranging from 3.4 to 2.3 g P/ kg DM (Schröder *et al*., 2005a). Most P in faeces will be in the inorganic form subject to P leaching after manure application.

The N use efficiency from excreted to soil-incorporated manure depends on the magnitude of gaseous N losses from stables and storage facilities, and on losses from manure application and grazing. Most losses at this stage, as already indicated in previous sections, is in the form of NH_3 and a small fraction of losses due to denitrification (N_2, N_2O and NO_x).

Ammonia losses can be reduced by measures that lower the NH_3 content of manures in the first place (i.e. additions of materials high in C: N ratio). Dietary measures, formerly explained, may also reduce the amount of N or TAN in the excreta. Manure types and techniques that improve the match between crop demand and manure inorganic N supply also improve the efficiency of N use. Chemical treatment of manure, especially acidification and mechanical treatment have also been proposed. Storage systems which are closed or with less surface are likely to result in lower NH_3 losses too. Grazing generally reduces the overall NH_3 losses from dairy systems, relative to situations where the herd is confined in housings (Bussink and Oenema, 1998).

The N use efficiency from soil-incorporated manure to harvestable crops depends on fertiliser management strategies such as nature of fertiliser, rate, timing, place, proportion in solid or liquid form and also depends on crop effects (Schröder *et al*., 2005b).

Even when the long-term N fertiliser value is correctly accounted for, the efficiency of organic inputs may not be as high as that of mineral fertilisers. The reason is that

mineralisation may partly occur outside of the growing season of crops. In grasslands managed at moderate intensity the long-term efficiency values from organic fertiliser may be 0.4-0.8 for N and 0.7-1 for P appear attainable (Schröder *et al*., 2005a). Corresponding values for mineral fertilisers can be as high as 0.5-0.9 (N) and 0.8-1 (P).

It is generally impossible to meet the N requirements as a whole with manure only, if excessive applications of P are to be avoided. The reason for this is the fact that the N: P ratio in most crops average>6, whereas the ratio of effectively available N and P in manures is generally<5. Hence, sustainable systems (i.e. in which P inputs do not exceed P outputs) are always short of N. The relative N deficiency can be met by the presence of legumes or by mineral N fertilisation (Schröder *et al*., 2005a).

Controlled-release forms of N fertiliser have been shown to improve N use efficiency, decrease N losses, cut labour and application costs, and increase yields (Giller *et al*., 2004). However, sales of such materials have always been inhibited by their high costs (Goulding, 2007).

Nitrogen should be water-soluble during the growing season to be available to plants, whereas it should be organically bound from late summer to spring in order to avoid losses. Practices resulting in both water-soluble N forms during the growing season and organically-bound N forms during the rest of the year are likely to overcome synchronisation problems.
The efficiency by which soil nutrients are converted to harvestable crops also depends on crop choice, on crop rotation and on cutting regimes. Genetic variation in nutrient acquisition and assimilation by plants show that further increases in efficiency are possible through plant breeding.

Nutrient budgeting is being used increasingly by farmers and policy makers. A nutrient budget is the summary table of the book-keeping of nutrient inputs and outputs of a system (Oenema *et al*., 2003). It is also widely used to study nutrient efficiency and losses. Oenema and Heinen (1999) distinguished 3 basic approaches in nutrient budgets studies, though there are variants within each of these: (i) farm gate budget: records the amounts of nutrients that enter and leave the farm via the farm-gate, (ii) soil surface budget: records the nutrients that enter the soil via the surface and that leave the soil via crop uptake and (iii) soil system budget: records all nutrient inputs and nutrient outputs, including nutrient gains and losses within and from the soil.

Nutrient surpluses of these budgets can be used as performance indicators of the efficiency of N and P use in farming systems. Although, it is widely accepted that they are useful tools to provide a general indication of the farm nutrient performance, they are generally not useful to evaluate for instance the effect of management on losses as the relationship between nutrient balance and nutrient loss has been found to be weak. Budgets also have the problem of the very large uncertainties associated with them (Oenema *et al*., 2003). The whole cause-effect chain needs to be considered, as nutrient surpluses may also change through changes in the agroecosystems (Oenema *et al*., 2003).

1.5. Modelling approaches to simulate the cycling, transformations and losses in the N and P soil-animal-plant farming systems.

During the last 30 years, there has been considerable progress in the quantification of the N pools and fluxes, due to mainly the development of new techniques for measurement of N losses (i.e. denitrification: Ryden *et al*., 1979; volatilisation: Lockyer, 1984; N_2O: Velthof and Oenema, 1995; NO: Harrison *et al.,* 1995) and net N mineralisation (Jarvis *et al*., 1996a). These new data have been used in the construction, calibration, verification and testing of mathematical models of the pasture N cycle (Reuss and Innis, 1977; Molina *et al*., 1983; Parton *et al*., 1987; Thornley and Verberne, 1989; Bergström *et al*., 1991; Cabon *et al.,* 1991; Hansen *et al*., 1991; Rijtema and Kroes, 1991; Scholefield *et al*., 1991; Van de Ven, 1992; Riedo *et al*., 1998), looking the cycling of N at different scales (i.e. Anger and Kuhbauch, 1999; Lin *et al*., 2000; Rotz *et al.,* 2005b, Macleod *et al*., *in press*), focussing on specific processes such as mineralisation (i.e. Matus and Rodriguez, 1994; Wu and McGechan, 1998) or losses to the environment such as NO_3^- leaching (i.e. Rodda *et al*., 1995; Scholefield *et al*., 1996; Di and Cameron, 2000; Vellinga *et al*., 2001), NH_3 emissions (i.e. Hutchings *et al*., 1996; Menzi *et al*., 1998; Sommer and Olesen, 2000; Ross *et al*., 2002; Webb *et al*., 2001, 2004), N_2O (Li *et al.,* 1992; Conen *et al.,* 2000; Parton *et al*., 2001; Schmid *et al.,* 2001) and NO_x emissions (Yienger and Levy, 1995; Parton *et al.,* 2001).

1.5.1. Modelling the N cycle.

1. 5.1.1 Modelling soil N mineralisation

These may be broadly categorised as: (i) simple functional approaches to predict net N mineralisation and (ii) mechanistic approaches that include a description of microbial biomass processes to predict long-term C and N turnover in soils.

The simple approaches try to quantify one or more active fraction of organic matter with associated rate constants to predict net N mineralisation. These approaches do not tend to consider the processes of ammonification and nitrification separately and their parameters are generally obtained from laboratory incubations studies by fitting N mineralisation data to the time of incubation.

(i) We can classify the simple modelling approaches depending on the number of fractions involved:

The single-fraction approach is the simplest one and involves only one active fraction. Standford and Smith (1972) defined soil N mineralisation potential as the quantity of soil organic N susceptible to mineralisation at a rate of mineralisation (k) according to first-order kinetics:

$$N_m = N_0 (1\text{-}\exp(-kt))$$

(1)

Where N_m is the N mineralised in time t and N_0 is the initial amount of substrate or the potentially mineralisable N.

The first-order kinetic model has been used to describe N mineralisation kinetics of soils under different edapho-climatic and crop conditions (Campbell *et al.,* 1984; Hadas *et al.*, 1986; Cabrera and Kissel, 1988). Other authors, such as Macduff and White (1985) and Addiscott (1983) found that their incubation data fitted well to a zero-order kinetics approach instead:

$$N_m = k_1 t$$

(2)

Where K_1 is the net mineralisation rate and was obtained from an estimate of the rate of net mineralisation, K_1 is a constant rate that does not depend on substrate amount. K_1 may be a

function of temperature and water content in the soil (Macduff and White, 1985; Clay *et al.*, 1985).

The multi-fraction approach considers more that one pool or fraction of organic N being mineralised. Each fraction has its specific rate of decomposition. Various authors (Molina *et al.,* 1980; Nuske and Richter, 1981) have divided the soil organic N into different fractions, each of them being assumed to follow first-order kinetics. In the simplest form 2 main fractions of organic N mineralises at different rates (Deans *et al.,* 1986; Wang *et al.*, 2004). One fraction consists of N compounds of easily (fast) decomposable plant material, while the second fraction represents the more resistant or recalcitrant (slow) plant fraction which accumulates within the soil:

$$N_m = N_{FAST}\,[1\text{-}\exp(-k_{FAST}\,t)] + N_{SLOW}\,[1\text{-}\exp(-k_{SLOW}\,t)] \quad \textbf{(3)}$$

Where N_{FAST} and N_{SLOW} represent potentially mineralisable N in the easily decomposable and resistant organic N fractions, respectively, and k_{FAST} and k_{SLOW} are the corresponding rate constants.

Some authors (i.e. Beauchamp *et al.*, 1986) indicated that this equation was inadequate to simulate the effect of drying-rewetting of soil and suggested improved equations. These equations were based on the assumption that the killed microbial biomass N pool is effectively used up by 7 days and N mineralised subsequently originates entirely from the soil organic N pool.

Other adopted a 3-fraction approach in order to account for fast decomposable plant material, recalcitrant decomposable plant material and dead biomass N (Richter *et al.*, 1982; Ando *et al.*, 1992)

Mixed first and zero-order kinetic approaches have been also proposed. Bonde and Rosswall (1987), for instance, suggested a degenerate of the double exponential model:

$$N_m = N_1\,[1\text{-}\exp(-k_1 t)] + Kt \quad \textbf{(4)}$$

In which N_1 represent the amount of mineralisable N in the easily decomposable fraction at the start and k_1 is the rate constant (first-order) and K is the zero-order rate constant.

Diverse empirically derived equations such as polynomials and parabolic functions have been proposed to describe net N mineralisation (Broadbent, 1986; Marion and Black, 1987; Pereira *et al*., 2005).

(ii) The mechanistic approaches for simulation of mineralisation-immobilisation turnover can be exemplified by non-compartment models and food-web models (Benbi and Richter, 2002). The mechanistic approaches represent the basic mechanisms that influence mineralisation. They attempt to simulate gross mineralisation and associated mineralisation (mineralisation-immobilisation turnover).

The mechanistic models have the advantage that model algorithms represent the basic mechanisms believed to influence mineralisation. However, it is difficult to validate the models as some of the presumed functional pools cannot be quantified by physical, chemical and biological techniques. Consequently, the models have to be calibrated by adjusting the rate coefficients and pool sizes (site-specific) to fit the measured data (Benbi and Richter, 2002).

1. 5.1.2. Models to simulate NH_3 emissions from fertiliser application

Empirical models have been described in different forms. The simple ones are obtained by relating experimental data to fitted equations. The rate of NH_3 volatilisation, for instance, has been described by a logistic (Stevens *et al.,* 1989b), sigmoidal (Sommer and Ersbøll, 1996) or Michaelis-Menten (Misselbrook *et al*., 2005b) equation.

Mechanistic models attempt to mathematically describe the physical, chemical and biological processes and interactions leading to NH_3 emissions (i.e. Van der Molen *et al.*, 1990). However, they are often difficult to validate and can be too complex for use in farmer/advisor orientated decision support systems (Misselbrook, 2005).

Models can also be split into those which only simulate NH_3 emissions from a limited number of factors (1) and models which simulate NH_3 at a broader scale (2). Examples of both types of approaches are shown as follows:

(i) Models that simulate NH_3 emissions for a limited number of factors:

Rachhpal-Singh and Nye (1986) developed a mechanistic model to predict NH_3 volatilisation loss following application of urea to the soil. This process combines the process of NH_3 volatilisation with the simultaneous transformation and movement of urea

and its products in soil. The process of NH_3 volatilisation is the transfer of NH_3 gas in the soil air from the soil surface to the immediate atmosphere. The rate of NH_3 is given by the following equation:

$$F_{Ng} = K_a \Delta N_g$$

(5)

Where F_{Ng} is the flux of NH_3 gas and ΔN_g the NH_3 gas concentration difference across the soil surface-atmosphere air boundary layer and K_a the mass transfer coefficient, which depends on factors such as: surface roughness, temperature and the wind speed over the soil surface.

Genermont and Cellier (1997) developed a detail mechanistic model to predict NH_3 volatilisation following manure slurry application in the field. The model consisted of 6 submodels; the first 3 submodels deal with the transfer of NH_3-N in the soil/atmosphere and the other 3 submodels simulate heat and water transfer in the soil and are included to account for the temperature and soil water concentration dependent equilibrium as NH_3 is transported with water in the soil: (i) Physical and chemical equilibrium of NH_4^+-N in the soil, (ii) aqueous and gaseous NH_3-N transfers through the soil, (iii) gaseous NH_3 transfer from the soil to the atmosphere, (iv) water tranfer in the soil, (v) heat transfer in the soil, (vi) energy budget, water and heat exchange between the soil and atmosphere.

(ii) An example of models which simulate NH_3 at a broader scale:

Pinder *et al*. (2004) developed an integrated model of a dairy farm that predicts monthly NH_3 emission factors based on farming practices and climate conditions, including temperature, wind speed, and precipitation. The model tracks the volume of manure and mass of NH_3-N as the manure moves through the housing, storage, application, and grazing stages of a dairy farm. Ammonia is volatilized from the surface of a liquid solution and is then transported to the free atmosphere. The per cow volatilisation of NH_3 was described as:

$$\text{Emissions} = A\,[\text{TAN}]\,H\,r^{-1}$$

(6)

Where A is the fouled surface area per cow (m^2 cow^{-1}), [TAN] is mass concentration of NH_3 and NH_4^+ in solution expressed as kg (as NH_3) m^{-3}, H^* is the effective Henry's Law constant (dimensionless), and r is the mass transfer resistance (day m^{-1}). Mass transfer of gas phase NH_3 was inhibited by the transport resistance, r. High wind speeds cause these resistances to

decrease. The surface resistance arises from diffusion through the top layer of soil or a surface crust formed on the top of stored manure. It is meant to capture poorly understood processes that are specific to the stage of the model. This parameter is tuned to match empirical data. Manure volume is increased by the rate of manure loading and by precipitation. Evaporation and infiltration reduce the solution volume. Urea mass is added at the manure loading rate multiplied by the concentration of urea in newly deposited manure.

Urea is transformed to TAN by hydrolysis. TAN is subsequently decreased by emissions and by infiltration. Manure is instantaneously transferred from the housing to storage once a day. For farms that apply manure monthly or more frequently, 90% manure is assumed to be transferred from storage during application. If the manure is applied seasonally, this fraction varies with each month. Three different types of storage are considered by this model: lagoon, slurry tank, and earthen basin. Manure is transferred from storage to the application stage daily, weekly, monthly, or seasonally. The NH_3 in the intercepted manure is subject only to volatilisation, so all of the NH_3 is emitted to the atmosphere. The remaining fraction either volatilizes or infiltrates into the soil.

Webb and Misselbrook (2004) developed a mass-flow model to estimate NH_3 emission from agriculture based on different NH_3 emission factors (Efs). Ammonia is emitted from the pool of TAN in livestock excreta. This pool may be increased by mineralisation of organic N during manure management and is depleted by gaseous emissions, leachate loss and immobilisation in litter. At each stage of manure management a portion of TAN is lost, mainly as NH_3, and the remainder passed to the next stage. The model allows rapid and easy estimation of the consequences of abatement at one stage of manure management on NH_3 losses at later stages of manure management.

1. 5.1.3. Models to simulate (i) denitrification and (ii) N_2O from soils

A number of different approaches have been used to develop denitrification submodels in N-cycling models (Parton *et al*., 1996): (i) microbial growth models, (ii) soil structural models and (iii) simplified process models. The microbial growth models consider the dynamics of microbial organisms responsible for the N cycling processes (Leffelaar, 1988; Li *et al.,* 1992ab; Riley and Matson, 2000). The soil structural models consider gaseous diffusion of gases into and out the soil aggregates. The distribution of these aggregates is considered and

denitrification only occurs in the anoxic parts of the aggregates. Examples of these models can be found in Arah and Smith (1989), Grant (1991), Vinten *et al.* (1996) and Kremen *et al.* (2005).

The simplified process models are easier to use and do not consider microbial processes or gaseous diffusion. Denitrification is assumed to be determined by easily measurable parameters such as degree of saturation [expressed as for instance %water-filled pore space (%WFPS)], soil temperature and NO_3^- content in the soil. Such models are practical to use in studies where denitrification at field scale is to be determined. Examples of these models can be found in Scholefield *et al.* (1991) and Well *et al.* (2001), for instance. The majority of the denitrification models can be given by the following general mathematical function to describe actual denitrification either at the local point scale or from a certain soil layer (Heinen, 2006):

$$D_a = \alpha f_N f_S f_T f_{PH}$$

(7)

Where D_a is the actual denitrification rate, α is the parameter depending on the exact formulation (i.e. potential denitrification or first-order denitrification coefficient, in both cases α can be a constant parameter or related to C dynamics), f_N is a dimensionless reduction function for NO_3^- content in soil, f_S is a dimensionless reduction function for water content in soil, f_T is a dimensionless reduction function for temperature in soil and f_{PH} is a dimensionless reduction function for soil pH. All these dimensionless function are generally in the range [0, 1].

The response to NO_3^- content in soil is generally described by a Michaelis–Menten relation. At high NO_3^- concentrations NO_3^- is not limiting (zero-order process), while at low NO_3^- concentrations NO_3^- becomes limiting (first-order process). Therefore, in most models the NO_3^- reduction function f_N is considered to be of Michaelis–Menten form (or Monod form):

$$f_N = N/(K+N)$$

(8)

Where N is the NO_3^- content of soil, or NO_3^- concentration K (same units as N) is the half-saturation constant, i.e., the NO_3^- content or concentration at which $f_N = 0.5$. Under natural

conditions the NO_3^-–N content is relatively low, which explains why in many studies a first-order decay denitrification function is used (Heinen, 2006).

The response to soil water contents is generally described by steep, non-linear relationships. As the water content increases, the air-filled porosity decreases, thus affecting oxygen supply rate. Many models use a power reduction function (i.e. Grundmann and Rolston, 1987). However, other forms of water reduction functions have been also used. Some authors used linear (broken-line) (Birkinshaw and Ewen, 2000), exponential (Kersebaum, 1995) or Michaelis-Menten (Priesack *et al*., 2001) type of relationships to describe the effect of soil water content on denitrification.

The response to temperature may be described by an exponential increase defined by Q_{10}-Arrhenius functions. Typical values of Q_{10} are 2 to 3. However, one must be aware that, although mostly considered to be constant, Q_{10} is dependent on the temperature range it was determined for. In a few models the temperature function is split in parts so that different types of denitrifying bacteria can be simulated to operate at each temperature interval (Hansen *et al.*, 1991).

The response to pH is generally described by bell-shaped relationships, where an optimum in denitrification rate is generally around pH = 7 to 7.5 and denitrification almost ceases for pH < 4 or pH > 10 (Heinen, 2006).

Under normal agricultural conditions it is not likely that pH will fluctuate much. However, the inclusion of pH as a parameter is generally much needed when simulating fields that have been limed.

(ii) Modelling N_2O emissions from soils: many current models of trace gas fluxes are based on simple scaling-up of a relatively limited database, and a black box approach to the soil-plant system. The easiest first step is performing simple regression analyses. The success or failure of this approach appears to depend on the simplicity of the system studied.

Normally, not more than 50 % of the variation of the change in the measured flux can be explained.

Conen *et al*. (2000) and Schmidt *et al*. (2000) using a 'Boundary line approach' developed empirical model of N_2O emission from agricultural soils. Both studies were based on the relationships between N_2O and three soil parameters (mineral N in soil, %WFPS and temperature).

Mosier *et al*. (1983) proposed an empirical N_2O model including as independent variables: soil relative water content, soil NH_4^+ and soil NO_3^-. A more mechanistic equation was developed afterwards:

$$E_{N2O} = M_d E\psi\ E_d^1 + M_N E\psi\ E_n \quad \textbf{(9)}$$

Where M_d is the maximum denitrification rate and M_N is the maximum nitrification rate. $E\psi$ is the effect of soil moisture on N_2O flux. E_d^1 is the effect of soil NO_3^- on N_2O flux. E_n is the effect of NH_4^+ on N_2O loss, $E\psi$, E_d^1 and E_n represents the normalized (0 to 1) effect of NO_3^-, $NH_4^+$and soil relative water content (RWC) on N_2O evolution.

NGAS-DAYCENT (Del Grosso *et al.,* 2000; Parton *et al.,* 1996) is one of the more sophisticated empirical models, which predicts denitrification and its product stoichiometry (N_2O/N_2) as a function of NO_3^- content, soil respiration, and diffusion constraint. The diffusion constraint is a function of soil moisture, total porosity, and the pore-size distribution. The product stoichiometry (N_2/N_2O) is controlled by a combination of soil moisture and respiration rates.

The DNDC model (Li *et al.,* 1992ab) simulates N_2O based on the kinetic processes of N_2O production where denitrification is activated by a rainfall event that saturates the soil. It consists of 4 submodels: thermal-hydraulic, crop growth, decomposition, and denitrification. Soil temperature and moisture are the key factors controlling both decomposition and denitrification.

1. 5.1.4. Principles to simulate NO_3^- leaching

The chemical transport and transformation model embodies the following elements (Jury and Flühler, 1992):

(i) A mass conservation law for the chemical processes, (ii) a division of N mass into appropriate phases requiring separate description (i.e. nitrification, mineralisation…), (iii) a flux law for each mobile phase, describing the rate of transport of mass of NO_3^- per unit area in that phase, (iv) a series of interphase mass transfer describing movement of water and solute between the phases, (v) a reaction term describing the rate of appearance or disappearance of mass of NO_3^- per unit of volume.

In this section I will focus on elements iii and iv, thereby mainly on the simulation of transport of solute down the soil profile. The movement of water and solute through the soil can be divided into 3 components: the mobile flow through the soil matrix, the slow-mobile flow through the soil matrix and the macropore flow (preferential flow). The three components are best defined in clay soil, where large aggregate blocks, containing the mobile and slow-mobile flow components, are separated by macropores. By contrast, in sandy soils, where the soil grains are of similar size, the water and solute moves predominantly under the mobile phase. The modelling of the transport of NO_3^- through the soil profile has to account for these 3 different flow mechanisms.

Modelling approaches to simulate the transport of NO_3^- through the soil profile can be broadly divided into those based on the soil-water theory (highly mechanistic) and those with empirical or functional basis (generally capacity type approaches). Among those functional approaches, Burns (1974) developed a simple empirical model to predict the distribution of non-adsorbed solutes (i.e. NO_3^-) subject to leaching and upward movement. He assumed that the soil was made up of a number of layers and that the input of rain to these layers controlled the downward movement of the solute. The model also assumed piston flow, whereby water which was input to the system was instantaneously mixed with the solution, and displaced the same volume of solute through each layer. This piston flow was described by the following equation:

$$F_S = [R/R+\theta]\ z \qquad \textbf{(10)}$$

Where F_S is the fraction of solute washed out to below a depth z, R is the amount of rain which infiltrates the soil and θ is the soil volumetric moisture content. This model was limited however, to sandy soils since it was unable to account for the mobile/immobile water within the soil profile. No water content above field capacity could be simulated. Transport of NO_3^- through the soil profile in heavy soils, however, is generally due to preferential flow.

Preferential flow, as opposed to uniform flow, results in irregular wetting of the soil profile as a direct consequence of water moving faster in certain parts of the soil profile than in others. Hendrickx and Flury (2001) defined preferential flow as ‘all phenomena where water and solutes move along certain pathways, while bypassing a fraction of the porous matrix’. Thus, an important characteristic of preferential flow is that during wetting, part of the

moisture front can propagate quickly to significant depths while bypassing a large part of the matrix pore-space. Water and solutes may move to far greater depths, and much faster, than would be predicted with the Richards equation using area-averaged moisture contents and pressure heads (Beven, 1991). Another important characteristic of preferential (non-uniform) flow is its non-equilibrium nature. Recent studies show that the occurrence of preferential flow due to heavy rainfall events, for example, is the rule rather than the exception in many soils (Flury and Flühler, 1994; Stamm *et al*., 1998; Lennartz *et al*., 1999; Jaynes *et al*., 2001).

Preferential flow in structured media can be described using a variety of dual-porosity, dual-permeability, multi-porosity, and/or multi-permeability models (Pruess and Wang, 1987; Jarvis, 1998a). Dual-porosity and dual-permeability models both assume that the porous medium consists of two interacting regions, one associated with the inter-aggregate, macropore, or fracture system, and one comprising micropores (or intra-aggregate pores) inside soil aggregates or the rock matrix. While dual-porosity models assume that water in the matrix is stagnant, dual-permeability models allow for water flow in the matrix as well.

A simple and functional dual-porosity model (SLIM) was developed by Addiscott *et al*. (1986) and Addiscott and Whitmore (1991). In the Solute Leaching Intermediate Model (SLIM) the soil is divided into a number of layers, similarly to Burns, each of which, in contrast, contains mobile and immobile categories of water and solute. SLIM, thereby is able to simulate the effect of preferential flow. Nitrate is prevented from leaching as long as it remains in the immobile phase. Water movement through the smallest soil pores are considered negligible and water flow in the soil matrix is not considered. The immobile category of water is not decreased by drainage, but can be diminished by evaporation. Water and solute entering a given layer from the layer above, or from rainfall, are added to the current mobile water and solute categories, respectively. A proportion of the new mobile water and solute categories, determined by the rate parameter α, moves to the next layer. Solutes and water move laterally by diffusion and the limits imposed by diffusion can be described by partially equalizing concentrations between mobile and immobile categories, using a 'hold-back' factor (the capacity parameter β). If the layer is the top layer and it reaches saturation further additions of water do not pass through the soil matrix. The model adjusts it so that they are lost by run-off. The parameters α and β of the SLIM model can be

calibrated or estimated from readily-available information (the clay percentage and aggregate size distribution: Addiscott, 1983), which is an advantage over more complex approaches.

Other functional approaches have been suggested by Rodda *et al*. (1995) and Scholefield *et al*. (1996), by which wholly empirical relationships between NO_3^- load, NO_3^- concentration and the volume of drain flow were constructed. These relationships were used to predict the outcome of preferential flow, so that for a given drainage volume and a given soil texture, which are supplied by the user, the percentage of soil N that is actually leached could be calculated. In these studies, relationships between the load of leached N and its concentration in drainage water were also derived.

Dual-porosity models with a mechanistic structure have long been applied to solute transport studies. For example, van Genuchten and Wierenga (1976) based the dual-porosity formulation on a mixed formulation of the Richards equation to describe water flow in the macropores and a mass balance equation to describe moisture dynamics in the matrix. An alternative approach for flow in the macropores was suggested by Germann and Beven (1985). They used a kinematic wave equation to describe gravitational movement of water in macropores. One advantage of this approach is that no water retention properties of the macropore region are required, and hence that the number of parameters can be reduced. Disadvantages over the dual-porosity models based on the Richards equation are that the kinematic wave equation is limited to vertical gravity-driven flow and can not describe upward flow during evaporation periods (Simunek *et al.*, 2003). These two dual-porosity approaches simulate solute transport by a formulation based on the convection-dispersion and mass balance for the macropores and matrix, respectively.

Dual-permeability models in which water can move in both the inter- and intra-aggregate pore regions are now also becoming more popular (i.e. Jarvis, 1994). Dual-permeability models differ mainly in how they implement water flow in and between the two pore regions, especially with respect to the degree of simplification and empiricism. Approaches to calculate water flow in macropores or inter-aggregate pores range from those invoking Poiseuille's equation (Ahuja and Hebson, 1992), the Green and Ampt or Philip infiltration models (Chen and Wagenet, 1992), the kinematic wave equation (Germann and Beven, 1985; Jarvis, 1994), and the Richards equation (Gerke and van Genuchten, 1993). Multi-

porosity and/or multi-permeability models are based on the same concept as dual-porosity and dual-permeability models, but include additional interacting pore regions (Gwo *et al*., 1995; Hutson and Wagenet, 1995). They can be simplified immediately to dual-porosity/permeability models.

A new approach to predict and model the flow of water and solute is to employ an explicit, precise but simplified model of the soil's void structure. For example, Peat *et al.* (2000) proposed a network model (Pore-Cor). This network comprised an infinite array of connected unit cells with periodic boundary conditions, each unit cell containing up to 1000 cubic pores connected by up to 3000 cylindrical throats. The geometry of the unit cell is adjusted so that the void network has the same porosity and water retention characteristics as the experimental sample.

1.5.2. Modelling the P cycle.

There are several models that describe the cycling (i.e. Oyanarte *et al*., 1997, Modin-Edman *et al., in press*) and/or loss of P (i.e. PSYCHIC: Davison *et al*., *in press*) at different scales and with different purposes. A limitation to model use in most cases is often the lack of adequate parameterisation data. Modelling P losses to the wider environment (water sources) normally requires scales larger than the farm. The development of adaptable databases of, for example, soils and weather data would help to expand the application of models as quantitative assessment tools.

Models based on export coefficients (i.e. Johnes, 1996) from various agricultural pathways and sources have been widely used. Interpretation of export coefficient data is always complicated by different farming systems (or land use types), hydrological pathways (which are also scale-dependant), and the forms of P that can be transferred and determined. Export coefficients are empirical, are often based on estimations which involve simple assumptions or extrapolation from small data sets and therefore have limited interpretative value (Haygarth and Jarvis, 1999).

Statistical or empirical models have also been proposed to model P loss including models that involve regression or other techniques, which relate water quality measures to various characteristics of the watershed (for instance). These models range from purely regression equations (i.e. Driver and Tasker, 1990) to relatively sophisticated derived-distribution

approaches for prediction of the frequency distribution of loadings and concentrations (i.e. DiToro and Small, 1984).

Process-based models such as SWAT (Arnold *et al*., 1998) explicitly simulate watershed processes. These types of models typically involve the numerical solution of a number of governing differential and algebraic equations that are a mathematical representation of processes such as rainfall run-off, infiltration leaching, P application method, rate and timing, land management and fate and chemical transformation of added P in soil (Sharpley, 2007).

1.6. Modelling dairy farm sustainability. Integration of system components.

For all levels of integration a systems approach is needed, where the systems approach toolbox, data needs and data availability are linked in such a way that the research or application question can be addressed in the most effective and simple way (Fig 9).

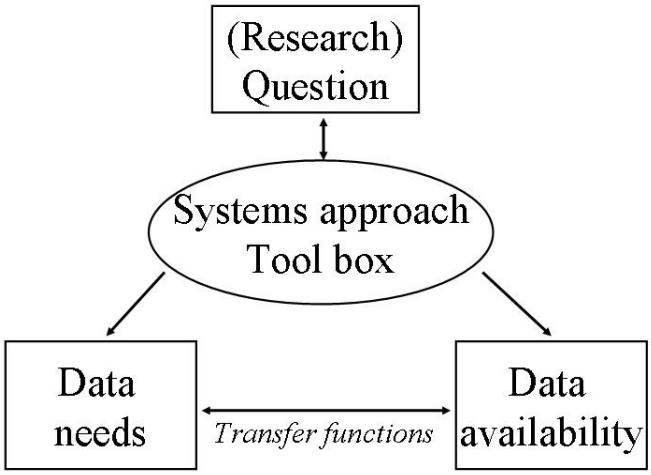


Figure 9. Flexible methodology for using systems approaches in agroecosystems (after Kropff *et al*., 2001)

Farming systems, due to their complexity, require integrated modelling approaches as most mitigation options to reduce pollution involve important trade-offs. For instance, as much as one-half of the climate mitigation potential of some C sequestration options could be lost when increased emissions of other GHG (N_2O and CH_4) were included (Smith *et al.,* 2000, 2001c).

Systems approaches based on Efs have been proposed to quantify the on-farm and off-farm GHG from dairy production systems as affected from management (i.e. Lovett *et al*., 2006) and to model the uncertainty associated with the implementation of adaptations required (i.e. Gibbons *et al*., 2006).

Climate change, and emissions of GHG, unfortunately, account for only a part of the whole challenge in farming systems. Farming is also subject to other pressures, including environmental (i.e. eutrophication, erosion, and acidification), socio-economic and sustainability issues. Identification of win-win strategies requires development of appropriate modelling systems together with the acquisition of field and farm data (Scholefield *et al.,* 2005). There is need to develop models that explore farming systems in an holistic way (McMichael *et al*., 2003).

Following this idea, some studies have formulated abatement strategies and evaluated their economical cost for single issues that are affected by nutrient management in a farm such as: pollution of: GHG (Jarvis, 2001), P (Haygarth, 2004) or NO_3^- leaching (Scholefield, 2004). Other more complex approaches have been proposed that incorporate the simulation of other losses (NH_3, NO_3^- leaching, P losses) and in some cases the incorporation of economics too. The development of whole farm approaches for the mitigation of pollutants has been taken up recently by several research groups in Europe (Schils *et al*., *in press*). Models may vary considerably on many aspects. Whereas for instance DairyWise (Schils *et al*., 2006ab) and Farm GHG (Olesen *et al*., 2006) are mainly empirical and based on Efs, FarmSim (Saletes *et al*., 2004) and $SIMS_{DAIRY}$ (del Prado *et al*., 2006d; del Prado and Scholefield, 2006) are based on semi-mechanistic approaches. More differences between these models can be shown in table 1. Some of these 4 models (DairyWise and $SIMS_{DAIRY}$) can also evaluate farm economics.

In other examples (Berentsen and Giesen, 1994; Van de Ven, 1996; Pacini *et al.,* 2004), modelling frameworks were developed using an economic linear programming modelling approach and coefficients resulting from different ecological models. Pacini *et al.* (2004) also included the potential risk for pesticides and herbaceous plant biodiversity coefficients.

Table 1. General characteristics of whole farm GHG models (taken from Schils *et al., in press*)

	DairyWise	**FarmGHG**	**$SIMS_{DAIRY}$**	**FarmSim**
Model type	**Empirical**	**Empirical**	**Semi-Mechanistic**	**Semi-Mechanistic**
CH_4 and N_2O emissions	x	x	x	x
CO_2 emissions	x	x		x
C sequestration				x
NH_3 and NO_3^- emissions	x	x	x	x
P cycling	x		x	
Pre-chain emissions	x	x		
Economics	x		x	

Broader attempts to develop fully integrated approaches to access sustainability in dairy farms include models (based on indicators) such as that developed by Van Calker *et al.* (2006) where overall sustainability is assessed in 4 aspects: economic (profitability), internal social (working conditions), external social (food safety, animal welfare, animal health and landscape quality) and ecological (eutrophication, groundwater pollution, dehydratation of the soil, acidification, global warming and ecotoxicity). An objective sustainability function per stakeholder group included was subsequently used as a criterion to compare farm sustainability.

1.7. Modelling as a tool

1.7.1. What are systems and systems analysis?

A system is a group of elements that are joined together in some regular interaction of interdependence toward the accomplishment of some purpose (Banks and Carson, 1984). Leffelaar and Ferrari (1989) define a system as a limited part of reality that contains interrelated elements. A system is a limited part of reality, so that a border has to be chosen. Example of living systems range from a plant cell organelle to an animal respiratory system to a dairy farm or an ecological system. Living systems are so immensely complex that they have resisted mathematical analysis by the classical methods successfully used by chemists and physicists. Systems analysis consists of studying the status of the system at a given

moment or its behaviour as a function of time in response to perturbations. Certainly, to perform system analysis using the real system is in most cases not practical or convenient.

Therefore, it is necessary to develop a model of the real system which captures its main attributes. A model is any representation of a real system, and may deal with the structure or function of a real system. The model may involve words, diagrams, mathematical notation, or physical structures in representing the system. A model will always involve varying degrees of simplification or abstraction.

1.7.2. What is a mathematical model?

It is a set of relations that attempts to formally describe the behaviour of a system. The accuracy and validity of the analysis will depend upon the capacity of the mathematical model to properly represent the functional relationships among the different components of the real system.

1.7.3. What is computer simulation?

Banks and Carson (1984) defined simulation as the imitation of the operation of a real-world process or system over time. Spain (1982) states that simulation in its simplest form involves implementing of a mathematical model on the computer to produce simulation data. In this way, the output of the mathematical model may be readily compared with experimental data from the real system in order to verify the model. Once the model is verified, it can be used for system analysis. Implementing a simulation model on a computer involves programming the mathematical expressions, and assigning various rate constants and coefficients. By using the calculus capability of computers we can simulate systems which would be impossible to investigate experimentally because of the amount of time and space involved.

The best model is always that which achieves the greatest realism with the least parameter complexity and the least model complexity (parsimony principle). It is a particularly important principle in modelling since our ability to model complexity is much greater than our ability to provide the data to parameterise, to calibrate and validate.

1.7.4. Objectives of building models.

There are numerous reasons for building models. Some of these reasons are listed below (Colella *et al*., 1974; Spain, 1982; Stockle, 1989; Thornley and Johnson, 1990; Thornley 2006): (i) implement actions upon living systems where such implementation in the real world, under specified operational conditions, may be risky, (ii) identify those parts of the system that are poorly understood and require further study, (iii) separate the physical problem from the design or management decision to be evaluated, (iv) allow researchers to carry out experiments on the system model that lie outside of the normal range of normal experimentation, (v) analyse systems involving multiple, non-linear interactions, such as physiological and ecological systems (systems with numerous variables interrelated to each other by positive and negative feedback loops), (vi) to integrate knowledge leading to an understanding of a complex system, (vii) develop computer-assist tools which can be used for engineering design, educational and training purposes, (viii) to foster multidisciplinary knowledge and (viv) to seek an optimal solution outcome to a problem (optimisation).

1.7.5. Classification of models.

There are multiple classifications of models. Jørgensen and Bendoricchio (2001), in a book on fundamentals of ecological modelling, proposed 2 classifications: (i) to define the most appropriate type of model to solve a given problem and (ii) to define models which differ in the choice of components used as state variables.

The models in the first classification can be shown as pairs:

- Research *vs.* management models: research models are used as a scientific tool whereas the application of the management models is to manage a certain problem.
- Deterministic *vs.* stochastic models: whereas in the deterministic models values are computed exactly in the stochastic ones values depend on probability distribution.
- Reductionistic *vs.* holistic models: the reductionistic modeller will attempt to incorporate as many details of the system as possible to capture its behaviour. He believes that the properties of the system are the sum of the details. The holistic, on the other hand, attempts to include in the model system properties of the ecosystem working as a system by using general principles. Here the properties of the system are not the sum of all the details considered.

- Descriptive *vs.* explanatory models: whereas the descriptive model shows the existence of relations between the elements of a system without explanation, explanatory models attempt to give an explanation of these relationships (de Wit, 1999). These 2 models are often referred as empirical (descriptive) and mechanistic (explanatory).
- Static *vs.* dynamic models: whereas in the static models the variables defining the system are independent of time in the dynamic models these variables are a function of time (or perhaps of space).
- Distributed *vs.* lumped models: the parameters are considered functions of time and space in the distributed models whereas in the lumped models the parameters are within certain prescribed spatial locations and time, considered as constants.
- Linear *vs.* non-linear models: the linear models used consecutively first-degree equations whereas the non-linear models have one or more equations which are not first-degree.
- Causal *vs.* black box models: in the causal models the inputs, states and the outputs are interrelated by using causal relationships whereas in the black–box model the input disturbances affect only the output response. No causality is assumed.

The models in the second classification can be defined as:

- Biodemographic models: if the model aims for a description of a number of individuals, species or classes of species, the model will be called biodemographic and it is based on the principle of conservation of genetic information.
- Bioenergetic models: a model that describes the energy flows is called bioenergetic and it is based on the principle of conservation of energy.
- Biogeochemical models: a model that considers the flow of material and the state variables are indicated as units of mass per unit of area or volume and it is based on the principle of conservation of mass.

It must be pointed out that model will generally be a combination of these definitions and sometimes will have different submodels which will be defined as both components of a classification pair.

1.7.6. Modelling elements

In its mathematical formulation, a model has 5 components:

- Forcing functions (external variables): functions/variables which influence the state of the ecosystem. They may also be refereed as control functions (subclass of forcing functions) when they are under our control (fertiliser N rates inputs) or just forcing functions/external variables when they are not (i.e. climatic variables). Some of these driving variables (e.g. fertiliser application rates) can be also categorised as environmental or management variables (Thornley, 1998).
- State variables: they describe the state of the system (i.e. N_2O emissions).
- Mathematical equations: they represent biological, chemical and physical processes and are used to describe the relationship between forcing functions/external variables and state variables. Some modellers may call them submodels.
- Parameters: they are coefficients in the mathematical representation of processes. They may be constant or ranges. Constant parameters are of less value than ranges as the many feedbacks in real ecosystems may make constant parameters unrealistic.
- Universal constants (i.e. GWP for CH_4).

1.7.7. Steps to follow in the modelling process

- Verification: is a test of the internal logic of the model.
- Calibration: Attempt to find the best accordance between computed and observed data by variation of some selected parameters. In some static or simple models, which contain only a few well-defined, or directly measured (empirical), parameters, calibration may not be required.
- Validation: it consists of and objective test of how well the model outputs fit the data. We can distinguish between structural (qualitative) and a predictive (quantitative) validity. The model exhibits structural validity if the model structure represents accurately the cause-effect relationship of the real system. The model exhibits predictive validity if its predictions of the system behaviour are reasonably in accordance with observations of the real system.

1.7.8. The modelling procedure

The first modelling step is the definition of the problem. We need to define time, space and which, is generally more difficult, subsystems to be incorporated in the model. System thinking is important; you must try to grasp the big picture.

More complex models (more subsystems) do not necessarily imply more accurate accountancy of the reactions of a real system as they generally require more parameters and each parameter has its associated uncertainty (error) and this uncertainty is carried through in the model. The success of the calibration and validation will be closely linked to the quality and quantity of the data.

Chapter 2
Scope and objectives of the study

2. Scope and objectives of the study

The amalgamation of several fields of study, for example, those of plant, soil, animal, atmospheric and aqueous environmental losses, as well as nutrient management, edapho-climatic conditions and economic factors are required to formulate effective policies for the nutrient use in dairy farms. The development and manipulation of such policies are difficult due to the complex interactions existing between the components of these systems and the conflicts between the multiple objectives which must be met.

Modelling tools that are capable to investigate these interactions can fulfil these requirements. So far, existing modelling approaches have generally been either too biased on single specific issues (e.g. socio-economics, NO_3^- leaching) and/or too soft-science based (emission factors, export coefficients or simple indicators) and/or insensitive to the main controls, hence only partially capturing the key factors and key processes and showing a partial reflection of the complex chain of causes and effects. Therefore, there is a need for modelling approaches that can overcome these shortcomings.

Taking into account these previous considerations the following specific objectives have been pursued in this thesis:

1. To develop simple simulation mathematical models (NCYCLE_IRL and NUTGRANJA 2.0) capable of integrating in an annual time-step the key processes of nutrient cycling of N and P in grassland-based systems and capable of studying the N use efficiency at different spatial scales (field and farm scale).
2. To evaluate the effect of management and edapho-climatic variables on N_2O and NO emissions in 2 experiments at 2 spatial scales (greenhouse and field/farm scale) and to asses the scope to use the derived empirical relationships for predictive purposes.
3. To develop a decision support system (NGAUGE DSS) that simulates grassland N flows with a shorter time-step (monthly) and is capable of optimising mineral N fertiliser distribution to meet environmental (N losses) and economic (herbage productions) goals.
4. To investigate how NGAUGE DSS can be used to study the effect of nutrient management on non-point pollution at 2 spatial scales (farm and landscape scale) and

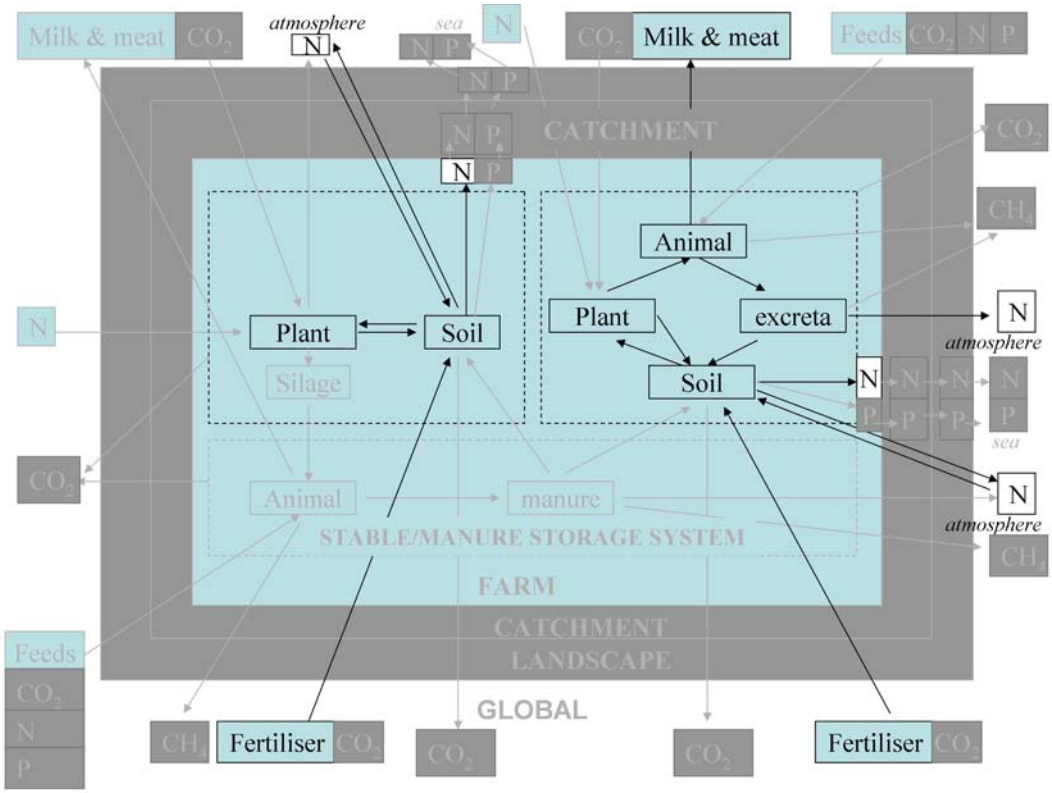
how NGAUGE DSS can provide novel abatement measures that can improve those already in place through existing policies [i.e. Nitrate vulnerable zones (NVZ) action program].

5. To development a modelling framework ($SIMS_{DAIRY}$) which integrates the key dairy farm components/attributes which define the overall sustainability of a dairy farm and that can optimise nutrient management to find more sustainable dairy systems at present or future.
6. To demonstrate how $SIMS_{DAIRY}$ can be used to find dairy farms which are more sustainable by using a weighted multi-criteria optimisation.

In order to achieve these objectives this research work has been structured in 3 types of studies: (i) development of new modelling approaches [models (chapters 3, 4 and 7) and frameworks (chapters 9 and 10)], (ii) applications of these modelling approaches for specific issues (chapters 8 and 11) and (iii) evaluation of the effect of some management and edapho-climatic variables on N_2O and NO emissions (chapters 5 and 6).

Chapter 3

Principles of development of a mass balance N cycle model for temperate grasslands: an Irish case study



3. Principles of development of a mass balance N cycle model for temperate grasslands: an Irish case study.

Abstract

Because of current environmental legislation in European grass-based farming, there is a need to develop tools that can link nitrogen (N) production with losses to the environment. A mass balance empirical model (NCYCLE) is proposed to fulfil this role. This study describes the principles and stages to develop a mass balance N cycle model for Irish grasslands using the basis of the existing NCYCLE model. The model was reconstructed and validated using empirical data from herbage cutting experiments in different Irish conditions and new functions were incorporated to improve the predictions. Irish data on agroclimatic regions and atmospheric deposition were used to provide site specific calculations. Outputs from the model are presented and appear to agree reasonably well with measured data from Ireland.

3.1. Introduction

Temperate grassland agriculture is responsible for much of the world's production of meat and dairy produce. It occupies about 30 % of the land area of Europe. Associated with productive grassland agriculture are serious environmental impacts that are now subject to legislative constraint. These include legislation on greenhouse gas emission (Kyoto protocol: Anon, 1997), ammonia (Gothenburg protocol: UNECE, 1999) and water quality (EU Nitrate Directive: Anon, 1991). It is considered that in many European countries the most intensive grassland farmers will face difficulty complying with the EU Nitrate Directive as implemented through the management of nitrate vulnerable zones (NVZs). Methodologies are required to enable a quantitative linkage between the production arm of sustainability and N losses to the environment, in this case nitrate (NO_3^-) leaching for grassland farms located in NVZs, for both policy makers and farmers. Mathematical models offer this capability. In order to fulfil this role, models need to have qualities of robustness and be sufficiently simple to be used by the lay person while being sufficiently complex to

embrace the full complement of soil, plant and animal processes involved in grassland N cycling.

The NCYCLE (Scholefield *et al.,* 1991) modelling approach allows the complexity of the N cycle to be encompassed: NCYCLE is a mass balance empirical model that was developed in the UK for grassland and calculates the annual N transformations, fluxes and losses for cut and grazed grassland at the field scale, according to inputs specifying climatic zone, soil texture and drainage class, sward management and age and fertiliser input. The annual leachable NO_3^- load is predicted on a per hectare basis. The model also enables the overall efficiency of N use to be calculated, so that the feasible trade-offs between production and environmental impact can be identified. Gaseous N losses from ammonia (NH_3) volatilisation and denitrification are also calculated and account for possible N pollution swapping to be identified.

NCYCLE model is different from other empirical approaches because it employs submodels that allow a high degree of application in relation to climate zone, soil conditions and land management so has the potential to be developed for many temperate grassland sites. In this paper we describe the general principles for reformulation of NCYCLE for application to N cycling in other temperate grasslands with specific reference to Ireland.

The steps to construct the new model were as follows:

1. Identification of grassland agroclimatic areas.
2. Consideration of the case for the inclusion of a range of fertiliser types (e.g. urea or ammonium nitrate.
3. Development of a new mineralisation submodel according to climatic zone and plant residue quality.
4. Addition of an Irish map in which different values of atmospheric N from deposition at field scale are associated to different areas of Ireland.
5. Modification of N uptake and partitioning in the plant.
6. Refinement of harvesting of herbage by cattle, N capture by the rumen and partitioning into product and excreta according to feed characteristics and animal type.
7. Simulation of partition of excreta into N in urine and dung according to feed characteristics.

8. Modified NH_3 production from urine and dung according to climatic zone and feed quality.
9. Derivation of the denitrification and leaching submodel according to climatic zone.

As a demonstration of the principles by which such a model can be developed we now present a case study of model reformulation for Irish grassland agriculture. Agriculture is an important area of economic activity in Ireland. Livestock and grass-based animal production enterprises account for almost 80 % of gross agricultural outputs. Although traditionally the use of N in Ireland is generally low, there has been a dramatic increase in the use of fertiliser N since 1945: the most recent fertiliser survey (Coulter *et al.,* 2002) showed that average use of N on grasslands was 136 kg N ha^{-1} yr^{-1} (48 and 176 kg N ha^{-1} yr^{-1} on beef and grazed dairy grassland, respectively and 95 and 151 kg N ha^{-1} yr^{-1} on beef and dairy grassland for silage, respectively). Beef and dairy production systems in Ireland have traditionally been based on grazed grass during the summer and feeding conserved grass during the winter. About 82 % of all farms make silage, producing a total of 4.4 million tonnes of silage dry matter (DM) yield per year (O'Kiely *et al*., 1998).

As in many other countries in Europe, agricultural land is regarded as the main source of NO_3^- in most rivers and groundwaters (82 % in Ireland, Environmental Protection Agency (EPA), 2002). Although the EPA (2002) concluded that water quality in Ireland was generally good in comparison with that in most European countries, it also identified eutrophication of inland fresh waters as "probably Ireland's most serious environmental pollution problem".

Average NO_3^- concentrations rarely exceed the EU legislated limits (11.3 mg NO_3^--N l^{-1}) in Irish waters. Nevertheless, increasing levels of NO_3^- have been reported in the last few years. The new model, NCYCLE_IRL, provides a means by which NO_3^- peak and average concentration in drainage water may be predicted for different soil, climate and management scenarios.

3.2. Original NCYCLE and existing developments and applications

The NCYCLE model was developed at the Institute of Grassland and Environmental Research (IGER), North Wyke, Devon, UK, using the results of measurements made on 10 long term field grazing systems. NCYCLE is an empirical, deterministic and mass balance model which calculates average annual fluxes of N per hectare within a beef or dairy grazing system (Fig 1) and cutting only system.

The input parameters are: soil texture, drainage status, land use history, age of sward, climatic zone and atmospheric deposition zone. The model is user friendly and does not require a detailed knowledge of computing. The key sub-model in NCYCLE uses linear regression to partition the annual flux of soil inorganic N between 'plant N' and the surplus of mineral N in the system which is available for gaseous and leaching losses. Sward age and management, climatic zone and soil characteristics exert an important influence on the amount of N mineralised within a year.

The proportion of plant N that is ingested by the animal can then be adjusted according to grazing pressure. Ingested N is then partitioned between product N (meat or milk) and excreted N (urine and dung), which is returned to the N pools in the soil. Inorganic N can be then lost via volatilisation (from urine and dung), denitrification and leaching. Nitrogen lost by denitrification is calculated using a sub model based on soil texture and drainage status. The surplus N that is neither volatilised nor denitrified is accumulated in the leachable N pool.

Components of NCYCLE have been tested against independent data-sets (e.g. Scholefield and Blantern, 1989) and the output from similar, empirically based models, such as GRASMOD (Van de Ven 1989). NCYCLE has also been used as a basis for calculating N balances on dairy farms (Jarvis, 1993) and different modelling applications have been developed using the original NCYCLE approach as a basis for: (i) NO_3^- leaching from UK pig production systems (Worthington and Danks, 1992), (ii) NO_3^- leaching at a catchment scale in the UK: NCATCH (Rodda *et al.,* 1995; Scholefield *et al.,* 1996) and MAGPIE (Lord and Anthony, 2000), (iii) N fluxes in ley-arable rotations in the UK (Smith *et al.,* 2001a), (iv) a decision support system (DSS) to optimise fertiliser in order to meet

environmental and economic optimum goals in the UK (Brown *et al.,* 2005) and (v): a GIS framework for N leaching from terraced agricultural systems in Nepal (Collins *et al.,* 1998).

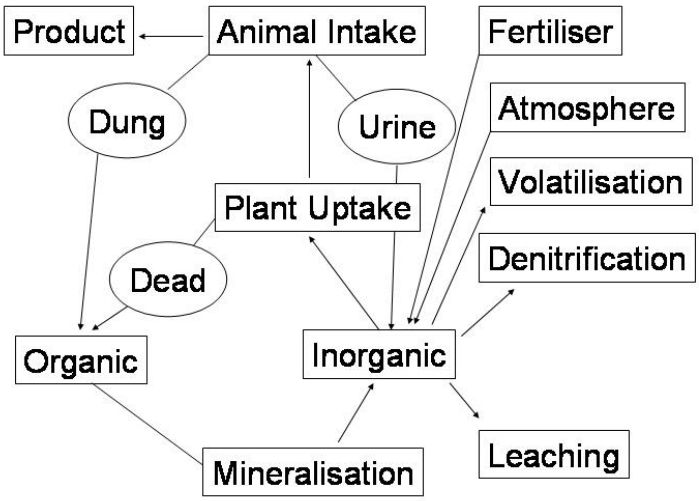


Figure 1. A flow diagram of the N transformations within NCYCLE (after Scholefield *et al.,* 1991).

3.3. Steps to the reformulation of NCYCLE into NCYCLE_IRL

The original NCYCLE was coded in PASCAL. NCYCLE_IRL was coded in DELPHI 5, an object oriented PASCAL -based programming language.

3.3.1. Development of grassland agroclimatic areas for Ireland

In order to asses the applicability of NCYCLE to Irish conditions, climatic variables from 30 year data-sets were used to compare weather patterns in Ireland with the corresponding ones in Great Britain. Monthly average temperature and rainfall in 6 stations in Ireland were graphed along with the corresponding values from 6 climatic regions in Great Britain. The patterns indicate that in general, the temperature and rainfall values in Ireland are within the range of values in the Great Britain. It was noted, though, that Irish locations tended to show higher temperature values in winter than the British sites (e.g., Fig 2). Therefore, small differences should be expected in processes that are highly dependent on temperature (mineralisation, plant uptake, denitrification and indirectly, leaching). The growing and

probably the grazing season in Ireland could be expected to be slightly longer than in Great Britain.

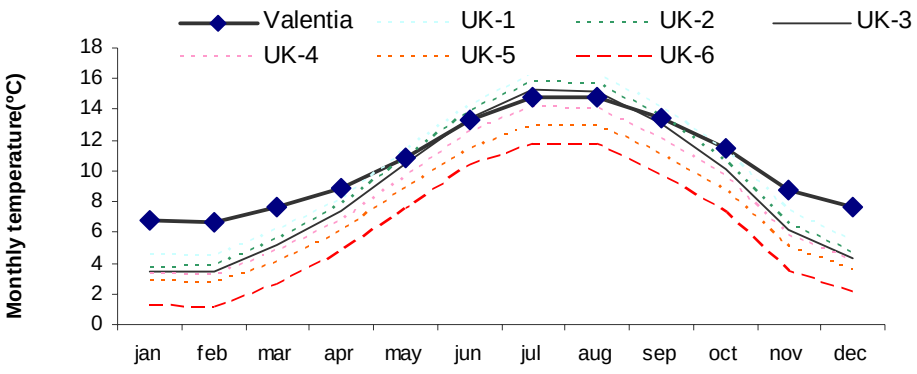


Figure 2. Comparison of monthly average temperature from a south west Irish location (Valentia) with temperature from 6 UK climatic regions.

Variability of grass production across Ireland has not been studied in detail. However, the results derived from the experiments of Ryan (1974ab, 1976) in different locations and soil types showed some variation if the same type of soils were compared in different locations. Some studies used the growing degree-days approach with little emphasis on grass production (Burke, 1968; McEntee, 1978), other studies such as Brereton (1995) used grass growth models that take the climatic variables (radiation, temperature and rainfall) into account and the most recent and complete study is that of Holden and Brereton (2004), who used hydro-thermal climate in conjunction with a statistical clustering technique to relate grass yield to climate data using crop simulation models.

In order to evaluate and quantify the differences in grass production among Irish grassland climatic zones, should they exist, site specific herbage N and DM yields from trials of Ryan (1974ab, 1976) were allocated to the agroclimatic zones defined by the study of Holden and Brereton (2004). This study indicated the existence of different general agroclimatic zones in Ireland and some qualitative references are made with respect to grass. The results of Ryan (1974ab, 1976) obtained from the same soil types but in a different region were compared and factors were produced and tested against the approach of Holden and Brereton (2004).

In NCYCLE, the main differences in herbage yields are caused by differences in the annual fluxes of soil available N. Therefore, the main differences in N fluxes when

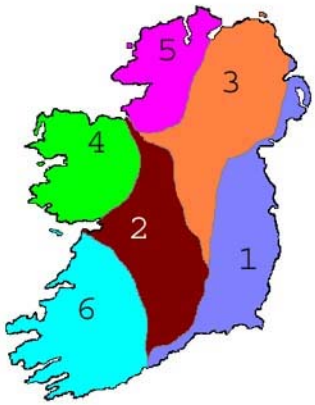
comparing different agroclimatic regions are originated from different mineralised soil N. Annual mineralised N from the different soils and regions were derived from data obtained from the zero-fertilised plots of Ryan (1974ab, 1976). By assuming that the total harvested herbage N yield would be 70 % of the total N in the plant, plant N uptake was obtained and related to the total annual N flux by using the following function derived from the original NCYCLE:

$$\text{N in dead plant} + \text{mineralised N from soil} + \text{atmospheric N} = 0.0007 * \text{plant N uptake}^2 + 0.8135 * \text{plant N uptake} + 14.804 \quad \textbf{(1)}$$

As there were records of fraction of clover DM in the yields, the grass yield from N fixed from clover swards was estimated and subtracted from the total herbage yield assuming a N content in clover of 4 % (Thomas, 2004). Nitrogen released to the soil from dead plant material was also accounted for using a NCYCLE function that relates the N that has not been removed from the total N in the plant as herbage with the N concentration in the herbage.

Atmosphere-derived N was also estimated for different regions of Ireland by using the atmospheric-deposition map information of Jordan (1997). As a result, mineralised N from the soil was obtained from equation 1.

When the effect of the soil type and drainage on rate of N mineralisation was separated, the data of Ryan (1974ab, 1976) resulted in a reasonably good agreement with yields measured in these agroclimatic zones: Ryan's data indicate that highest mineralisation rates occurred in the zone 6 (South and south-west Munster), followed by zones 2, 1, 4 and 3 (Fig 3). Some of the Ulster area was not explored by Ryan's trials and therefore assumptions were made for zone 5 in order to cover the entire island (Fig 3). Figure 3 shows the different mineralisation adjustment factors for every zone. For instance, grasslands within zone 4 for a similar soil and history would have 77% of the N mineralised in zone 6.



Zone 6 (factor 1.00)

Zone 2 (factor 0.87)

Zone 1 (factor 0.84)

Zone 4 (factor 0.77)

Zone 3 (factor 0.70)

Zone 5 (factor 0.60)

Figure 3. Agroclimatic regions in Ireland (after Holden and Brereton, 2004).

3.3.2. The case for the inclusion of a range of fertiliser types

The impact of this major fertiliser source application on Irish grassland soils was investigated to assess the necessity of including urea fertiliser for simulation within NCYCLE_IRL. Neither the original NCYCLE (Scholefield *et al.,* 1991) nor the trials of Ryan (1974ab, 1976) were of use for this purpose as they are based on calcium ammonium nitrate (CAN) fertiliser applications. Hence, literature on losses and herbage yields in Irish grasslands had to be reviewed: according to the last Irish fertiliser survey (Coulter *et al.,* 2002), most of the surveyed farms used CAN for grazed grasslands (40 %) and high N compounds (i.e. 23:2.5:5) for grasslands for silage production (49 %). Nevertheless, urea plays a significant role in Ireland accounting for about 17 % of N fertiliser used in both types of grasslands.

Some studies have investigated the efficiency of herbage production in Ireland using different fertiliser types and for different seasons: Murphy (1969) and Keane *et al.* (1974) found no difference between three different N sources (CAN, AN, urea) applied at same rate of N, either in total annual yields or yields in the first harvest. Herlihy (1980) concluded that only at mid-late season was grass production higher in grasslands fertilised with CAN than in those fertilised with urea. Stevens *et al.* (1989a), in Northern Ireland, analyzed the effect of date of application and form of N on herbage production in spring: a range from -0.6 to 1.1 extra t DM ha^{-1} with urea use was found compared with CAN.

Evidence may suggest, therefore, that urea fertilisation could result in some cases in slightly lower herbage yields and thus, probably greater and different forms of N lost. Nevertheless, the effect does not seem to be greater than a 10 % difference (sometimes no difference). Application of urea in grasslands during the driest and hottest months of the year generally results in lower N fertiliser efficiency, which may be attributed to enhanced NH_3 volatilisation under these conditions. Currently, the Irish code of best practice points out this fact and discourages farmers from using urea during late spring and summer (Humphreys *et al.,* 2003).

Therefore, the inclusion of urea fertiliser as a factor to include in NCYCLE_IRL was ruled out because of the facts that: (i) urea has only, and not systematically, been found to result in lower herbage yields during late spring and summer and (ii) as the use of annual urea is not very high, the fertiliser survey does not indicate the seasonal usage of urea.

3.3.3. Development of a new mineralisation submodel

Within NCYCLE, mineralisation is considered to have two components:

(i) That derived from the mineralisation of previous years' organic N pools influenced by the previous years' management.

(ii) That from mineralisation of dead plant tissue from the current year's herbage growth and excreta (if grazed).

For NCYCLE_IRL, as noted in the previous section, this mineralisation rate was derived from a multi-site trial involving 8-10 year old cut grass swards from long term grasslands, a range of representative soil textures and a range of annual fertiliser N application including zero (Ryan, 1974ab, 1976). The mineralisation starting values were derived from the total grass herbage N yield (prior to subtraction of clover N yield) of plots receiving no fertiliser N multiplied by a factor of 1.4 to allow for unharvested shoot and root material dying and mineralising during the season. Nitrogen deposited from the atmosphere was also taken into account. It was assumed that the amount of dead plant tissue at the end of the year was equal to that at the beginning. Four soil types and 5 regions were considered, applying extrapolations where insufficient data were available. To moderate the values for a wider range of soil types, ages and locations, the same factors as in the original NCYCLE were

used (see Scholefield *et al.,* 1991). The factors are as follows: history of the grassland (long-term grassland, mixed-ley arable and long-term arable), sward age (<2, 2-3, 4-6, 7-10, 11-20, >20 years), soil texture (sandy loam, loam, peat and clay loam) and drainage status of the soil (good, moderate and poor).

The factors in Table 1 indicate the fact that when grassland is cultivated and reseeded, there is a large increase in the mineralisation of soil N in the first year (Young, 1986) that is reflected in a higher yield (Culleton and McGilloway, 1995). In Ireland, Culleton and McGilloway (1995) and Culleton *et al*. (1989) reported a DM yield gain of about 40 % and 60 %, respectively, during the first year after reseeding a long term grassland.

The starting value for the mineralisation of soil organic N calculations depended on the history class of the grassland (long term grassland: 280, mixed-ley arable: 105 and long-term arable: 42 kg N $ha^{-1}yr^{-1}$) and this value was subsequently modified by applying multiplicative adjustment factors to account for the age of the sward, zone of the country (see section 1), soil texture and drainage status (Scholefield *et al.,* 1991). The multiplicative values are shown in Table 1 and 2 and Fig 3.

Table 1. Adjustment factors applied to the amount of N mineralised from soil organic matter on the basis of previous cropping history of the field and age of existing sward.

Previous Land Use	Age of sward (years)					
	1	2-3	4-6	7-10	11-20	>20
Long term grassland	2.5	1	1	1	1.25	1.5
Ley/Arable	2.5	2.25	2.25	2.5	3	3.5
Long-term arable	2.5	2.5	3	3.5	4	5

Addition of an Irish map in which different values of atmospheric N from deposition at field scale are associated to different areas of Ireland.

The model uses the information on rainfall chemistry presented by Jordan (1997). Two maps showing the regional variation of NO_3^--N and ammonium-N (NH_4^+-N) during the period of 1992-1994 were incorporated into the model (Figure 4). Nitrate deposition is shown to be < 5 kg N ha^{-1} yr^{-1} for most of Ireland. This value is only exceeded in Wexford, part of South Wicklow and part of Donegal. Regarding NH_4^+ deposition, for most of the island the annual mean deposition is < 6 kg N ha^{-1} yr^{-1}, only being exceeded in North East Antrim and some small areas in Wicklow and Dublin counties.

Table 2. Adjustment factors applied to the amount of N mineralised from soil organic matter on the basis of soil texture and drainage class.

Drainage	Soil Texture			
	Sandy Loam	Loam	Clay Loam	Peat
Poor	0.38	0.72	0.50	0.50
Moderate	0.60	0.80	0.90	0.66
Good	0.75	1	1.15	1.03

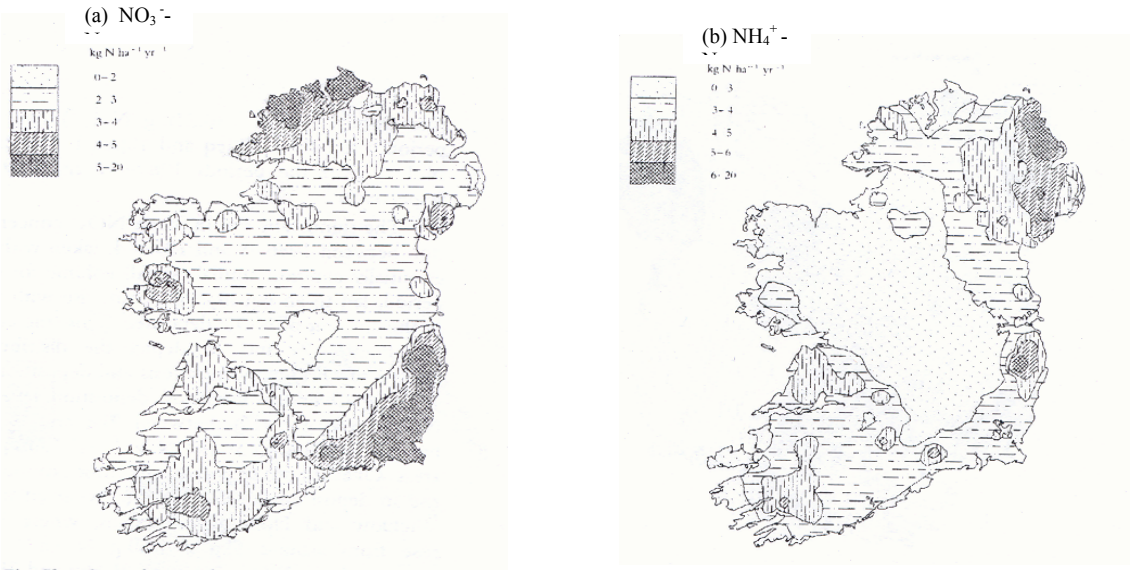


Figure 4. Maps of Ireland showing levels of deposition of (a) NO_3^--N and (b) NH_4^+-N from the atmosphere (after Jordan, 1997).

3.3.4. Simulation of N uptake and partitioning in the plant

Using the same approach as the original NCYCLE, the N uptake by the plant competes with the processes of N loss for the mineral N pool in the soil. The proportion of plant uptake from the total inorganic N flux in the soil is calculated as a function of the total N flux in the soil. This relationship was found to be linear and negative, resulting in a higher proportion of mineral N flux being lost as gaseous and leaching losses with increasing amounts of mineral N in the soil (Scholefield *et al.,* 1991).

A proportion of the total plant N does not reach the animal, nor the silage, but decays in the soil, adding to the soil organic N pool that is subject to mineralisation. The difference between plant N and this dead tissue is herbage N. Different studies have estimated the N

recovered by herbage and ranges between 45 % (Ourry *et al.,* 1988) and 77 % (Hansson and Petersson, 1989) have been recorded. Although in the original NCYCLE, 62 % (from Ball and Field, 1987) was proposed as the default value, Ryan's cut herbage results (Ryan 1974ab, 1976) suggested changing this value to 70 % in Ireland. In any case, this value can be changed by the user in order to investigate the effect of changing this proportion (e.g. by changing grazing pressure) on N fluxes.

The proportion of dead plant that is mineralised during the grazing season is regarded as being related to the concentration of N in the herbage. It is assumed firstly, that the mean concentration of N in the leaf litter and dead roots undergoing decomposition is 45 % of that in the herbage. The proportion of the dead plant that is then mineralised is obtained from the mean concentration of N in that fraction, as proposed by Jenkinson (1982). More details are given in the original NCYCLE paper (Scholefield *et al.,* 1991).

Studies from Ireland have shown different herbage responses to different N fertiliser applications, soil types, regions, cutting regimes, reseeding times and different sources of N applied, but very few (e.g. Ryan, 1974ab, 1976) include more than two of these factors as variables.

3.3.5. Simulation of harvesting of herbage by cattle, N capture by the rumen and partition into product and excreta

In the last decades, many changes have been made to ensure better efficiency of N use by animals by introducing new breeds and different diets. Incorporation of sensitivity to these changes would increase the accuracy of N predictions made by the NCYCLE model. Therefore, the approaches to the fate of ingested N used in the original NCYCLE were tested and compared with new approaches: Kebreab *et al.* (2001) analyzed the amount and form of N excreted under different dairy cattle production systems.

To estimate the relationship between N intake and excretion, experiments containing similar diets that only differed in their level of proteins were studied. Mathematical representations of these relationships were obtained. Moorby (2003) reviewed literature on dairy cow dietary N efficiency and investigated the main reasons for inefficiencies in the use of dietary N leading to excretion products in the dairy cows.

Comparisons were made of simulated NCYCLE_IRL results obtained using the original NCYCLE functions and the functions proposed by Kebreab *et al.* (2001) using the data obtained from the review by Moorby (2003). The results are shown in Figure 5.

Results shown in Figure 5 indicate that both NCYCLE and NCYCLE_IRL would make predictions within the range of results reported by Moorby's literature review. On the other hand, NCYCLE tends to slightly over-predict N in urine and under-predict N in dung with most of the reviewed literature. The fact that the original NCYCLE uses functions that take into account the rate of protein: energy in the dairy cow feed intake (% N in the herbage) results in some poor predictions when trying to simulate intensive farms, which would normally be using different feed concentrates or supplements with a different protein: energy content.

As a possible way to overcome this shortcoming, the relationships proposed by Kebreab *et al.* (2001) were adopted, which relate total N intake and amount and forms of excretion and averages the effect of the different protein: energy content diets during the grazing period. These new findings, therefore, suggest that the current dairy cow performance is best simulated by the Kebreab *et al*. (2001) approach and the total N in milk (kg N ha^{-1} yr^{-1}) is calculated as follows:

$$\text{N dairy cow excreta} = 0.17 * \text{N Animal Intake} + 12.702 \quad \textbf{(2)}$$

$$\text{N dairy cow milk} = 0.17 * \text{N Animal Intake} - \text{N dairy cow excreta} \quad \textbf{(3)}$$

The proportion of the N in the herbage that is transformed to beef animal product (liveweight gain) remained in NCYCLE_IRL as it was proposed by Scholefield *et al.* (1991). This proportion is related to the herbage N concentration according to a relationship derived from Agricultural Research Council (ARC) (1980).

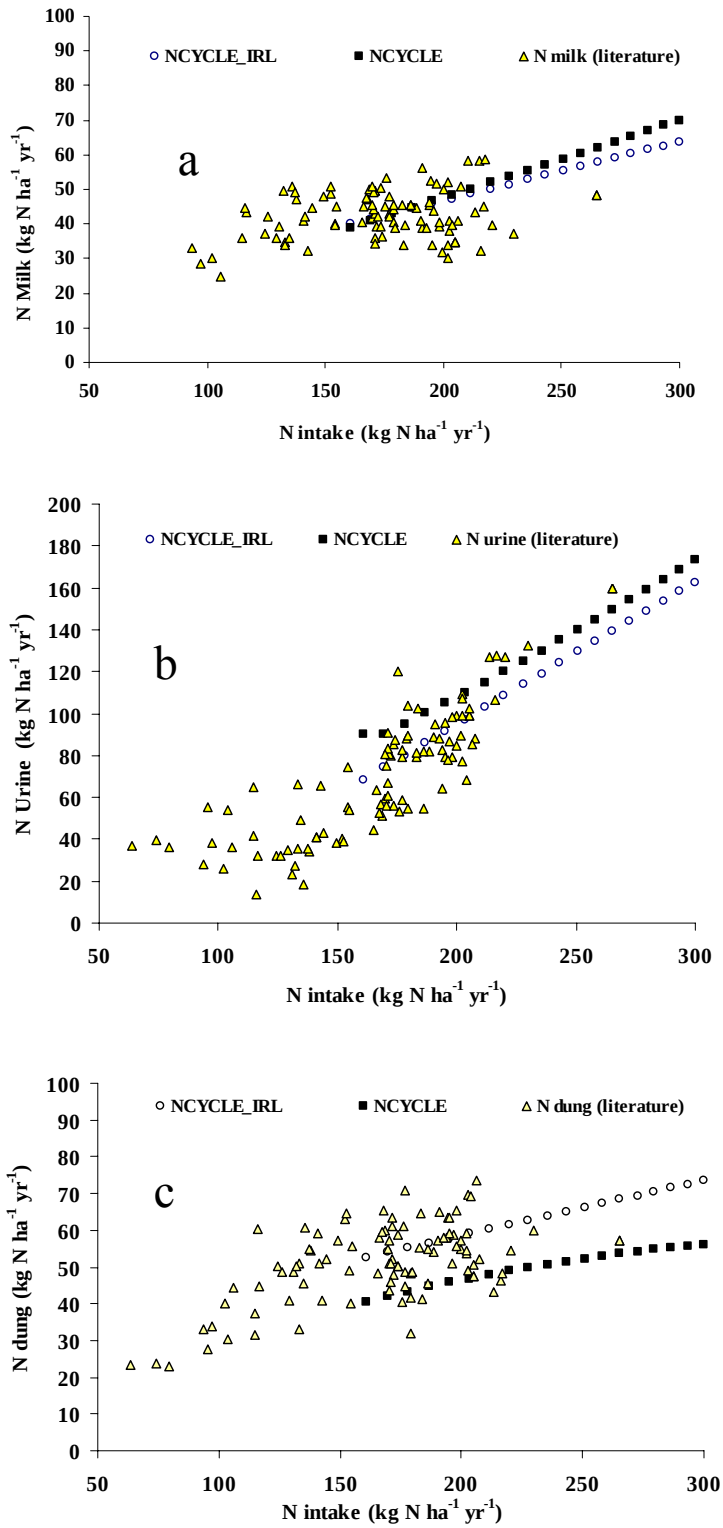


Figure 5. Comparison of NCYCLE_IRL°, NCYCLE■ and literature$^{\Delta}$ values of N in (a) milk, (b) urine and (c) dung over a range of N intakes (kg N ha^{-1} yr^{-1}).

The total N beef product (kg N ha^{-1} yr^{-1}) is calculated as shown by the following equation:

N beef product = N Animal Intake*((6.357 + 51.268*0.47143 Percent N Diet)*0.01)

(4)

Steen and Laidlaw (1995), in Ireland, showed a liveweight gain per hectare of 20.5 % and 22.5 % when applying 360 kg N ha^{-1} yr^{-1} as opposed to 60 kg N ha^{-1} yr^{-1} in a low stocking rate and a high stocking rate grassland respectively. The model NCYCLE_IRL predicts that on average for this particular situation and for zone 4 (Galway area) and for a clay loam soil, a N liveweight gain of 21.7 % is obtained when comparing a grazed beef grassland fertilised with these two fertiliser rates.

3.3.6. Simulation of partition of excreta into N in urine and dung

Nitrogen excreted in faeces by dairy cows is reported to be rather constant in proportion to DM intake, about 0.6 % of the dietary DM intake (Van Soest, 1994). Urinary N excretion, on the other hand, appears to be more variable. Increases in dietary protein or N intake generally lead to substantial increases in urinary loss (Van Soest, 1994) with almost all N ingested in excess of animal requirement excreted in urine (Peyraud *et al.,*1995).

In the original model, excreta from beef animals are calculated from the subtraction of N in beef product from the total N intake. The partitioning of excreted N between dung and urine reflects the concentration of N in the diet. It predicts that, with 1.5 % N in the diet, 45 % of the excreted N occurs in the urine whereas, with 4 % N in the diet, 80 % occurs in the urine (Scholefield *et al.,* 1991). The fraction of excretion resulting as urine N was linearly related to the % N in the diet, represented by an equation as follows:

N beef cow urine = 0.1369 * % N in the diet+ 0.262

(5)

Functions from Kebreab *et al.* (2001) were incorporated within the dairy cow urine and dung calculations: To estimate the relationship between N intake and excretion, Kebreab *et al.* (2001) conducted experiments in which similar diets that only differed in their level of

proteins were fed to dairy cows. As a result, linear correlations were found for the relationship between excreted N and N intake. In NCYCLE_IRL the dairy cow excreta is calculated from the subtraction of N in milk from total N intake.

In the same study, N in dung (kg N ha^{-1} yr^{-1}) was found to be linearly correlated with N intake and the equation was:

$$\text{N dairy cow dung} = 0.15 * \text{N Animal Intake} + 28.47 \quad \textbf{(6)}$$

Urine was then calculated from total N in the excreta minus the N in dung. It is assumed that most of the urine N is mineralised within hours. It is also considered that 25 % of the dung N is readily mineralisable and will contribute to the inorganic pool in the soil and to NH_3 volatilisation.

3.3.7. Simulation of NH_3 production from urine and dung

Agriculture is considered to be the principal source of NH_3 emissions in Ireland. It accounted for 90 % of the emission of 130 kt in 1998 (Humphreys *et al*., 2003).

Studies on NH_3 emissions from animal excreta were reviewed to investigate different approaches from that implemented in the original NCYCLE: In the original NCYCLE, the proportion of the urine N volatilised as gaseous NH_3 is considered to be 15 %, this being the mean value of the results obtained using wind tunnels by Ryden *et al*. (1987), Vertregt and Rutgers (1987) and Lockyer and Whitehead (1990). This proportion can also be altered manually by the user in the model. The proportion of dung N volatilised was assumed to be 3 % based on the results of MacDiarmid and Watkin (1972) and Ryden *et al.* (1987).

Different studies, though, have indicated broader ranges of volatilised NH_3 from: (a) urine, between 4 and 41 % of the N (Ball and Ryden, 1984; Lockyer and Whitehead, 1990; Ryden *et al.,* 1987; Vallis *et al.,* 1982; Vertregt and Rutgers, 1987; Whitehead and Raistrick, 1993) with an extreme of 66 % and (b) dung, ranged from 1 to 13 % of the N (MacDiarmid and Watkin, 1972; Sugimoto and Ball, 1989; Vertregt and Rutgers, 1987; Ryden *et al.,* 1987). Therefore and in order to account for the variation of the proportion of N volatilised from the excreta, NCYCLE_IRL incorporated two relationships as an additional refinement to the

existing sub-model from the original NCYCLE: the fraction of excreted N lost as NH_3 (Vfrac) was related to the average dietary N concentration (ND: g kg^{-1} DM) as follows:

For dairy cows: Vfrac = 2.717 10-7 * ND 3.389 (Bussink, 1996)

(7)

For beef cows: Vfrac = 1.267 10-4 * ND 1.853 (Jarvis *et al.,* 1989)

(8)

3.3.8. Production of the denitrification and leaching submodel

The original NCYCLE model calculated the total N lost through denitrification and leaching as the difference between the inputs to the soil inorganic N (fertiliser, atmosphere, mineralisation, urine, dung and dead plant material) and uptake by the plant component in the sward + NH_3 volatilisation from urine and dung (Scholefield *et al.,* 1991). The proportion of the remaining loss attributable to denitrification loss is then derived according to soil and drainage class from the matrix in Table 3, which is based on Scholefield *et al.* (1988). Leachable N is then obtained by difference.

For NCYCLE_IRL, the same factors were used based on the fact that the denitrification and leaching mechanism proposed by NCYCLE suggests that the main differences in the splitting are based on physical properties of the soil (universal factor), which indirectly influences the denitrification process rate by influencing the capacity of different kind of soils to retain water and thus altering the redox potential. Temperature also affects denitrification, many studies have suggested that Q_{10} is normally about 2 within 15 to 35˚C (Scholefield *et al.,* 1997). Within the model temperature is accounted for when selecting different Irish agroclimatic zones. The temperature then influences the amount of N that flows in the soil and thus the amount of total N subject to denitrification or leaching losses.

As a change to the original NCYCLE proposed by Scholefield *et al.* (1991), NCYCLE_IRL was upgraded to produce actual N leached per hectare and peak and average N concentrations in the leachate using information from Scholefield *et al.* (1993), Scholefield *et al.* (1996) and Rodda *et al.* (1995).

Table 3. Proportion of N due to denitrification as a proportion of the loss due to denitrification and leaching, allocated on the basis of soil texture and drainage class.

	Drainage		
Texture	Good	Moderate	Poor
Loam	0.25	0.45	0.65
Sandy Loam	0.15	0.3	0.55
Clay Loam	0.3	0.55	0.75
Peat	*0.3*	*0.55*	*0.75*

In these studies, relationships between the load of leached N and its concentration in drainage water were derived. Wholly empirical relationships between NO_3^- load, NO_3^- concentration and the volume of drain flow were used to predict the outcome of preferential flow, so that for a given drainage volume and a given soil texture which are supplied by the user, the percentage of soil N that is actually leached can be calculated. Well-fitted linear regressions of peak NO_3^--N concentration on total leached soil NO_3^--N were obtained for soils of different texture under grassland management. Average NO_3^- concentration was defined as the total amount of NO_3^- leached divided by the drainage volume.

3.4. Validation using field data

3.4.1. Herbage

When annual DM herbage yields from different field experiments (Ryan 1974ab; O'Connell, *pers comm.*) were compared with those modelled using NCYCLE_IRL for a range of fertiliser rates (0-600 kg N ha^{-1} yr^{-1}), a reasonably good agreement between modelled and measured values ($r^2 = 0.55$) was found (data not shown).

Some of these scenarios on different soils and zones were selected (Table 4) and used to plot modelled and measured DM herbage yield values for a range of fertiliser rates (Fig 6).

On loam (sites A and D) and sandy loam (sites Q and R) soils, not only did NCYCLE_IRL predict herbage yields according to soil texture quite well, but it also succeeded in accounting for the effect of drainage and agroclimatic zone. For instance, a moderately drained loam soil in the agroclimatic zone 6 (site A) resulted in up to 13 % more herbage DM yield than that in the agroclimatic site 1 (site D). Herbage yield on clay loam soils tended to be well predicted with poor (site T) and moderate drainage (data not shown).

However, herbage yield was over-predicted in well-drained soils (site L). This discrepancy could not be further checked as we only had one site with this type of soil and drainage.

Table 4. Characteristics of the simulated field scenarios to compare predicted and measured herbage yields.

Site	Location	NCYCLE_IRL zone	Soil texture	Drainage
A[¥]	Baltimore	6	loam	moderate
D[¥]	Kilmeaden	1	loam	moderate
L[¥]	Bunclody	1	clay loam	good
Q[¥]	Tuam	4	sandy loam	good
R[¥]	Tuam	4	sandy loam	moderate
T[¥]	Ballinamore	3	clay loam	poor

[¥]After Ryan (1974 ab, 1976)

Either an over-prediction of the mineralisation rates from previous years or an incorrect assumption of the drainage class may have caused this discrepancy. The model simulates average weather conditions and therefore could not be expected to make good predictions of herbage from years of particularly good or bad growing conditions.

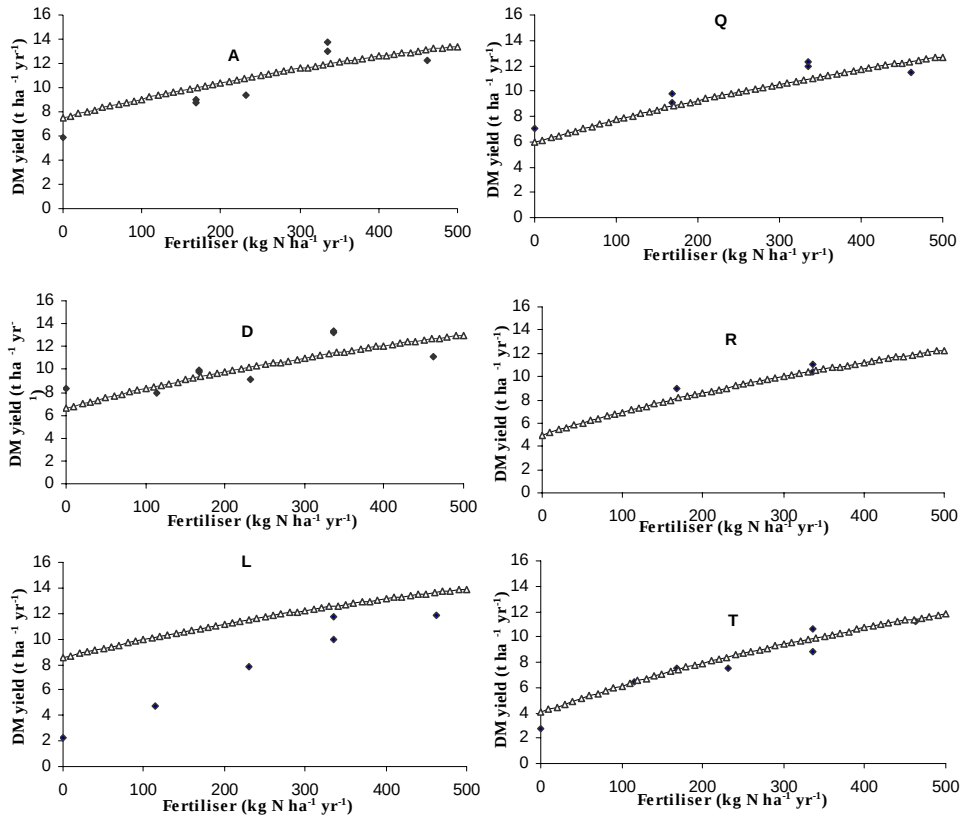


Figure 6. Predicted[Δ] and observed[♦] annual herbage values (t dry matter ha^{-1} yr^{-1}) for a range of fertiliser rates in sites A, D, L, Q, R and T.

3.4.2. Denitrification

Jordan (1989), in studies carried out in Northern Ireland, obtained annual denitrification losses in the range of 31 to 79 kg N ha^{-1} yr^{-1} from swards on a poorly drained clayey soil receiving a rate of 300 kg N ha^{-1} yr^{-1} as mineral fertiliser. NCYCLE_IRL predicts in the range of 33 to 65 kg N ha^{-1} yr^{-1}, which accords well within Jordan's range. However, denitrification rates from Ryan *et al.* (1998) were compared with simulated results from NCYCLE_IRL and the predictions resulted in an over prediction by NCYCLE_IRL of about 50 % for grazed grass on loam and sandy loam soils.

3.4.3. Leaching

Ryan (1999) reported N leaching values for 5 sites and during 2 years. Measured (M) range and predicted (P) results are shown in Table 5. Account was taken of mineral N resulting from manure applications and annual net drainage was assumed to be over 500 mm.

Table 5. Predicted and ranges of observed values in the 5 sites (after Ryan, 1999).

SITE	CAS		CLO		ELT		OAK		RAT	
Leached N	M[a]	P[a]	M[a]	P[a]	M[a]	P[a]	M[a]	P[a]	M[a]	P[a]
(kg N ha^{-1} yr^{-1})	17-20	20	57-77	90	44-87	76	58-81	73	39-84	33

* CAS= Castlecomer (poorly drained clay loam deep soil), CLO = Clonroche (well drained loam-clay loam deep soil), ELT = Elton (well drained loam deep soil), OAK = Oakpark (well drained sandy loam shallow soil), RAT = Rathangan (poorly drained loam-clay loam deep soil).
[a] Measured (M) and predicted (P) results from Ryan (1999) and NCYCLE_IRL respectively.

There is generally a good agreement between predicted and observed values. In only one of the 5 soils (Clonroche) NCYCLE_IRL appears to over predict the N leaching by about 25 %.

3.5. Model applications

3.5.1. Example of the effect of soil type on N losses

Fig 7 shows two examples of the effect of soil type on the form and quantity of N losses: NCYCLE_IRL predicts that the amount of mineral N flowing in the system is greatly influenced by the texture and drainage state of the soil. Well-drained soils mineralise greater amounts of N partly due the enhanced aerobic conditions of the soil. Higher N losses in well-drained soils compared with those from poorer drained soils would also be expected due to

this greater mineral N flux and the reducing efficiency of N uptake by the plant when increasing the available soil N. This fact can be observed in Fig 7 a, b when total losses are compared: within the 0-500 kg N ha^{-1} yr^{-1} fertiliser range, an average of about 20 % more total N losses are predicted to occur in the well drained soil (a) than in the poorly-drained soil (b).

Texture and drainage status of the soil also greatly influence the soil water retention thus exerting a large influence on soil anaerobiosis and solute transport. As expected, whereas the well-drained sandy loam soil is predicted to lose most of the N surplus via NO_3^- leaching, the poorly-drained clay loam loss is mainly via denitrification losses (Figure 7 a, b).

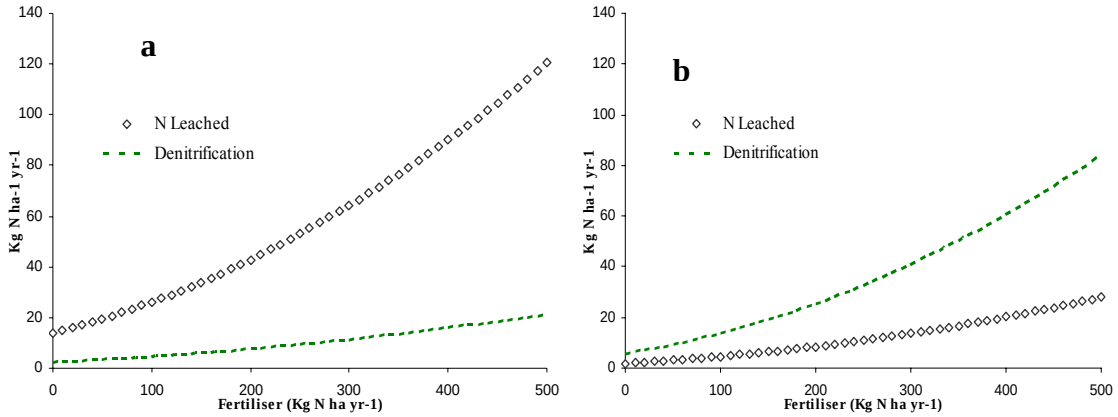


Figure 7. N leaching and denitrification losses from a well drained sandy loam soil (a) and poorly drained clay loam soil (b).

3.5.2. NCYCLE_IRL as a tool to analyse N leaching in Ireland

In order to investigate the status-quo of the dairy farming systems in Ireland in terms of N leaching, the model NCYCLE_IRL was used to simulate two different types of managed grasslands in Ireland using data from the survey of fertiliser use during 2000 (Coulter *et al.*, 2002).

This study was divided into two subsections for different management of grasslands:

(i) Grazed dairy grasslands.

(ii) Grasslands for silage production.

(i) Grazed dairy grasslands

According to the last survey of fertiliser use in Ireland (Coulter *et al*., 2002), Irish farms follow different fertiliser application rates (kg N ha^{-1} yr^{-1}) for grazed grasslands according to different stocking rates (SR). Assuming that in Ireland a dairy cow of 550 kg equals 1 livestock unit (LU) and 1 LU produces about 85 kg N yr^{-1} as excreta, the amount of organic N associated with different SR and therefore to different fertiliser rates can be easily estimated (Table 6).

In this exercise, NCYCLE_IRL was used to simulate grazed grasslands with different SR and fertiliser rates. As the survey of fertiliser use (Coulter *et al.,* 2002) does not specify the sites of the farms, these farms were simulated to have the same location (South) and Annual Hydrologically Effective Rainfall (HER) was assumed to be that from Cork (median of last ten years= 800 mm). Three different types of soils were used in order to see the effect of soil type on N leaching (Table 6).

According to our calculations based on the survey (Coulter *et al.,* 2002), approximately 45 % of the grazed dairy grasslands in Ireland exceed the amount of organic N (170 kg N ha^{-1} yr^{-1}) proposed as a limit to be applied to the land in a National Action Plan area. Farms generally also own grasslands for silage production and hence, part of this organic N from the animal excreta would be generated when the animals are housed and spread to grasslands for conservation, making this percentage lower in reality.

Table 6. Predicted values of annual N leaching (average concentration in the leachate) for different stocking rates (SR) and texture and drainage state in the soil in grazed fields located in the south of Ireland.

S R	organic N	Fertiliser N	No of farms	Leaching		
LU ha^{-1}	kg N ha^{-1}	kg N ha^{-1}		(average concentration) mg l^{-1}		
				*SL-Good	*L-Mod	*CL-Poor
<1.2	<102	58	41	5.8	4.3	0.7
1.2-1.5	102-128	101	55	7.7	5.6	1.1
1.5-1.9	128-162	137	128	9.5	6.8	1.5
1.9-2.25	162-191	182	153	11.8	8.4	2
2.25-2.6	191-221	248	89	15.7	10.9	3
2.6-2.9	221-247	297	31	18.7	13	3.8
>2.9	>247	348	16	22.1	15.2	4.6

* SL= Sandy Loam, L=Loam, CL= Clay loam and Mod=Moderate.

Texture and drainage status of the soil exert a big influence on the extent to which N can be leached. When average concentration in the leachate is considered (Table 6), N leaching

increases as SR increases. Predicted values for different type of soils ranged: (i) 0.7 to 4.6 mg N l^{-1} in poorly drained clay-loam soils, (ii) 4.3 to 15.2 mg N l^{-1} in moderately drained loam soils and (iii) 5.8 to 22.1 mg N l^{-1} in well drained sandy loam soils.

(ii) Grasslands for silage production

N fertiliser used for silage grasslands and classified by Irish region (Coulter *et al.,* 2002) was used in order to explore the current differences in N leaching from farm fields located within different Irish regions. The most widespread texture, drainage status of the soil and net annual drainage volume were assumed for every region (Schulte, *pers comm.*).

Results shown in Table 7 indicate that a great variability in the herbage production and N loss results can be expected for different locations. In terms of silage production, NCYCLE_IRL predicts a range of average DM yield of about 7 ('border' and 'west') to about 10.5 t ha^{-1} yr^{-1} ('south'). These 3 regions comprise about 55 % of the total number of farms surveyed.

According to this survey (Coulter *et al.,* 2002), whereas farms in 'border' and 'west' areas normally have farms with low SR, farms in the 'south' tend to be intensively managed.

Table 7. Predicted annual values of N leaching (load, average and peak concentration in the leachate), DM yield and denitrified N in grasslands for silage production in different sites in Ireland.

Region	Fertiliser	farms	Soil type	DM	leached N			denitrified N
				yield	Load	peak	average	
	kg N ha^{-1}	No		t ha^{-1}	kg ha^{-1}	mg l^{-1}		kg N ha^{-1}
South-east	136	138	*L-Mod	9.9	23.5	18	4.3	19.2
Dublin	126	8	*L-Mod	9.5	16.7	16.5	5.6	17.2
Mid-east	141	93	*CL-Poor	7.5	4.8	5.8	1.1	15.1
Midlands	137	98	*SL-Good	9.6	32.5	33.6	6.5	5.7
Border	116	172	*CL-Poor	7.1	4.1	5.5	0.8	12.8
South-West	123	116	*CL-Poor	8.2	6.4	6.4	0.6	19.2
South	151	219	*SL-Good	10.4	42.3	43.3	5.3	7.5
West	102	167	*CL-Poor	7.1	4.2	5.5	0.6	12.7

* SL= Sandy Loam, L=Loam, CL= Clay loam and Mod=Moderate.

As expected, risks of N leaching losses are high in the areas with predominantly well drained soils and low in the areas with predominantly poorly drained soils. When average concentration in the leachate is considered, all the farms appear to comply with the EU legislated limit even at the NCYCLE_IRL leaching scale (leached N below the root zone).

3.6. Practicality of the NCYCLE approach

Empirically-based, mass balance models have the advantages of producing an acceptably accurate prediction based on relatively few input data and are easy to use. In contrast, mechanistically based models, which are often considered more scientifically robust, have large data demands (e.g. DNDC, Li *et al.,* 1992ab) which in many instances will be difficult to fulfil, resulting in increased uncertainty in model output.

Their scope is often fairly narrow because they were originally developed for specific goals and may not be applicable to the whole system of N cycling in grasslands. Currently, there is a trend towards more integrated modelling approaches, often using combinations of existing models e.g. STONE (Wolf *et al*., 2005), LANAS (Theobald *et al.,* 2004) and MAGPIE (Lord and Anthony, 2000). This enables complex problems to be addressed but exacerbates the difficulties of data availability, model run-time and the level of expertise required. The best models for assessing compliance with environmental constraints need to be transparent, simple and robust so that they may be applied and understood equally by those policing environmental constraints and those operating under them. We assert that mass balance models, like NCYCLE, best fulfil this role.

The development of the NCYCLE model for Ireland is presented as a case study and could be undertaken for any temperate grassland system. This kind of reformulation relies on good quality, integrated data over a number of years to encompass the range of weather patterns within and between regions. This modelling exercise has made use of most of the current available data on N cycling in Irish pasture. While the construction of a highly mechanistic model may not have such a large data requirement, the use of such a model may be prohibited by the paucity of site-specific data available in the present case.

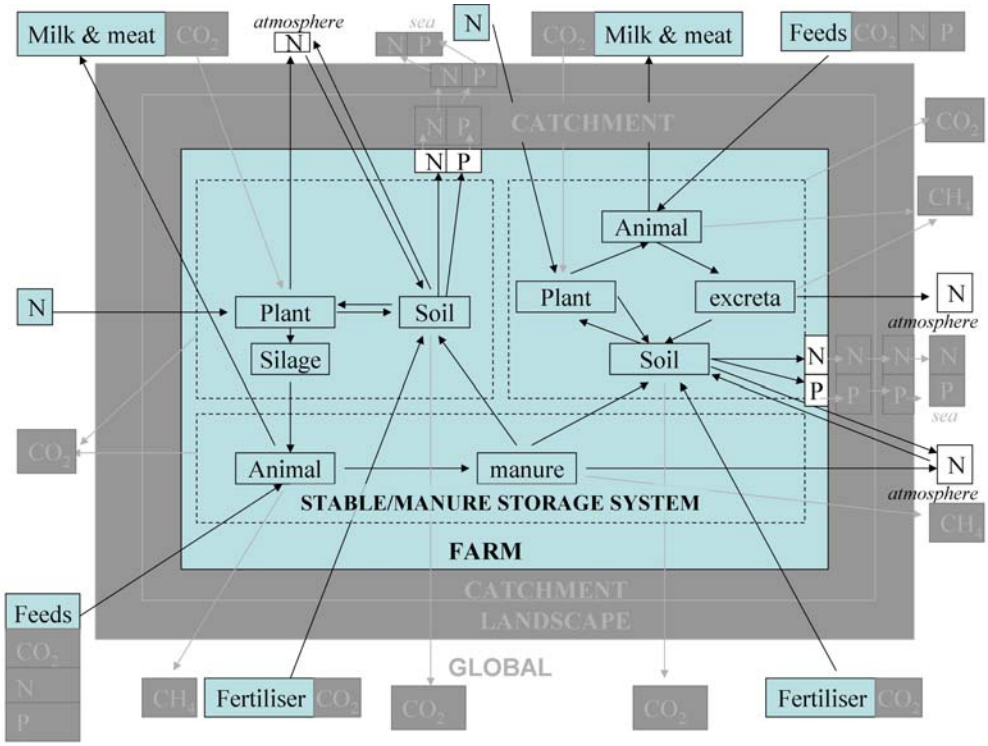
3.7. Conclusions

NCYCLE_IRL represents one of the first efforts to integrate all the available data on N cycling in Irish grasslands. Modifications of the existing functions of the original NCYCLE (animal capture in the rumen, partition of excreta, NH_3 volatilisation) and values for existing

parameters (N from atmosphere, N from mineralisation from previous years) improved the predictions from the original version. The applicability of the model was also enhanced by incorporating the peak and average N concentration in the leachate, which could be useful for investigating the implications to different environmental legislations such as the EU Nitrate Directive. The model also succeeded in incorporating the existing Irish agroclimatic and atmospheric N deposition studies into a simple and integrated approach. The predictions of N losses and yields for Irish conditions proved to agree well within the expected and measured ranges. Further extension of the applicability of the model should consist of more studies, the up-scaling to a farm level and the introduction of a shorter time-step, possibly monthly.

Chapter 4

NUTGRANJA 2.0: a simple mass balance model to explore the effects of different management strategies on N and P losses in dairy farms



4. NUTGRANJA 2.0: a simple mass balance model to explore the effects of different management strategies on N and P losses in dairy farms.

Abstract

European dairy farming has evolved mainly in response to economic drivers but additionally is now being given environmental goals. There is a need to reconcile these economic and environmental pressures in the form of more sustainable systems.

Farm management has been identified as the single most important factor determining the economic and environmental performance of dairy farming systems. Cattle diet manipulation, for instance, has been regarded as a very important means to improve the efficiency of nitrogen (N) and phosphorus (P) utilisation. Because of the complexity of nutrient flows and transfers within dairy systems, there is a need to develop simple and robust tools which enable scientists and policy makers to study dairy farming systems. We propose as one of these tools a new simulation model (NUTGRANJA 2.0).

In this paper we describe the development of this model. NUTGRANJA 2.0 is an annual mass-balance empirical model developed in order to simulate the main transfers and flows of N and P in a dairy farm. Nitrogen and P flows are simulated through different stages of the farm management. The internal flows form a cycle through which energy and mass (N and P) are calculated in multiple iterations through the four main cycle compartments (soil, plant, cattle and excretion) until a steady state for N and P flows is reached. Each of these compartments is differently affected by external driving forces such as climatic, soil and management factors.

A sensitivity analysis exercise was carried out which showed that field-related factors such as % clover in the sward, % sward on flat ground and annual fertiliser rate had a large effect on most of the state variables of the model. As a result, the effect of some field factors in the field had a large influence on losses and production variables.

4.1. Introduction

Dairy farming in Europe is regarded as a major source of non-point pollution. The issues of greatest concern with regard to losses from dairy farming are nitrogen (N), phosphorus (P) and methane (CH_4) as their release into the environment is associated with issues such as: water eutrophication (mainly nitrate (NO_3^-) and P), soil acidity (ammonia (NH_3) and nitric oxide + nitrogen dioxide (NO_x)) and climate change (greenhouse gases: nitrous oxide (N_2O) and CH_4). Growing concern about N and P losses from dairy farming systems to the wider environment is already forcing farmers to address them, for instance under legislation for Nitrate vulnerable zones. Although these losses are affected by site-specific factors such as soil properties and climatic characteristics, changes in farm management, for example reduced use of N fertilisers or improved systems of animal slurry application, are considered to offer substantial scope for reducing loss and hence the impact to the environment (Van der Meer, 1994).

To date, although different approaches have been proposed such as N and P budgets or the use of indicators, there is still a need to develop more flexible, robust and yet simple (i.e. with easily available user-inputs) tools in order to explore strategic dairy farming management options with a focus on the environment. Simulation models can fulfil this role. We have developed a new mass balance simulation model (NUTGRANJA 2.0) that calculates N and P use efficiency and losses from dairy farming systems as function of climate, soil and farm management. The model is modified from a version developed for the European context (NUTGRANJA 1.0: del Prado *et al.*, 1999, 2000a, 2002). In NUTGRANJA 2.0 the model has been specifically developed for the Basque Country (Spain) dairy farms although the same principles should apply to any other dairy farming systems in the Atlantic area.

4.2. Materials and methods

4.2.1. General principles of the model

NUTGRANJA is a mass balance empirical model that simulates internal and external dairy farm N and P fluxes in an annual time-step. The internal flows form a cycle through which energy and mass of N and P are calculated in multiple iterations through the four main cycle

compartments (soil, plant, cattle and excretion) until a steady state for N and P flows is reached. Each of these compartments is differently affected by external driving forces such as climatic, soil and management factors. A flow diagram of N and P of the model is shown in Fig 1.

The largest flows between the soil and the animal are through the forage ingested by the animals, and their excreta, which is recycled in the soil. Dairy farm cows can be fed on grazed or ensiled grass/ white clover, arable crops and concentrates. Although many dairy farmers, in practice, may grow different arable crops to meet some of the cattle requirements, to simplify our dairy system, we defined our farm land arable use as maize. The model simulates the plant growth response to soil available N and P as a function of management factors and edapho-climatic conditions.

Annual N available for the plant comprises NO_3^- and NH_4^+ pools from fertiliser addition, atmospheric deposition, hydrolysed excreted urine and N mineralised from: previous years organic N, recycled manure, dung and dead plant material. Phosphorus is recycled through dung, manure and dead plant material. For a given lactating herd type (i.e. dairy cow /young cattle numbers, milk yield/cow, % butterfat in milk and % protein in milk) and diet profile (i.e. proportion of the DM intake needs during the grazing period which is met by grazing, grass silage, maize silage or concentrates), the model predicts the land area of grass/ white clover which is actually grazed by matching the total predicted grazed grass/white clover intake (DM) and requirements (energy and proteins) with predicted supplies of grazed grass/white clover per unit area (DM, energy and N). The land area utilised for grass and maize silages is computed similarly by matching the predicted total animal requirements from these sources (during grazing and/or housing period) with the predicted silage yields per unit of area. The amount of N or P which does not result in milk is assumed to be excreted as urine and dung during grazing or manure during housing.

The manure produced during the housing period is stored and either applied or exported outside the farm. Nitrogen may be lost as gaseous losses during the different stages from deposition in the house to application to the soil.

Numerous studies describe dairy farms as very ‘leaky’ systems (i.e. Jarvis *et al*., 1996b). Inefficiencies occur in many of the main processes that are present in these systems. In NUTGRANJA 2.0, losses of N and P are predicted to occur in the following stages: silage

making, animal feeding, manure storage, animal housing, manure application, grazing activity, soil leaching/ run-off and soil nitrification and denitrification.

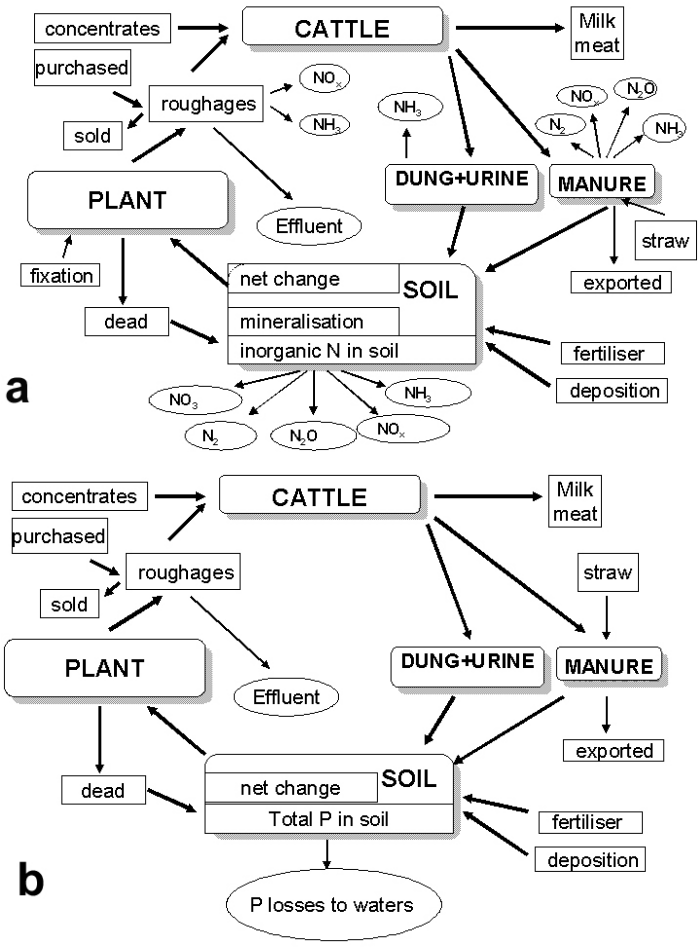


Figure 1. Flow diagram of (a) N and (b) P of the model NUTGRANJA 2.0

4.2.2. Description of the model. Order of calculations in order to carry out the farm-scale simulation of N and P flows

4.2.2.1. Inputs needed to run the model

The model interface displays a climatic map of the area of study, which for this version is the Basque Country (Fig 2). Climatic average parameters are accessed by selecting a location inside the map. Any site in the map can be defined in terms of average climatic conditions

through values of annual rainfall, annual temperature, temperature in August, temperature in January and hydrologically effective rainfall (HER).

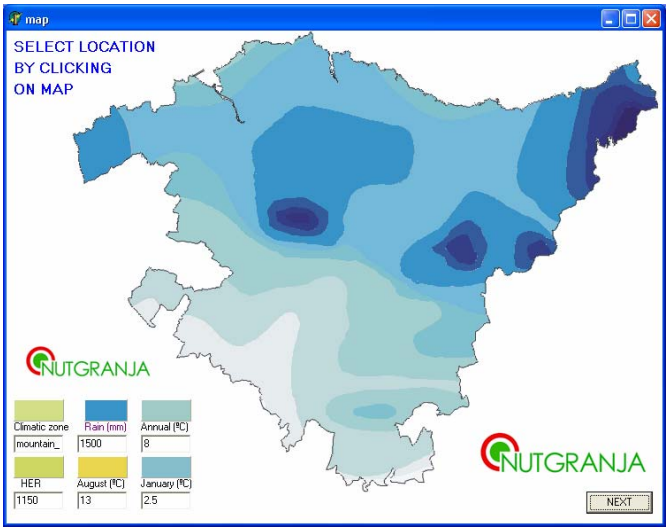


Figure 2. Example of NUTGRANJA 2.0 screen displaying the climatic map input user for the Basque Country.

NUTGRANJA 2.0 requires information on animal inputs (cows diet profile, animal types, animal number, replacement rate, animal grazing days), which will be used to predict the herd nutrient requirements. The model assumption is that the whole herd can be described by describing an average dairy cow and an average follower.

The land use in the farm is defined through dividing the whole area into distinctive areas described by:

(i) Agronomic use: grazed grass, cut grass (% of total area) and maize (% of total area).

(ii) Soil type: texture (sand, sandy loam, loam, clay loam and clay), drainage type (good, average, poor) and soil quality.

(iii) Sward type: natural or sown, botanic composition, clover content (% clover of total DM), history of the field (long term grassland or long term-arable), sward age (<2, 2-4, 4-7, 7-11, 11-20, >20 years), slope (none, medium and steep).

(iv) Management: mineral fertiliser N and P inputs, type of mineral fertiliser (urea, AN, NO_3^--based and NH_4^+-based), manure application rate, method and season of application and manure type for every area of agronomic use.

The type of housing generally will also have a strong influence on the type of manure generated. The model distinguishes 2 types of system: slurry- and straw (FYM)-based housing. Each of them will also have different options for storage and soil application

methods. The steps of calculation are illustrated in the simplified flow chart of the whole model shown in Fig 3.

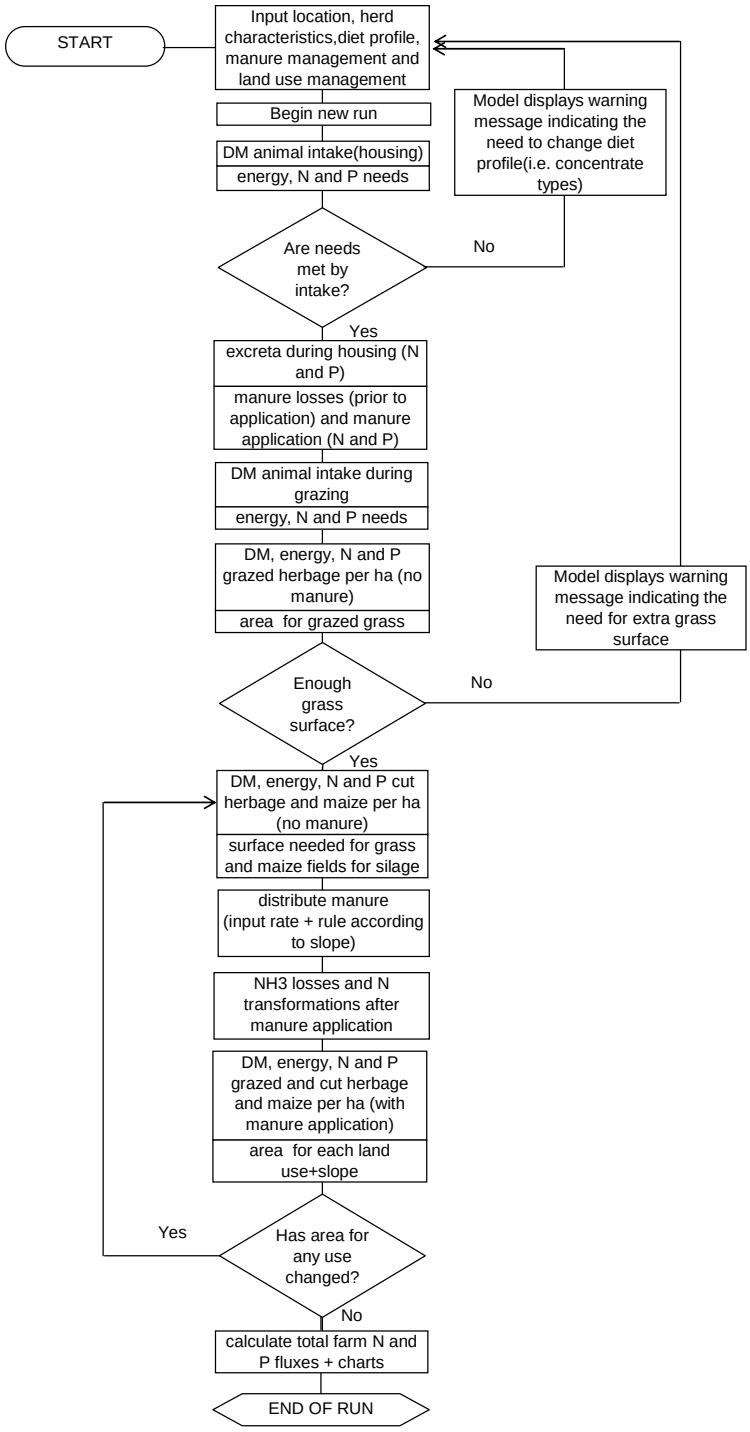


Figure 3. Simplified flow chart of NUTGRANJA 2.0.

4.2.2.2. Calculation of N and P pools during the housing period: interactions between diet, milk, manure and NH_3 and denitrification losses

NUTGRANJA 2.0 calculates the N and P excreta generated in the stable during the housing period by subtracting the N and P in the milk from that ingested. Subsequently, these excreta (manure) undergo storage and application or export. NUTGRANJA 2.0 simulates these N and P flows and transformations through different stages:

(1) For a chosen farm type defined by: (i) number and type of young and dairy cows, (ii) average daily milk yield (L milk cow^{-1}), (iii) % butterfat and protein in the milk, (iv) grass: maize: concentrate ratio, (v) concentrate type and (vi) housing days; total animal DM intake is predicted by using the improved nutritional modelling approach 'Feed into Milk' (Thomas, 2004). According to this approach, daily DM intake per dairy cow is a function of the type of cow (breed, condition score and weight), milk yield target, butterfat % milk concentration and stage of lactation. Although calving pattern may vary greatly in real dairy systems, for modelling purposes, we assumed that our dairy herd calving structure was such that we would have equal numbers of cows calving every month and, thereby, the total milk yield per farm and unit of time remained constant during the year. For a given milk yield target, NUTGRANJA 2.0 assumed an average week of lactation which equalled that resulting in average DM requirements of a whole lactation period (Fig 4).

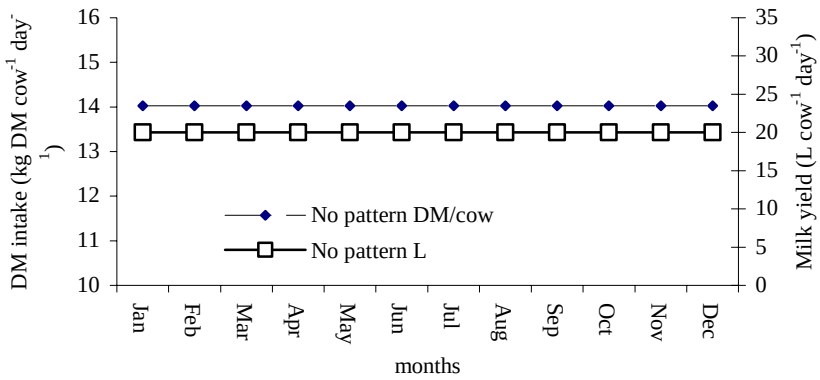


Figure 4. Example of monthly milk yield and dry matter voluntary intake for a given herd yielding an average of 20 L milk cow^{-1} day^{-1} at a no-seasonal calving pattern.

Young cattle herd structure was assumed to be such that, on an annual average, it would equal to an all-yearlings herd. Energy and protein requirements were calculated based on the approach in 'Feed into Milk' (Thomas, 2004).

Although there is a lack of information about the minimum intake level of P at which dairy cows can maintain health and milk production, we propose an equation from Valk and Beynen (2003) to estimate the P requirements per day for a dairy cow:

$$\text{P requirements (g/day)} = [19 + (0.14 * \text{L milk}) + (\text{L milk} * 0.9) / (0.70) \quad \textbf{(1)}$$

Animal requirements must match supplies in terms of energy, proteins and P. If this match is not achieved, the model displays a warning message and the user is prompted to select a different diet profile. No P requirements *vs* supply test was incorporated for the young cattle.

The model assumes that cow milk on average contains 0.95 g P/kg. Manure N and P, at this stage, is hence calculated by subtracting milk N and P output from the diet N and P requirements.

(2) Manure N losses during the housing period and storage via NH_3, N_2O and N_2 are subsequently calculated in the model following the approach by Webb and Misselbrook (2004). In this approach , NH_3, N_2O and N_2 emissions are calculated from the pool of total ammonium (NH_4^+)-N (TAN) in cow excreta (manure N) according to Emission factors (Efs) for different manure management types and stages (Webb *et al*., 2006).

NUTGRANJA 2.0 offers the capability to simulate slurry and farm yard manure (FYM) based dairy systems. An input of annual straw DM use per dairy cow is needed as straw may be a substantial fraction of the total manure, especially in FYM-based systems. The model assumes N and P concentrations in straw of 3 g/kg (Jarvis, 1993) and 0.8 g/kg (Mengel and Kirby, 1987), respectively. The annual ratio of initial manure TAN: total N is predicted as a function of protein % in the diet (Brown *et al*., 2005). Some N immobilisation is allowed for FYM. Manure collection and transport system was assumed to efficiently drive all wastes into storage and hence, as P is not subject to volatilisation, it was assumed that there were zero P losses at this stage.

4.2.2.3. Calculating the plant nutrient pools from fields and silage making

NUTGRANJA 2.0 simulates the efficient use of grass for grazing and hence assumes that the grazed area is never undergrazed. Using this assumption, the surface of grass in the farm that is actually grazed is calculated by matching the total N, DM, energy and P total requirements for grazed grass with that of herbage production per unit of surface. The rest of grass and maize is used for silage making. If the predicted area required for grazing is smaller than the user-input grass area, NUTGRANJA 2.0 displays a warning message so that the user can correct this input. The areas with grass for silage and maize for silage are calculated in the same way, by matching total requirements for silage with predicted results for grass cut and maize cut per hectare. The silage (also maize) that exceeds the animal needs of the farm is assumed to be sold or stored.

NUTGRANJA 2.0 carries out these calculations in an iterative way, by which in each iteration total manure is distributed within the different grassland and maize areas. These are defined by a combination of: land use (grazed grassland, cut grassland and maize) x areas with different slopes (flat, slight-sloped and steep-sloped). Those areas with a steep slope are assumed to be undesirable for manure application. NUTGRANJA 2.0 assumes that manure is applied at the intended rates (in m^3 ha^{-1}) with preference first to the maize areas, second to grass flat areas and ultimately to the slight-sloped areas. Once the manure is distributed, NUTGRANJA 2.0 calculates the N transformations resulting from the applications and re-calculates grass herbage and maize yield per hectare, which is again used to re-calculate the surface needed for each land use. The iterations stop once each surface value reaches a steady state (Fig 3).

The calculation in the model for harvestable crop N production is based on a non-orthogonal response curve which relates N inorganic flux in the soil and potential crop DM yield (after Van de Ven, 1992, 1996). For this version of the model, the potential annual DM yield in grasslands of the Basque Country for different type of swards (natural, sown), Basque climatic areas (oceanic, mountain-oceanic, oceanic-mediterranean and mediterranean), land use average slope and botanical composition (gramineae species, white clover) was obtained from existing studies (Rodriguez, 1990 and Oyanarte *et al*., 1997).

The concentration of N in cut and grazed grass was calculated using relationships between fertiliser N and % N in herbage, derived from Morrison *et al*. (1980) and the model

NCYCLE (Scholefield *et al*., 1991), respectively. Potential maize yield was obtained for the different climatic regions in the Basque Country (Ibarra *et al*, 2003 and Artetxe, 1996) and % N in maize was calculated using an existing relationship between maize DM yield and maize N production (after Van de Ven, 1992; 1996).

Grass-white clover swards are simulated using two equations incorporated from the existing model NFIX-CYCLE (Scholefield *et al*., 1995), in which: (i) grass DM response is predicted by the proportion of sward clover in equilibrium and normalised by the existing factors which have an effect on grass and (ii) mineral N fluxes in the soil regulate the inhibitory effect of NO_3^- on the N_2 fixation activity of established clover root nodules and hence, the ratio of N $Fixed_{clover}$: N $Uptaken_{clover}$ (Nesheim and Boller, 1991). A constant N concentration in white clover of 4.25 % is assumed (Artetxe, 1996). This approach may have some limitations as it does not account for the dynamics of a grass-white clover sward from year to year or the improved structure of the soil in swards with clover (Holtham *et al.*, 2002). Nevertheless, it can be of great use to predict the main differences in N fluxes between pure grass swards and mixtures with white clover. Table 1 shows examples of predicted inhibitory effect of mineral N in the soil (indirectly through different annual fertiliser rates) on biological fixation of the white clover nodules.

Although it is widely recognised that inorganic P in soil may increase the plant uptake returns, plant growth response to P is poor when the lower threshold limit in the soil is exceeded (soil index P= 2-3). Intensive dairy farming generally results in heavy addition of P in the soil through fertiliser or animal excreta and therefore soil indexes of P of 3 or greater are expected. This implies that soil P generally has little or no effect on grass yields in intensive farms. However, in northern Spain, where grasslands may be situated in hilly terrains, soil P can be limiting for grass growth due to high P losses through run-off (del Hierro *et al*., 2002).

A multi-site study in the Basque Country to examine the response of herbage to soil P status indicated that only grasslands with soil Olsen P values < 20 ppm resulted in productive responses to P fertilisation (Rodriguez and Dominguez, 1987). In NUTGRANJA 2.0, following the findings of this study (data not shown), a reduction in grassland DM yield of 10 % and 20 % for soil Olsen P<20 ppm and Olsen P<10 ppm, respectively was imposed. We assumed that the same Olsen P thresholds as those for grasslands also limit maize

production.

Table 1. Comparison of proportion of biological fixed over up taken N by white clover in grass-clover swards with different amount of clover.

Clover	Fertilisation	Manure	Fixed	No Fixed
%			Kg N/ha	
10	Low	Low	37	2
10	High	Low	29	10
10	Low	High	33	6
10	High	High	22	17
30	Low	Low	77	7
30	High	Low	42	43
30	Low	High	60	24
30	High	High	21	64

Since P deficiency in the soil may induce inhibition of N_2 fixation in white clover (Almeida *et al*., 2000), the model incorporated a simple relationship to alter the ratio of N $Fixed_{clover}$: N $Uptaken_{clover}$ when the soil Olsen P was<20 ppm.

The metabolisable energy (ME) and P content of cut and grazed grass and white clover (harvestable/grazed) are calculated from standard values (Thomas, 2004) and linear regressions (Artetxe, 1996), respectively. Metabolisable energy and P in maize were calculated using standard values (Thomas, 2004).

Inorganic N flux in the soil is calculated as the sum of N annual fluxes from mineral fertiliser, atmospheric deposition, mineralised organic N from different sources (previous years' management, manure application and dead plants) and hydrolysed urine from grazing cattle.

Annual P flux in the soils was calculated by using a simple approach where the annual initial total soil P input from previous years is computed with sources of P from the year's management simulation such as mineral fertiliser, atmospheric deposition, applied manure, dung and plant dead material.

A proportion of the total plant N and P does not reach the animal, nor the silage, but decays in the soil (roots and stubbles), initially adding N and P to the soil organic pool and subsequently contributing to an annual pool of mineralised N and P. The difference between plant N and P and this decaying material from plant roots and stubbles is the

harvestable/grazed N and P yield. Nitrogen and P recovered by different crops can range between 45 % and 77 % (del Prado *et al*., 2006a).

NUTGRANJA 2.0 assumed a default value of 62% (Scholefield *et al*., 1991), 70% and 90% for N and P in grass, white clover and maize, respectively. However, the user can manually alter this value to explore the effect of changing this proportion on the whole N and P cycle [e.g. to simulate the preferential tendency of clover intake instead of grass by cows in mixed grass-white clover swards (Rutter *et al*. 2004) or to simulate under-grazed pastures].

The grass/white clover and maize that is cut is ensiled and used as animal feed in the house. The silage making process may be far from being completely efficient in conserving all the mass of the fresh grass. Nitrogen and DM losses can range from 6 to 30 % of the initial harvested crop (Bastiman and Altman, 1985). In NUTGRANJA 2.0 the user can select the efficiency of grass/white clover and maize silage making. Nitrogen losses from silage making are a mixture of NH_3 and N oxides (Maw *et al*. 2002) and surface waste and liquid effluent. In NUTGRANJA 2.0, losses were initially split as (i) gaseous losses at 78 % and (ii) other losses which, may be attributed to surface waste and silage effluent at 22 % [from calculations derived from Mayne and Gordon (1986ab)]. Dry matter and P losses during conservation were assumed to be proportional to the loss of N (Schils *et al*. 2005). In the absence of sufficient quantitative data, gaseous losses were assumed to be split according to a 50: 50 ratio between NH_3 and NO_x losses. Nitrogen and P lost through surface waste and liquid effluent was assumed to be lost outside the boundaries of the farm.

4.2.2.4. Simulation of cattle grazing: N and P capture by the rumen, partition into product and excreta and NH_3 volatilisation losses from excreta and mineral fertiliser in grazed fields.

The same approach as that to predict animal feed requirements during the housing period was used to calculate the total DM intake, energy and protein requirements and hence, the excreta produced during the grazing period (N and P ingested minus N and P in milk). One of the main differences of the grazing period from the housing period is that animals mainly excrete on the grazed land. This excreta pool is split into pools of urine and dung N and P. Because the excretion of N in the dung per unit of DM consumed is fairly constant, changes in dietary N concentration are mostly reflected in the amount of N excreted in the urine. The

partitioning of excreted N between dung and urine was calculated according to relationships taken from NCYCLE (Scholefield *et al*., 1991).

It is assumed that most of the urine N is hydrolysed and mineralised within a few hours and hence, in NUTGRANJA 2.0, this pool of N is considered as inorganic N. However, only a proportion of the total dung N will be readily mineralisable as TAN and will contribute to NH_3 volatilisation.

Ammonia losses from urine and dung were calculated according to Efs used in NCYCLE (Scholefield *et al*., 1991) and NARSES (Webb and Misselbrook, 2004). The proportion of the urine and mineralised dung TAN volatilised as NH_3 was considered to be 8 and 3 %, respectively.

The model assumes that all the ingested P not partitioned into milk is excreted as dung. No P was assumed to be transferred in urine (Haygarth *et al*., 1998).

NUTGRANJA 2.0 simulates the NH_3 emission from fertiliser applications according to a study by Misselbrook *et al.* (2004). This study uses Efs which are expressed as a function of factors such as: fertiliser types (urea, NH_4^+-based, AN and NO_3^--based), land use, application rate, rainfall and temperature.

4.2.2.5. Simulation of mineralisation and losses through NH_3 volatilisation from applied manure

NUTGRANJA 2.0 considers mineralisation from 4 different sources: (1) previous years´management, (2) dung, (3) applied manure and (4) decaying of plant roots and stubbles.

Annual mineralised N from previous years´management is well known to be sensitive to climatic factors, soil texture, drainage status of the soil and sward age (Scholefield *et al*., 1991). There are very few studies which have investigated mineralisation of soil organic N in grasslands or land used for maize in either the Basque Country or the north of Spain. Using one of the existing studies, Estavillo *et al.* (1997), calculated N fluxes in a natural grassland on a clay loam poorly drained soil. The data from the zero-fertilised plots in this study were used to derive apparent annual mineralised N.

In order to estimate net mineralisation from zero-fertilised mown grassland plots we assumed (del Prado *et al*., 2006a): (i) that there are no N losses, (ii) that the total harvested

herbage N yield would be 70 % of the total N in the plant and (iii) that if white clover is present in the sward, N fixation is accounted for in the N balance. Nitrogen plant uptake was subsequently calculated and related to the total annual inorganic N flux by using the approach from Scholefield *et al*. (1991).

Estimation of the study by Estavillo *et al.* (1997) annual net N mineralisation from these plots was 140 kg N ha^{-1} yr^{-1} and 252 kg N ha^{-1} yr^{-1} for year 1 and 2 of the study, respectively. The two years differed greatly in temperature and rainfall conditions, year 1 being much drier than year 2 (Estavillo *et al.*, 1997). Although the rate at which mineralisation occurs is the result of complex interactions between biological, chemical, and physical components of the soil and is subject to many external influences, it is widely held that soil texture, soil temperature and soil water are the most important factors controlling this rate (i.e. Jarvis *et al*., 1996a).

Their effect on net mineralisation can be represented by zero (Macduff and White, 1985) or first-order kinetics (Stanford and Smith, 1972). As a way to simulate the average effect of soil temperature and soil moisture, and thereby, the average effect of site (agroclimatic area) on net mineralisation from previous years' management, monthly rainfall and temperature data were obtained for year 1 and year 2 of the study by Estavillo *et al*. (1997) and for different agroclimatic sites. Measured mineralisation values from year 1 and year 2 were associated to grassland areas on clay loam poorly drained with an average monthly rainfall and temperature pattern similar to that in year 1 and year 2 in the study. Extrapolations were made for the rest of the agroclimatic sites by using 2 modifier functions accounting for the effect of moisture and temperature differences. The value for each climatic site was subsequently modified by applying adjustment factors to account for the age of the sward, history class of the grassland (long term grassland, mixed-ley arable and long-term arable), soil texture and drainage status (Scholefield *et al*., 1991 and Brown *et al*., 2005).

As mentioned in the previous section, NUTGRANJA 2.0 assumes that a proportion (25 %) of the total dung N is readily mineralisable in a year and will contribute to the inorganic N pool in the soil and to NH_3 volatilisation. The rest of the dung N remains as an organic N fraction (recalcitrant organic N) which is mostly protected from losses and plant uptake.

Two main general types of manures (slurry or FYM) can be used in the farm and are associated to the type of housing system chosen (slurry or straw-based). Furthermore, the

user can also define the properties of slurry in terms of % DM and the age of FYM (fresh or aged: after Brown *et al*. 2005). Application of manure N to the soil results in a proportion of the N applied being lost as NH_3 while some joins the soil N pool. Three different sub-pools of manure N in the soil can then be identified according to their mineralisation rate: one sub-pool is rapidly mineralised into ammoniacal N (TAN) and subsequently nitrified to NO_3^-, a second sub-pool is mineralised throughout the following months (semi-recalcitrant organic N) and a third pool remains as organic N within the simulated year (recalcitrant N). The proportion of the total manure N as an initial TAN pool is calculated according to the urine N: dung N ratio excreted in the stable. This ratio is related to the protein content in the diet during housing.

Ammonia emissions from manure application are calculated as a basis the approach from Chambers *et al.* (2000). In this approach Efs for NH_3 volatilisation from manure application on grassland and maize land are determined according to: (i) properties of the slurry (% DM), (ii) its application date (for soil moisture content), (iii) incorporation timing after application, (iv) method of application and (v) method of incorporation.

Once NH_3 volatilisation is calculated, the remaining N from slurry or FYM is assumed to be subject to loss or plant uptake (inorganic N), mineralised (semi-recalcitrant N) and, hence, to join the pool of inorganic N, or to accumulate (recalcitrant N). Mineralisation of semi-recalcitrant N is simulated according to Brown *et al*. (2005) by which, factors such as application date, manure type and cumulative degree days above 5^oC regulate the rate of mineralisation. Although NUTGRANJA 2.0 simulates annual N flows, manure application rates are specified quarterly by the user, following the concept of 4 main application periods within a year: February-April, May-July, August-October and November-January (Smith *et al*., 2001b).

It is assumed that 45 % of the roots and stubbles N undergo decomposition (Scholefield *et al.*, 1991). A proportion of the decaying plant roots and stubbles is mineralised annually and is calculated as a function of the concentration of N in the plant (Jenkinson, 1982).

4.2.2.6. Simulation of N losses through nitrification, denitrification and leaching/run-off in fields

Total N losses through nitrification, denitrification and leaching/run-off are calculated as the difference between the inputs to the soil inorganic N (fertiliser, manure, atmosphere, mineralisation, urine, dung and decaying roots and stubbles) and uptake by the plant component in the sward + NH_3 volatilisation from mineral fertiliser, urine and dung. NUTGRANJA 2.0 assumes that within a year all N from sources that, at least initially, have a fraction of NH_4^+-N in the soil (mineralised N, fertiliser N, atmospheric N) is either nitrified, absorbed by plants or lost as NH_3 or N oxides (N_2O and NO_x). Although it has been widely shown that NH_4^+ can be the major form of N available to plants under conditions that are unfavourable for nitrification such as poor aeration, soil acidity or cold temperatures (Clarkson *et al*., 1986; Watson, 1986; MacDuff and Jackson, 1991), in normal conditions plants prefer N as NO_3^- form from the soil. NUTGRANJA 2.0 assumes that 20 % of the annual nitrified NH_4^+ which has not been volatilised is taken up by the plant.

Nitrous oxide and NO_x from the soil are generally emitted through nitrification and denitrification processes, both processes being affected by a number of factors, such as rain, temperature, fertilisation, irrigation, pH, organic matter content and particle size (Tiedje, 1988). In NUTGRANJA 2.0 the proportion of the nitrified NH_4^+ neither taken up by the plant nor lost as NH_3 is assumed to be lost as N_2O and NO_x losses from nitrification. The sum of denitrified and leachable/run-off N is subsequently calculated by subtracting NO_3^- uptake by the plant from the remaining NO_3^- pool in the soil. The proportion of the remaining loss attributable to denitrification was calculated according to soil type and agroclimatic site, an approach which is partly based on Scholefield *et al*. (1991) and Brown *et al*. (2005).

Leachable/run-off N is then determined as the difference between total N losses and losses through nitrification and denitrification processes. From the fraction of leachable NO_3^--N, NUTGRANJA 2.0 calculates actual N leached per hectare and peak and average N concentrations in the leachate, using information from Scholefield *et al*. (1993*)*, Scholefield *et al*. (1996*)* and Rodda *et al*. (1995). These studies derived relationships between the load of leached NO_3^--N and its concentration in drainage water. Wholly empirical relationships between NO_3^- load, NO_3^- concentration and the volume of drain flow were used to predict

the outcome of preferential flow, so that for a given drainage volume and a given soil texture, both being supplied by the user, the percentage of soil N that is actually leached can be calculated. Well-fitted linear regressions of peak NO_3^--N concentration on total leached soil NO_3-N were obtained for soils of different texture under grassland management. Average NO_3 concentration was defined as the total amount of NO_3^- leached divided by the drainage volume.

Although NUTGRANJA 2.0 does not have an adequately small time-step to simulate the effect of events (i.e. daily rainfall and fertilisation) which may trigger N_2O, NO_x and N_2 emissions, it incorporates an attempt to predict the average effect of key factors (i.e. water, mineral N and temperature) on these emissions, based on the work of Brown *et al*. (2005).

4.2.2.7. Simulation of net changes of P in the soil

NUTGRANJA 2.0 attempted to identify the major pathways of P flows in the soil-plant-animal-manure system and where more efficient use of P may be made, but does not attempt to quantify in more detail the transfer rates of P in different forms.

NUTGRANJA 2.0 does not have sufficient mechanisms to simulate neither hydrological mechanisms nor transformations of P in the soil. However, based on the review by Haygarth and Jarvis (1999) we incorporated export coefficients for grazed grass, cut grass and maize. According to this study soil texture and grazing activity had an important influence on the magnitude of P losses. The ability of a soil to hold P within the soil matrix depends on particle size distribution, organic matter content and iron and aluminium content (Sharpley, 1995; Leinweber *et al.*, 1999). In general, sandy soils have a lower capacity to bind P than those with a high clay content (Sharpley, 1995; Leinweber *et al.*, 1999). The model simulates the net changes of P in the soil, these being calculated as:

$$\text{Net P change (kg P/ha/yr)} = \text{total soil P- plant P uptake- P Losses} \quad \textbf{(2)}$$

4.3. Sensitivity analysis

Model runs were conducted in which the values of some of the environmental/management (E/M) variables included in the model were varied in order to assess their relative influence on state variables such as (i) silage surplus export (kg N $ha^{-1}yr^{-1}$), (ii) total manure N (kg N $ha^{-1}yr^{-1}$), (iii) P soil net change (kg P $ha^{-1}yr^{-1}$), (iv) N_2O losses (kg N $ha^{-1}yr^{-1}$), (v) NH_3 losses (kg N $ha^{-1}yr^{-1}$) and (vi) average NO_3^--N concentration in the leachate (mg l^{-1}).
A 'standard' baseline farm scenario was specified in terms of site and management characteristics (Table 2).

Table 2. Inputs for 'standard' baseline farm scenario.

Climatic characteristics	**Manure management**
Atlantic oceanic	Slurry-based system
Annual rainfall=1300 mm	Storage= open tank
Temperature= 14 ºC	Application method=broadcast
HER=550 mm	Autumn-winter manure application=60% of annual manure
Animal management	**Fields Management**
Dairy cows=80 (6935 l milk yr^{-1} cow^{-1}, 3.3 % protein, 4.2% butterfat)	Farm mineral fertiliser rate (N)=168 kg N $ha^{-1}yr^{-1}$
Young cattle =60	Farm mineral fertiliser rate (P)=27 kg P $ha^{-1}yr^{-1}$
Housing period=200 days	Grassland with flat surface (60%)
Maize in diet=10 % of total DM (housing and grazing)	Clover in sward=0%
Concentrates in diet=40% of total DM (housing), 35 % of total DM (grazing)	Type of fertiliser=AN
Concentrate types = beans (80%), wheatfeed (10%) and oats (10%) of total concentrates DM	Soil type grassland=poorly drained clay loam
Silage in diet=50 % of total DM (housing)	Long term grassland past
Silage management quality=average	Average sward age=6 yrs

In turn, and keeping all other E/M variables at their 'standard' values, the value of each environmental/management variable was varied over a numerical (-30%, -10%, +10%, +30%) or class (i.e. soil type: sand, loam and clay) range and the surplus silage, total manure N, P net change, N_2O, NH_3 and average NO_3^--N concentration in the leachate calculated at each value. The range of values used for each E/M variable is given in Table 3 and Table 4 for numerical or class ranges, respectively.

Table 3. Environmental/management variables varied at a numerical range.

Model variable	% varied
Milk yield cow^{-1} yr^{-1}	-30%,-10%,+10%,+30%
Mineral fertiliser (kg N ha^{-1})	-30%,-10%,+10%,+30%
Mineral fertiliser (kg P ha^{-1})	-30%,-10%,+10%,+30%
Housing days	-30%,-10%,+10%,+30%
Manure in winter	-30%,-10%,+10%,+30%
Flat area of grassland (%)	-30%,-10%,+10%,+30%
Concentrates (%)	-30%,-10%,+10%,+30%
Clover in sward (%)	+10%,+30%

The sensitivity analysis for the E/M variables varied at a numerical range was defined as relative sensitivity (Sr), where Sr = % change in output ÷ % change in input. The sensitivity analysis for the E/M variables varied over a class-type range was assessed by comparing their outputs with the outputs from the 'standard' baseline farm scenario.

Table 4. Environmental/management variables varied over a class-type range.

Model variable	classes of variation
type of fertiliser	Urea
	NO_3-based
	NH_4-based
Housing system	FYM
Manure storage	tank: rigid cover
	tank: floating cover
	tank: crusted
	lagoon: open
	lagoon: rigid cover
	lagoon: floating cover
	lagoon: crusted
Manure application	Deep injection
	Shallow injection
	Band-spread
Silage making	poor
	good
soil type grass	moderately drained loam
	well drained sandy-loam
History of the grassland	arable past
Sward age	<2 yrs
	>20 yrs
climate	mediterranean-very dry
	mediterranean-transition-dry
	mountain oceanic- rainy

The results of these sensitivity analyses are given in Fig 5 and Fig 6.

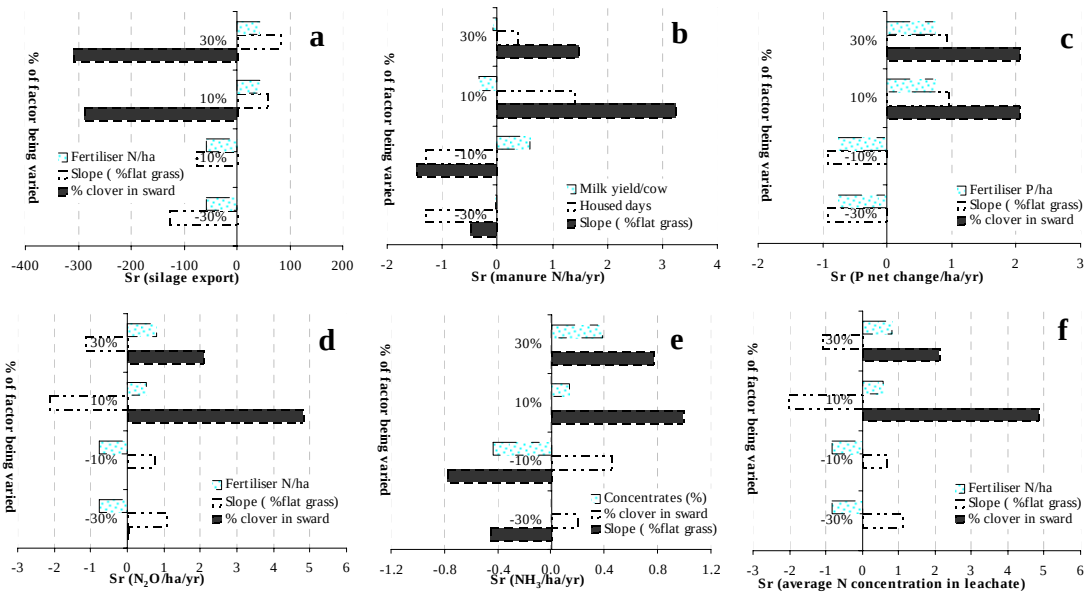


Figure 5. Output of sensitivity analysis of varying factors by -30%,-10%,+10% and +30% on silage export (a), manure N (b), net change P (c), N_2O losses (d), NH_3 losses (e) and average NO_3-N concentration in the leachate (f).

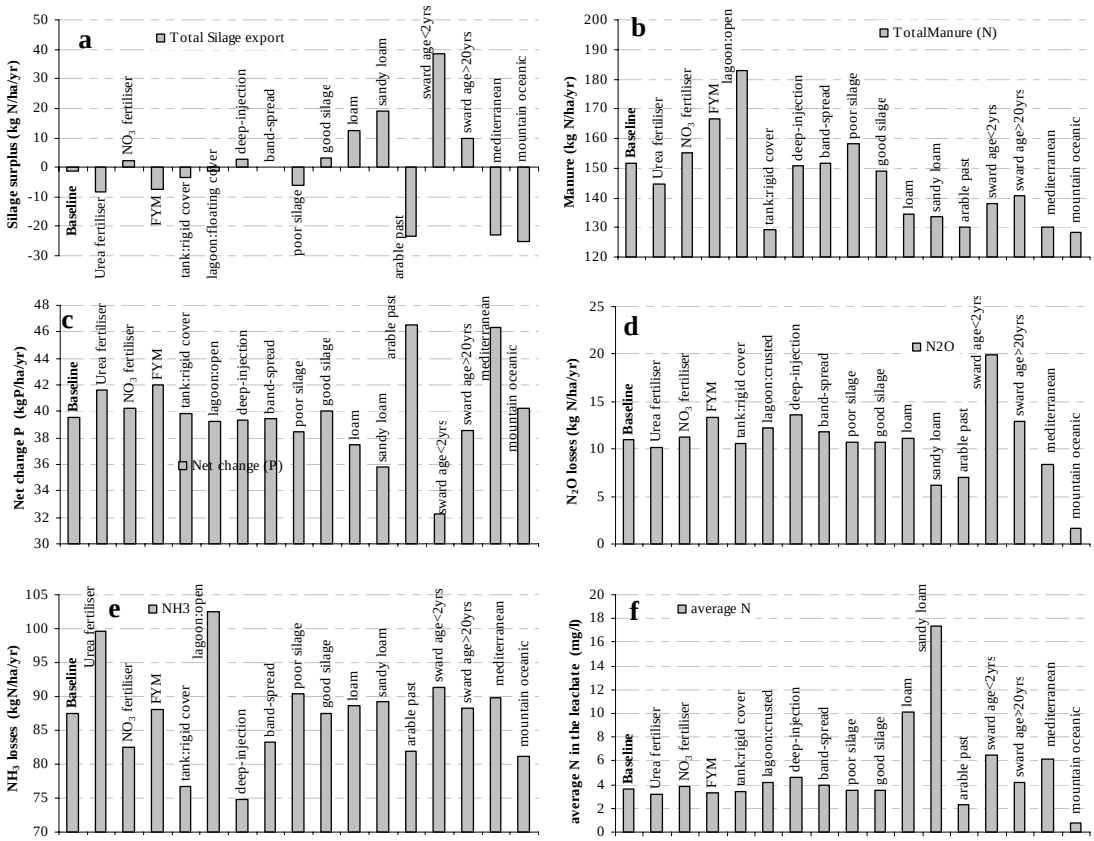


Figure 6. Output of sensitivity analysis of varying varied-by-classes factors on silage export (a), manure N (b), net change P (c), N_2O losses (d), NH_3 losses (e) and average NO_3-N concentration in the leachate (f).

All the state variables under analysis were sensitive to most of the varying E/M variables used. Farm silage N surplus was the state variable that was most sensitive to E/M variables being varied and net change P in the soil was the state variable that was lest sensitive. The E/M variables that numerically had a large effect on silage N surplus were, in decreasing order of magnitude, % clover in the sward, % sward with flat slope and annual fertiliser N rate (Fig 5a). These results reflect the fact that these 3 E/M variables had a large effect on herbage dry matter production. Mixed swards of perennial ryegrass and white clover resulted in much smaller DM yields productions than pure perennial ryegrass swards.

It should be noted that although this effect on DM yield has been also found by field experiment studies, although to a smaller degree (i.e. Schils *et al.*, 2000). It may be exaggerated in our analysis, as we assume that we apply the same mineral fertiliser and similar manure applications to a mixed clover ryegrass sward than to a pure ryegrass sward assuming also that these applications would have no effect on the proportion of clover in the sward, this being an input of the model. Sward age, especially young swards (sward age<2 years) resulted in large silage export values (Fig 6a). Culleton and McGilloway (1995) and Keating and O'Kiely (2000), for instance, in field experiments, reported a DM yield gain of about 40 % and 20 %, respectively, during the first year after reseeding a long-term grassland. Soil type and climatic conditions also had a substantial effect on herbage production and thus on silage export (Fig 6a). Soils with better drainage than the baseline (poorly drained clay loam soil) resulted in larger herbage productions and sites in dry (Mediterranean) or mountain areas resulted in smaller herbage productions than the baseline production situated in the wet Atlantic area. Other E/M variables to which silage export was sensitive, although to a lesser extent, were manure and fertiliser management and silage making quality (Fig 6a).

Fig 5b and 6b shows the difference in total manure N production per hectare for the different E/M variables varied. Of those E/M variables numerically varied, % sward with flat slope, duration of housed period and milk yield production per cow showed the largest effect on manure N. Increasing the % of flat sward surface had a direct and positive effect on the protein content of the grass (data not shown) and a positive effect on ingested N by the cow. Hence, on diets with the same DM ingestion per cow, more excreted N is simulated to occur. Housing days, as expected, had an influence on the split between excreta produced in the

stable and that deposited during grazing. Increasing, for instance, milk yield per cow increased N utilisation by cows. This could result in a certain decrease in manure N production when the increase in milk yield per cow was small. This decrease in manure, however, was partly counteracted by the differences in nutrient requirements for different lactating types of cows. Therefore, it showed almost no effect whatsoever when the cow yielded 30% more or 30% less milk than the baseline. Of those E/M variables that changed on class-basis, manure storage system, history of the grassland and climate exerted a large influence on manure N production in the farm (Fig 6b).

Changes in soil P were sensitive to % clover in sward, % sward with flat slope and annual fertiliser P rate (Fig 5c). The larger the proportion of clover in the sward, the larger the amount of net change of P in the soil, as less herbage is predicted to be produced, less silage is exported and more is recycled through the animals and back to the soil through their excreta. On one hand flatter areas had smaller losses of P from the soil. On the other hand, with a smaller effect on net change of P, flatter areas produce more herbage DM than those with a larger steeply sloping area, leading to less P being recycled through the animal and more silage being exported. The balance between these 2 opposite effects results in swards situated on flatter areas having increased P in the soil. The addition of more fertiliser P did not result in greater yields; part of this P was lost, but mostly was stored in the soil and, therefore, reflected in the net change of P in the soil. Other E/M variables that influenced the net change of P in the soil were sward age, climatic conditions and past history of the grasslands (Fig 6c).

Nitrous oxide loss and NO_3^--N concentration in the leachate were similarly affected by changes in % clover in sward, % sward with flat slope and annual fertiliser N rate (Fig 5d and 5f). Increasing fertiliser N rate and % clover in sward resulted in increasing N_2O emissions and average concentration of N in the leachate. Increasing clover in the sward resulted in larger transfers of N from the plant to the animal but smaller transfers from the soil to the plant, as a proportion of the N is fixed from the atmosphere through the clover symbiotic nodules. This increased amount of available N not taken up by the plant or recycled through the animal excreta increases the amount of N in the soil that can be subject to processes of denitrification or nitrification with consequent losses of N_2O and NO_3^-/run-off leaching losses.

Soil type, age of the sward and climatic conditions strongly affected both N_2O and average NO_3^--N in the leachate (Fig 6d and 6f). Soil type and climatic conditions have a control on physical factors such as soil anaerobicity, soil temperature and drainage. They also, indirectly, affect mineralisation rates and hence the amount of N in the soil available to the plant or subject to denitrification, nitrification and leaching processes.

Ammonia emissions were affected, in a lesser way than N_2O and NO_3^--N, by changes in % sward with flat slope, % clover in sward, and annual concentrates amount (Fig 5e). Increasing the % of sward with flat slope and the % of concentrates in the diet gave increases in NH_3 emissions through more N being eaten by the cattle and thereby increasing the total amount of excreted N. As expected, mineral fertiliser form, storage system and application method had a large effect on NH_3 emissions. On one hand, deep injection was the factor by which NH_3 was more successfully reduced, followed closely by the use of closed tanks to store manure. On the other hand, urea fertiliser and open storage lagoons resulted in substantially increased NH_3 emissions in the farm.

4.4. Conclusions

Existing data on N and P fluxes and existing modelling approaches were used to develop a new farm model (NUTGRANJA 2.0) for the Basque Country (also relevant for the Atlantic area of northern Spain). This model fills the gap of farm-scale models that are capable of integrating in a simple and transparent way all the main components of the N and P cycle.

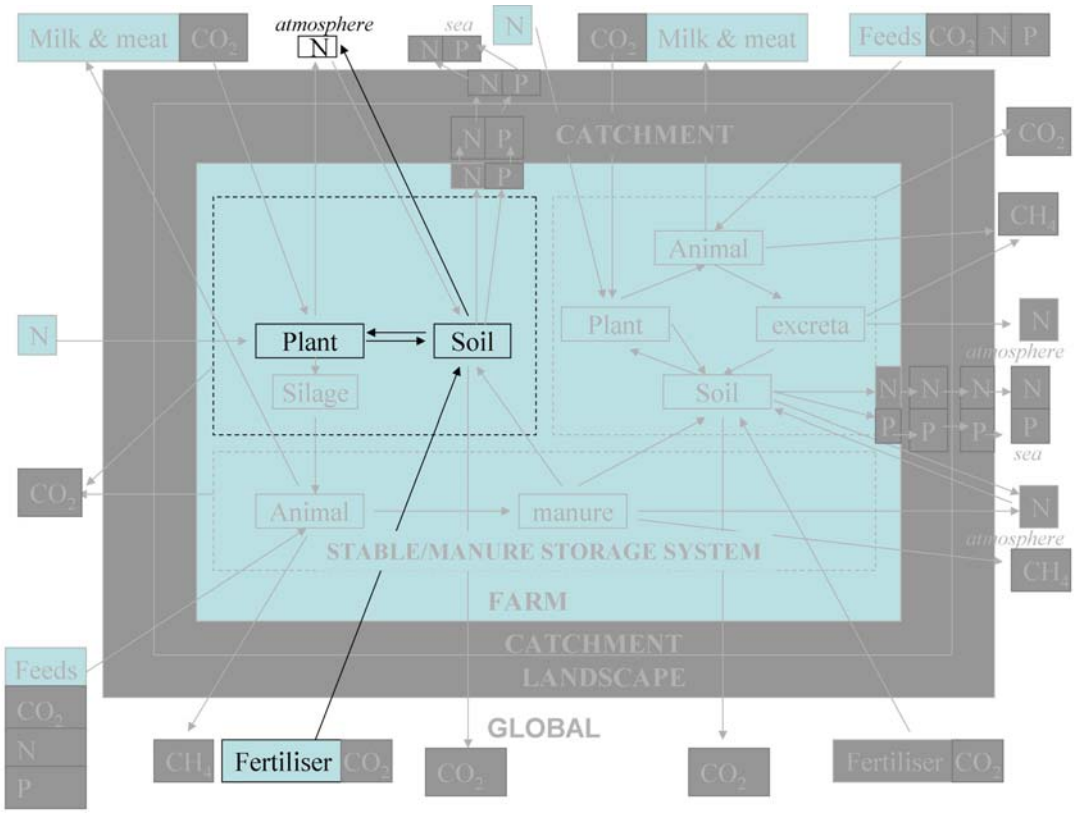
NUTGRANJA 2.0, using the mass balance criterion, is capable of simulating the effect, in a simpler way, of nutrient management and edapho-climatic conditions on the N and P flows, losses, efficiency and transformations in the soil-plant-animal dairy farm system. This study described the basis of NUTGRANJA 2.0 approach and showed to what extent modelled state variables, essentially those related to losses and production in the farm, were sensitive to E/M variables in the model.

The use of a yearly time-step in NUTGRANJA 2.0 intended to match the existing data available in the Basque Country. This allows the system to be studied at a suitable level of complexity to represent the functional relationships among the components of the farm

system. Further testing with future data from any of the components and processes of the plant-soil-animal system (from the Basque Country farms or northern Spain) and shorter time-steps to account for manure and fertiliser application timing will contribute to improvements in the predictability and robustness of the model. Furthermore, because of the combination of readily-available input data required to run the model, large sensitivity to combinations of management x soil x climatic factors and capability to simulate processes affecting internal and external N and P flows, NUTGRANJA 2.0, could be relevant to: (i) complement methodologies to estimate GHG from agriculture (i.e. IPCC) in the Basque Country and (ii) study the effect of Basque dairy farming systems on diffuse pollution to waters (NO_3^- and P losses within a catchment scale). The latter will require linking NUTGRANJA 2.0 with existing spatially-implicit hydrological models and will be remarkably useful in view of implementation of the Water Framework Directive.

Chapter 5

Nitrous and nitric oxide emissions from different N sources and under a range of soil water contents.



5. Nitrous and nitric oxide emissions from different N sources and under a range of soil water contents.

Abstract

Emissions of nitrous oxide (N_2O) and nitric oxide (NO) have been identified as one of the most important sources of atmospheric pollution from grasslands. Soils are major sources for the production of N_2O and NO, which are by-products or intermediate products of microbial nitrification and denitrification processes. Some studies have tried to evaluate the importance of denitrification or nitrification in the formation of N_2O or NO but there are few that have considered emissions of both gases as affected by a wide range of different factors. In this study, the importance of a number of factors (soil moisture, fertiliser type and temperature) was determined for N_2O and NO emissions. Nitrous oxide and NO evolution in time and the possibility of using the ratio NO: N_2O as an indicator for the processes involved were also explored. Dinitrogen (N_2) and ammonia (NH_3) emissions were estimated and a mass balance for N fluxes was performed. Nitrous oxide and NO were produced by nitrification and denitrification in soils fertilised with NH_4^+ and by denitrification in soils fertilised with NO_3^-. Water content in the soil was the most important factor affecting N_2O and NO emissions. Our N_2O and NO data were fitted to quadratic (r = 0.8) and negative exponential (r = 0.7) equations, respectively. A long lag phase was observed for the N_2O emitted from soils fertilised with NO_3^- (denitrification), which was not observed for the soils fertilised with NH_4^+ (nitrification) and was possibly due to a greater inhibiting effect of low temperatures on microbial activity controlling denitrification rather than on nitrification. The use of the NO: N_2O ratio as a possible indicator of denitrification or nitrification in the formation of N_2O and NO was discounted for soils fertilised with NO_3^-. The N mass balance indicated that about 50 kg N ha^{-1} was immobilised by microorganisms and/or taken up by plant roots, and that most of the losses occurred in wet soils (WFPS>60 %) as N_2 and NH_3 losses (>55 %).

5.1. Introduction

In grasslands, large quantities of nitrogen (N) flow through the animal-plant-soil-atmosphere system. A small quantity of this N is retained by the animal and exported to humans in meat or milk. The fate of the remaining N is not always easily accounted for due to the multiple complex interactions within the system, but one of the most important is gaseous loss as nitrous oxide (N_2O) and nitric oxide (NO).

Nitrous oxide has been identified as one of the main contributors to the greenhouse effect (Bouwman, 1990). Nitric oxide and N_2O are also involved in ozone layer depletion (IPCC, 1996). Nitric oxide also plays a major role in the chemistry of the tropospheric ozone (Bouwman, 1990) and in the formation of acid rain (Vos *et al.,* 1994).

Both NO and N_2O are formed in the soil generally through nitrification and denitrification and both are controlled by a number of soil class factors, including moisture content, temperature, fertiliser additions, pH, organic matter content, particle-size, nitrate (NO_3^-) and ammonium (NH_4^+) (Tiedje, 1988; Granli and Bockman, 1994).

Nitrate and NH_4^+ in the soil are subject to the following process dynamics. Nitrate may: (1) undergo denitrification to gaseous oxides of N and to N_2, (2) be taken up by organisms (assimilatory reduction), (3) be used by microorganisms as an electron acceptor and become reduced to NH_4^+ (dissimilatory reduction), (4) be leached or run off, or (5) accumulate in the soil. Ammonium may: (1) be taken up by plants, (2) be immobilised in microbial biomass, (3) nitrify to NO_3^- and partially be lost as gaseous oxides of N (4) be leached, (5) accumulate in the soil (Paul and Clark, 1996) or (6) volatilised as ammonia (NH_3).

The regulation of trace N-gas production via nitrification and denitrification has been described by the “hole-in-the-pipe” conceptual model (Firestone and Davidson, 1989). The rate of the processes (denitrification and nitrification) and the relative proportions of end products are controlled at two different levels. First level factors control the movement of N through the “pipe”. Second level factors control the partitioning of the reacting N species to N_2, N_2O, NO, or to a more oxidized product: factors, hence, control the size of the holes in the pipe through which the gases “leak”.

Numerous studies have investigated the contribution of nitrification and denitrification to the flux of N_2O and NO from soils using (i) laboratory (i.e. Anderson and Levine, 1986; Wrage *et al.,* 2004) and (ii) field techniques (i.e. Muller *et al.,* 1998).

Experiments have also been carried out to investigate the effect of key factors such as soil temperature, soil water, soil texture, soil pH and land use (Bandibas *et al*., 1994; Skiba *et al*., 1998; Dobbie and Smith, 2001) on N_2O, on N_2O and NO (Harrison *et al*., 1995; Yamulki *et al.,* 1997; Skiba and Ball, 2002) and on NO (Cárdenas *et al.,* 1993; Skiba *et al.,* 1997).

So far, in our conditions several field studies have been carried out in order to study the effect of land use (Estavillo *et al.,* 2002; Pinto *et al.,* 2004), grazing activity (Merino *et al*., 2001a) and nitrification inhibitors (Merino *et al.,* 2001b, 2002, 2005; Macadam *et al.,* 2003) on N_2O and NO emissions. In order to better understand the processes that have an effect on these emissions, we established an experiment to quantify N oxide losses and to study the relative importance of the different soil physical (moisture and temperature) and chemical (NO_3^- and NH_4^+) parameters that control these losses.

5.2. Materials and methods

5.2.1. Experimental set-up

A total of 108 intact soil cores (20 cm diameter x 15 cm length) were collected from a permanent grassland field in Derio (Spain) by inserting purpose-built PVC pots. Grass and clover shoots were removed both at the beginning and throughout the experiment in order to minimise plant impact on nitrification and denitrification. Previous studies (Whitehead, 1995) suggested that plants absorb NO_3^- and roots promote denitrification by providing dead cellular material and depleting oxygen concentration in the rhizosphere (Mahmood *et al.,* 1997). The shoots can also absorb NO_2, affecting the net flux of NO_x (NO + NO_2) from the soil (Bouwman, 1998) to the air.

The sward was a permanent grassland (60 % *Lollium perenne*, 31 % *Lollium rigidum* and 8 % *Trifolium repens*) and had been reseeded 3 months before the experiment was started. The soil was a poorly drained clay soil classified as a dystric gleysol and its characteristics are shown in Table 1.

The 108 pots with soil cores were placed in a greenhouse and separated into 3 groups of identical pots (3 x 36 core-sets). In order to minimize spatial variability among core-sets, the three soil samples were taken within a 10 cm distance of each other. The experiment lasted for 23 days. The first core-set was used to measure N_2O (for 23 days) and NO (for 16 days) fluxes and to determine mineral N content (NH_4^+ and NO_3^-) at day 23. The second and third core-sets were used to determine mineral N content at day 2 and day 16, respectively. Each core-set was subsequently subdivided into 3 types of fertiliser treatments of 12 soils ranging in water content (3 N treatments x 12 WFPS). Two different kinds of N fertiliser: $(NH_4)_2SO_4$ (a) and KNO_3 (b) were applied at a rate of 150 kg N ha^{-1} and an unfertilised control (c) was established. Each N treatment had a range of soil moisture from 30 % to 96 % water-filled pore space (WFPS). Soil subsamples for mineral N content determination were taken with 2.5 cm diameter x 10 cm length cores.

Table 1. Physical and chemical characteristics of the soil (0-10 cm).

Coarse Sand (%)	2.1	**pH (KCl)**	5.3	**Olsen P (mg l^{-1})**	60.8
Fine Sand (%)	36.2	**OM (%)**	2.01	**CEC (meq $100g^{-1}$)**	12.2
Silt (%)	34.6	**N (%)**	0.13	**Bulk Density**	1.36
Clay (%)	27.1	**C/N**	9	**Porosity (%)**	48.6

The required soil moisture in the pots was determined on the basis of bulk density, porosity and pot dimensions: soils were dried or wetted as required in order to reach the expected initial moisture content and once the experiment started, soils were weighed daily and subsequently watered in order to replace water lost through evaporation. Watering was carried out at least two hours before gas sampling in order to minimize possible gaseous pulses caused from the watering.

Extractable soil NH_4^+ and NO_3^- were analysed as follows: 100 g moist soil for each sample was extracted with 200 cm^3 1M KCl and the soil suspension was then filtered (Whatman No 1). The extracts were frozen until ready for analysis for NO_3^--N and NH_4^+-N using a segmented flow injection analyser (Alpkem 501). Ammonium-N was determined by the Berthelot reaction, adapted for automated methods (Alpkem, 1986, 1987). Nitrate-N was

determined from a diazo-based colour reaction with nitrite, after passing the sample through a cadmium column, which reduced the nitrate to nitrite.

5.2.2. Measurements of N_2O and NO

Gaseous N_2O and NO fluxes were measured at the same time of the day in order to minimise the impact of diurnal variation (Yamulki *et al.,* 2001). Nitrous oxide was measured following the closed flux chamber technique (Velthof and Oenema, 1995): the concentration of N_2O in the headspace was determined using a photo-acoustic infra-red gas analyser (Brüel and Kjaer 1302 Multi-Gas Monitor) after closing the flux chamber (internal diameter: 20cm, height: 15cm) at 0, 8, 16 and 24 minutes, N_2O emission rate was calculated from the change in concentration in the chamber over this time. The gas analyser was fitted with optical filters to selectively measure concentrations of N_2O, CO_2 and water vapour. Concentration of N_2O was compensated for interferences of CO_2 and water vapour.

Nitric oxide fluxes were measured using an open chamber technique as described by Harrison *et al.* (1995). Charcoal-filtered air was pumped through the chamber via polytetrafluoroethylene (PTFE) tubing at a rate of 2 l min^{-1} to remove ambient O_3 from the air stream, thus eliminating reactions between ambient O_3 and NO within the chamber. Concentrations of NO were measured at the air inlet and outlet of the chamber using an NO-NO_2-NO_x chemiluminiscence analyser (Unisearch LMA-4), fitted with a chromium trioxide NO to NO_2 converter. Fluxes of NO were calculated from the difference in concentration in inlet and outlet air, the flow rate of air through the chamber, and the surface area of the chamber.

5.2.3. Nitrogen balances

Nitrogen balances were carried out for the soils fertilised with NH_4^+ and NO_3^- (a and b treatments, respectively). Each treatment was subsequently split into two subtreatments of dry and wet soils (Four subtreatments: a-WFPS<60 %, a-WFPS>60 %, b-WFPS<60 %, b-WFPS>60 %). The forms of N losses which had not been directly measured were estimated in order to carry out the balances. Losses of N_2 were estimated following the modelling approach described by Parton *et al.* (1996). According to this approach the N_2: N_2O ratio can be predicted by the soil moisture content, soil NO_3^- and soil respiration rates. Ammonia emissions from soils fertilised with $(NH_4)_2SO_4$ were also estimated using the approach

described by Misselbrook *et al.* (2004). This study describes a simple model for estimating NH_3 emissions as a function of the following variables: fertiliser type, soil pH, land use, application rate, rainfall and temperature.

Apparent soil N immobilisation and roots uptake ($N_{immo\text{-}root}$) was calculated by mass balance in the following way: $N_{immo\text{-}root} = (N_{Fer} + N_{min0})-(N_{min1} + N_{N2} + N_{N2O} + N_{NO} + N_{NH3})$ where N_{Fer} = fertiliser N, N_{min0} = mineral N before fertiliser application (assumed as the initial measured mineral N from the unfertilised soil), N_{min1}= measured mineral N after fertiliser application, N_{N2}= estimated N_2 emissions, N_{N2O}= N_2O emissions, N_{NO}= NO emissions and N_{NH3}= NH_3 emissions. Losses were calculated from the cumulative emissions.

5.2.4. Statistical analysis

Data were subjected to statistical analysis (ANOVA and GLM regressions). Multiple comparisons among the means were made using Duncan´s Range Test. Significant differences are expressed at $p<0.001$, unless otherwise stated. Multiple regression analyses between the main variables measured in the soil and N_2O and NO were also carried out. Statistical analyses and graphical outputs of the results were carried out using Excel, SPSS, SAS 8.0 and Harvard Graphics 4.0.

5.3. Results

5.3.1. N_2O fluxes

A great variation in N_2O emission rate was recorded during the 23 days of the experiment: emission rates from individual pots ranged from 0 to 530 g N_2O-N ha^{-1} d^{-1}. Variability in daily N_2O emission rates was large for the 3 N treatments (mean of 12 WFPS) as shown by the standard error bars in Fig 1. On most days no statistical differences could be found between means of N_2O from different treatments (data not shown). Despite this lack of statistical significance on most days, soils under different treatments clearly showed different behaviour with time (Fig 1). We identified 4 different discrete response periods during the experiment:

(1) From day 2 to 4, only N_2O emission rates from soils fertilised with NH_4^+ were significantly (data not shown) greater than those from the unfertilised soils.

(2) From day 8 to 17, both soils fertilised with NO_3^- and with NH_4^+ resulted in greater (although not significantly different, data not shown) N_2O emission rates than the unfertilised soils. Emission rates from soils fertilised with NO_3^- were the greatest (not significantly different, data not shown).

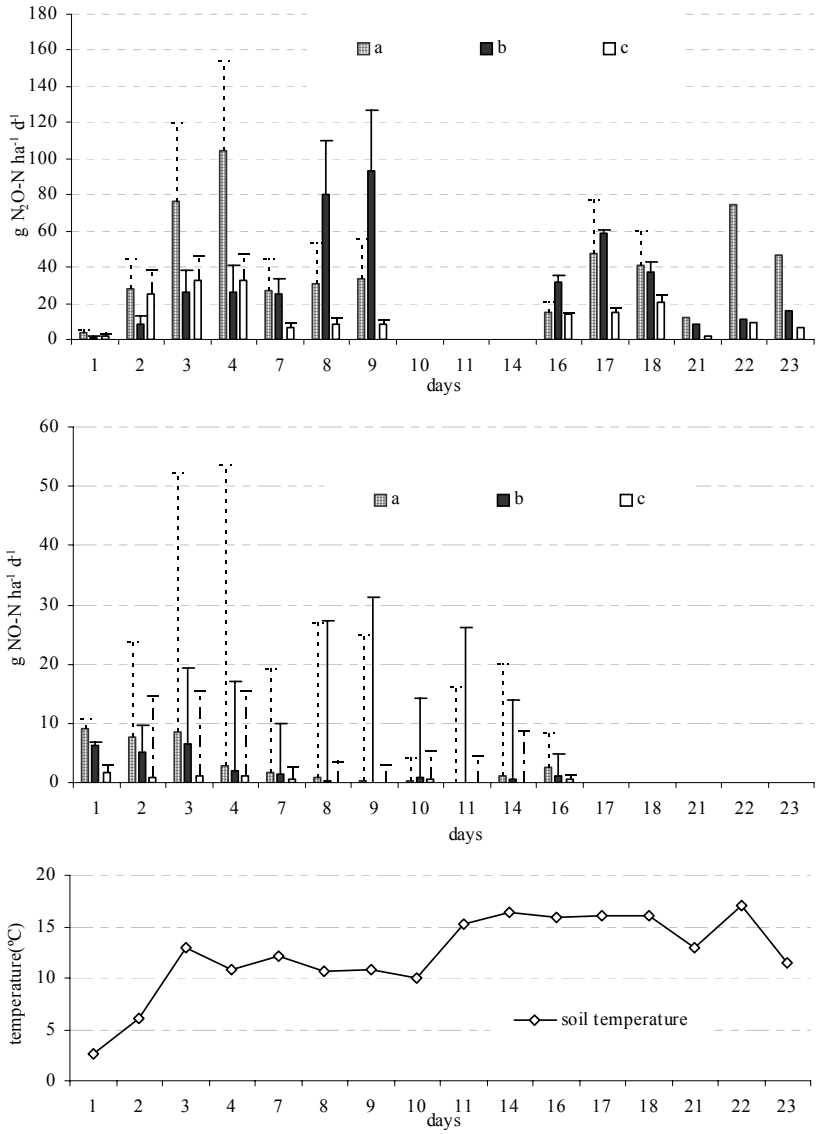


Figure 1. Evolution throughout the experimental period of mean N_2O and NO fluxes (mean of 12 WFPS), and soil temperature in soils fertilised with: (**a**) $(NH_4)_2SO_4$, (**b**) KNO_3 and (**c**) control. Vertical bars show standard errors.

(3) From day 18 to 21, both fertilised soils resulted in similar N_2O emission rates greater (not significantly different, data not shown) than the unfertilised soils.
(4) From day 22 to 23, soils fertilised with NH_4^+ again showed the greatest (not significantly different, data not shown) N_2O emission rates. No difference was found between soils fertilised with NO_3^- and unfertilised soils.

Nitrate and NH_4^+ content in the soil was significantly different across the 3 treatments ($p<0.05$, Table 2): as expected, soils fertilised with NH_4^+ showed the highest levels of NH_4^+ ranging from 84.7 to 57.9 kg N ha^{-1} on the day 2 and 23, respectively ($p<0.05$, Table 2). The NO_3^- content in soils fertilised with NH_4^+ was significantly smaller than that found in soils fertilised with NO_3^- and only significantly greater than in the unfertilised soils in day 23 ($p<0.05$, Table 2). Nitrate content varied from 14.8 to 38.1 kg N ha^{-1} on the day 2 and 23, respectively (Table 2).

Soils fertilised with NO_3^- showed the highest levels of NO_3^-, ranging from 141.3 to 94.1 kg N ha^{-1} on days 2 and 23, respectively ($p<0.05$, Table 2). The level of NH_4^+ in this soil, however, was always very low (<6 kg N ha^{-1}) and was not significantly different to that found in the unfertilised soils ($p<0.05$, Table 2). Taking into account that nitrification and denitrification are generally substrate-limited (Williams *et al.*, 1992), large amounts of denitrifiable N (NO_3^-) together with small amounts of nitrifiable N (NH_4^+) may indicate that in NO_3^- fertilised soils denitrification, and not nitrification, may have been the main process of N transformation.

Table 2. Evolution throughout the experiment of mean NO_3^- and NH_4^+ content in the soil for the different N treatments (mean of 12 WFPS).

	Day 2		**Day 16**		**Day 23**	
Treatment	**NH_4^+**	**NO_3^-**	**NH_4^+**	**NO_3^-**	**NH_4^+**	**NO_3^-**
$(NH_4)_2SO_4$	84.7 a	14.8 b	83.6 a	35.7 b	57.9 a	38.1 b
KNO_3	4.5 b	141.3 a	5.5 b	113.7 a	4.8 b	94.1 a
0N*	3.9 b	12.5 b	4.7 b	12.2 b	4.6 b	10.5 c

Figures followed by the same letter within each column are not significantly different according to Duncan´s multiple range test. ($p< 0.05$). *unfertilised soils.

The amount of nitrifiable and denitrifiable N at different times and for different N_2O responses can indicate different bacterial processes (nitrification or denitrification). For instance, at day 2, the NH_4^+ content in the soils fertilised with NH_4^+ was 21 times greater

(~85 kg NH_4^+-N ha^{-1}) than in soils fertilised with NO_3^- (~5 kg NH_4^+-N ha^{-1}). Nitrate content, however, was about 9 times smaller (~15 *vs* ~141 kg NO_3^- -N ha^{-1}). Nitrous oxide emissions in soils fertilised with NO_3^- were similar to those from unfertilised soils. Hence, NH_4^+ in the soil appeared to be the limiting N substrate for N_2O to be produced, and nitrification of NH_4^+ seemed to be the main bacterial process generating N_2O. However, the N_2O peak that occurred in the soils fertilised with NH_4^+ during the last 2 days of the experiment (response period 4) could have come from denitrification and/or nitrification as both nitrifiable N (NH_4^+) and denitrifiable N (NO_3^-) were not limiting at that time.

Soils fertilised with NO_3^- resulted in very small N_2O emission rates until day 8 of the experiment (beginning of response period 2). From this day, as previously commented, soils fertilised with NO_3^- resulted in greater N_2O emission rates than the rest. Since most N was in the form of denitrifiable N (NO_3^-) (Table 2), it could be suggested that N_2O emissions may have been produced by denitrification processes. From day 18, N_2O emissions in the soils fertilised with NO_3^- decreased.

Mean daily N_2O emissions were integrated over the time of the experiment (cumulative emissions). Different groups of soils with different N treatments and moisture contents (dry soils: moisture content<60% WFPS, wet soils: moisture content>60% WFPS and combined soils) were considered in order to study the effect of fertiliser type and soil moisture on N_2O cumulative emissions. Soils fertilised with NH_4^+ (mean of 12 WFPS) resulted in greater (not significantly different, data not shown) N_2O emissions than those fertilised with NO_3^-, being about 900 and 800 g N ha^{-1}, respectively. Fertilised soils, as expected, resulted in significantly greater (data not shown) N_2O emissions than the unfertilised ones.

Whereas under wet conditions (WFPS>60%) the fertilised soils (mean of 2 N treatments) gave cumulative N_2O emissions 3.5 times greater than the unfertilised ones (mean of unfertilised treatment), on drier conditions (WFPS<60%) this difference was a factor of about 1.5. Soils (mean of 3 N treatments) under wet conditions (WFPS>60%) showed significantly greater (data not shown) cumulative N_2O emissions than soils under dry conditions (WFPS<60%) did. Fertilised and unfertilised soils (mean of 3 N treatments) under wet conditions (WFPS>60%) resulted in about 10 times greater N_2O emissions than soils with the same treatments but under dry conditions (WFPS<60%). These differences were statistically significant for the fertilised soil but not for the unfertilised ones (data not

shown). Moreover, cumulative N_2O emissions from the dry (WFPS<60%) fertilised soils (mean of 2 N treatments) were almost 3 times smaller (not significantly different, data not shown) than from wet (WFPS>60%) and unfertilised soils (~140 g N ha^{-1} *vs* ~400 g N ha^{-1}), suggesting that water soil content may have been the main factor that controlled N_2O emissions in this experiment.

5.3.2. NO fluxes

A great variation in NO emission rates was recorded during the experiment (Fig 1). Emission rates from individual pots ranged between 0 and 25.6 g NO-N ha^{-1} d^{-1}, and daily standard errors for the 3 N treatments (mean of 12 WFPS) were substantial on most days (Fig 1). Large values of NO emissions occurred only at the beginning of the experiment (first 3 days). From day 4 to 14, NO emission rates decreased, and, from day 15 to 16, NO emission rates slightly increased. As in the case of N_2O emissions, fertilised soils emitted more NO than unfertilised ones (only statistically significant during the first 3 days, data not shown). Although NO emission rates from soils fertilised with NH_4^+ were generally greater than from those fertilised with NO_3^-, no statistical differences were found.

A separation of each N treatment based on soil moisture content (% WFPS) was carried out for NO emissions from soils under dry (<60 % WFPS) and wet (>60% WFPS) conditions, and, contrary to what was found for N_2O, no clear pattern was observed between the two groups (data not shown).

Although fertilised soils (mean of 12 WFPS) showed the greatest NO emissions during the first 3 days, these soils differed greatly from each other in NO_3^- and NH_4^+ content. Whereas in soils fertilised with NH_4^+, NH_4^+ level remained high and NO_3^- level (smaller than NH_4^+) increased (statistically significantly, data not shown) from 14.8 to 35.7 kg N ha^{-1} (Table 2), in soils fertilised with NO_3^-, NH_4^+ levels remained low (<6 kg N ha^{-1}) and NO_3^- was significantly greater than NH_4^+ ($p<0.05$, Table 2) and decreased (statistically significantly, data not shown) from 141.3 to 113.7 kg N ha^{-1}.

Nitrification is suggested to be the main process of NO formation in soils fertilised with NH_4^+ during the first days of the experiment since the content of nitrifiable N (NH_4^+) was greater than that of denitrifiable N (NO_3^-) throughout the experiment ($p< 0.05$, Table 2), and NO_3^- content significantly increased from day 2 to day 16 (Table 2). Denitrification is

suggested to be the main process of NO formation in the soils fertilised with NO_3^- during the first days as NO_3^- was the only source of N, the content of which was significantly greater than in unfertilised soils ($p < 0.05$, Table 2).

5.3.3. N balances

Ammonia emissions from soils fertilised with NH_4^+ (a) were estimated on the assumption that the main volatilisation loss would occur within the first week (Misselbrook, *pers comm.*). Estimated N_2:N_2O ratio (from all individual soils, data not shown) ranged from 0.01 (soil fertilised with NH_4^+ and WFPS = 30 %) to 23.9 (soil fertilised with NO_3^- and WFPS = 96 %) and N_2 cumulative emissions (from all individual soils, data not shown) ranged from 0 to 47 kg N ha^{-1}. Ammonia cumulative emissions (from all individual soils, data not shown) ranged from 5.7 to 6.2 kg N ha^{-1} in soils fertilised with NH_4^+.

Mass balances of N were estimated for the 4 subtreatments at the end of the experiment (Table 3). Dinitrogen and NH_3 losses together accounted for most of the N losses in all subtreatments (>55 %). Nitrogen losses from soils under wet conditions were greater than those from dry soils. The main loss in soils under wet conditions was generally N_2 and represented a loss of the N applied as NH_4^+ and as NO_3^- of 11 and 17 %, respectively. Soils under dry conditions and fertilised with NH_4^+ resulted in the greatest NH_3 emissions of all 4 subtreatments (4.1 % of the N applied). Both N_2O and NO losses were similar when soils under similar water conditions were compared: N_2O losses from soils under wet conditions were greater than those under dry conditions (0.9 % vs 0.1 % of the N applied) and, reversely, NO losses from soils under dry conditions were greater than those under wet conditions (0.05 % vs 0.03 % of the N applied).

When the N treatments were compared separately NO_3^- and NH_4^+ contents in soils under dry conditions were always greater than those under wet conditions. The estimated values of apparent N immobilisation and root uptake ($N_{immo\text{-}root}$) showed no differences between the 4 subtreatments at the end of the experiment ($N_{immo\text{-}root}$ range = 51-54 kg N ha^{-1}).

Table 3. Nitrogen mass balance (kg N ha^{-1}) for the 4 subtreatments during the experiment.

	a-WFPS<60 %$^{\Delta}$	**a-WFPS>60 %**$^{\Delta}$	**b-WFPS<60 %**$^{\Delta}$	**b-WFPS>60 %**$^{\Delta}$
N_{Fer}	150	150	150	150
NO_3^-	47.1	30.7	111.3	77.0
NH_4^+	64.8	52.3	5.1	4.5
N_{N2}	$2.4 \cdot 10^{-1}$	16.9	$2.5 \cdot 10^{-1}$	25.4
N_{N2O}	$1.5 \cdot 10^{-1}$	$5.1 \cdot 10^{-2}$	$1.5 \cdot 10^{-1}$	1.4
N_{NO}	$6.8 \cdot 10^{-2}$	1.4	$6.1 \cdot 10^{-2}$	$1.4 \cdot 10^{-2}$
N_{NH3}	6.1	5.9	0	0
$N_{immo\text{-}root}$	51.2	54.5	52.8	53.4

$^{\Delta}$Subtreatments: **a-WFPS<60 %**=soils fertilised with $(NH_4)_2SO_4$ under dry conditions (WFPS<60 %), **a-WFPS>60 %**=soils fertilised with $(NH_4)_2SO_4$ under wet conditions (WFPS>60 %), **b-WFPS<60 %**=soils fertilised with KNO_3 under dry conditions (WFPS<60 %), **b-WFPS>60 %**=soils fertilised with KNO_3 under wet conditions (WFPS>60 %).

5.4. Discussion

5.4.1. N_2O fluxes

Different response periods of N_2O from soils fertilised with different N forms suggest that N_2O emissions were greatly influenced by the N substrate form. In the soils fertilised with NH_4^+, as it has been described by other studies (Freney *et al.*, 1985; Murakami *et al.*, 1987), two N_2O peaks were observed: the first one coming from nitrification and the second one coming from nitrification and/or denitrification. In soils fertilised with NO_3^-, only one peak, possibly coming from denitrification and later than in the soils fertilised with NH_4^+, was observed. This delay may have been caused by a long lag period on the formation of the N_2O reductase enzyme. Shorter than in our experiment, this period has been previously reported by other authors (Firestone *et al.,* 1979; Weier *et al.,* 1993).

The fact that the temperature varied during the first 3 days of our experiment (soil average temperature ranged from about 3 to about 12 ºC) may have had a different impact on denitrification and nitrification processes. Low temperatures in the first days may have: (i) enhanced N_2O produced by nitrification (Maag and Vinther, 1996) and/or (ii) suppressed the formation of N_2O from denitrification by inhibiting the NO_2^- reductase enzyme (Dupain and Germon, 1990). Although theoretically, in nitrate fertilised soils NO_3^- can undergo processes of dissimilatory reduction and, thus, produce NH_4^+ instead of gaseous nitrogen oxides and/or N_2, the possibility of this occurring should be ruled out as soil NH_4^+ content was always very small.

As found by other authors in experiments of soils fertilised with mineral fertiliser (Conrad *et al.,* 1983; Dobbie and Smith, 2003; Ryden, 1983; Skiba *et al.,* 1992) or manure (Oenema *et al.,* 1997), N_2O emissions were large only when soil mineral N was not limiting and soil moisture was above a certain threshold. In our experiment, this soil moisture content threshold was around 60 % WFPS, which is similar to that found by Dobbie and Smith (2003). Soils fertilised with NH_4^+, as also indicated by Dalal *et al.* (2003), resulted in greater N_2O emissions than those fertilised with NO_3^-.

Correlations between N_2O emissions and the main measured factors (WFPS %, NO_3^- content, NH_4^+ content and soil temperature) were obtained for each N treatment and this comprised: (i) all the soils of a N treatment or (ii) dry soils of a N treatment (<60 % WFPS) or (iii) wet soils of a N treatment (>60 %WFPS). We found that these correlations were generally weak (Table 4). These results are in line with literature values (Aulakh *et al.,* 1992; Bronson and Mosier, 1993; Thornton *et al*., 1996). Being an important factor regulating both nitrification and denitrification (Williams *et al.,* 1992), temperature may have contributed to these poor coefficients as there was a great fluctuation in temperature values during the experiment. These correlations showed that soil moisture content (as %WFPS) was generally the factor best correlated with N_2O emissions. However, only dry (<60 % WFPS) and NH_4^+ (a) fertilised soils resulted in a coefficient greater than 0.5.

Table 4. Correlation coefficients (r) with N_2O emission rates, WFPS %, soil temperature, NO_3^- content and NH_4^+ content for all the soils and for the dry and wet range of soils. (α= 0.05).

	WFPS (%)			**Soil Temperature**			**NO_3^- content**			**NH_4^+ content**		
	*a	*b	*c	*a	*b	*c	*a	*b	*c	*a	*b	*c
All soils	0.26	0.46	0.22	0.10	0.12	0.04	0.02	-0.24	0.02	0	-0.09	-0.33
Soils (WFPS<60%)	0.55	-0.02	0.39	0.18	0.24	0.37	-0.20	-0.17	0.26	-0.18	-0.01	0.02
Soils (WFPS>60%)	-0.18	0.28	-0.12	0.14	0.16	0	0.30	-0.05	-0.13	-0.05	-0.10	-0.43

*Soils fertilised with: (a) $(NH_4)_2SO_4$, (b) KNO_3 and (c) unfertilised.

For each soil, average N_2O emissions were plotted against soil water content (Fig 2). We log-converted N_2O emissions as N_2O emissions have well been described to follow Ln-normal distributions (Velthof *et al.,* 2000; De Klein *et al.,* 1999). These values were fitted to a quadratic equation with a high and positive correlation (r = 0.8 and S.E = 1.1, 95 % confidence):

$$\text{Ln } N_2O \text{ (g } N_2O\text{-N ha}^{-1} \text{ d}^{-1}) = -0.002*WFPS^2+0.3*WFPS-8.5 \quad \textbf{(1)}$$

This equation showed that with increasing soil water content (% WFPS), N_2O emissions also increased until the soil water content reached approximately 75 % WFPS. Above this soil water content, N_2O emissions decreased with increasing soil water content, which partially could have accounted for the negative correlation coefficient between N_2O emissions and WFPS with wet soils only (a and c treatments) taken into account (Table 4).

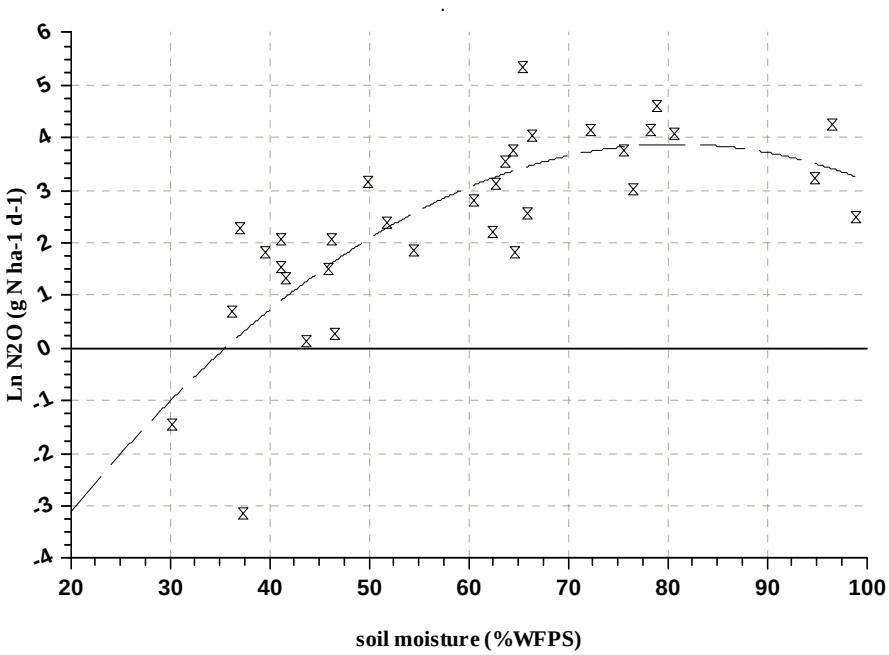


Figure 2. Average Ln N_2O emissions related to soil moisture content (% WFPS).

The most probable explanation is that N_2O emissions increased to a level where simultaneous denitrification and nitrification were at their maximum (75 %WFPS). Above this soil water content, denitrification was the main process producing N_2O and, as the soil became more anaerobic, emissions of N_2 became greater than those of N_2O.

This response appears to be similar to that found in other studies. However, the optimum water content for N_2O emissions can differ from soil to soil (Davidson, 1991; Bouwman, 1998). For instance, Schmidt *et al.* (2000), using a boundary line approach, proposed a bell-

shaped function to relate N_2O flux and % WFPS, and found an optimum WFPS value at 72 %.

Multiple regression analyses were carried out in order to study the relationship between the main soil variables measured (WFPS, temperature, NO_3^- and NH_4^+content) and N_2O emissions. These analyses were performed using 3 different groups of data: (i) the whole dataset (including the 3 N treatments x 12 WFPS), (ii) dry soils only (3 N treatments x WFPS<60%) and (iii) wet soils only (3 N treatments x WFPS>60%).

When the whole dataset was considered, the equation representing the best multiple regression was as follows:

$$\text{Ln } N_2O \text{ (g } N_2O\text{-N ha}^{-1}\text{ d}^{-1}) = -0.33+0.03\ W+3.22\cdot10^{-6}\ W^2\cdot A^2 \quad \textbf{(2)}$$

where W= WFPS (%) and A= ammonium content in the soil (kg NH_4^+-N ha^{-1}).

This equation explained 35 % of the variation and the regression was statistically significant at $p<0.001$. More complex equations were tested but none of them fitted the data better than this equation. The inclusion of both variables (WFPS and NH_4^+) and the positive sign associated to them supports the idea that nitrification may have played an important role in controlling N_2O emissions from our wet soils. In wet conditions, there is evidence that nitrification can occur (Aulakh and Bijay-Singh, 1997), generally restricted to shallow depths or local microsites (Abbasi and Adams, 2000).

Whereas the multiple regressions using data from dry soils showed no statistical significance, on wet soils, the best multiple regression explained 60 % of the variation ($p<0.001$). The equation of this regression was as follows:

$$\text{Ln } N_2O \text{ (g } N_2O\text{-N ha}^{-1}\text{ d}^{-1}) = 0.76+ 2.02\cdot10^{-4}\cdot N\cdot T^2+2.29\cdot10^{-6}\cdot W\cdot A^2 \quad \textbf{(3)}$$

where W= WFPS (%), N = nitrate content in the soil (kg NO_3^--N ha^{-1}), T= Soil temperature (ºC) and A = ammonium content in the soil (kg NH_4^+-N ha^{-1}).

All the tested variables were included in this equation. The fact that this equation (wet soils) included both NO_3^- (denitrifiable N) and NH_4^+ (nitrifiable N) and the whole dataset equation only included NH_4^+ (nitrifiable N) may support that N_2O from both denitrification and nitrification processes could have occurred in wet soils (Stevens *et al.,* 1997).

Other studies, using multiple regression analysis, have reported similar coefficients and correlating variables: Clayton *et al.* (1997) and Shepherd *et al.* (1991), for instance, accounted for only about 28 % of the variation. Skiba *et al.* (1994) found that N_2O was best correlated with NO_3^- and moisture content in the soil, and both factors together explained about 33% of the variation of the N_2O emission rates.

5.4.2. NO fluxes

Soils under different treatments with time clearly showed a similar NO emissions pattern. In addition, these soils (the 3 N treatments together) showed similar evolution of NO emissions in time to that from other studies (Slemr and Seiler, 1984; Skiba *et al.,* 1992): (i) NO emissions increased during the first three days after N fertiliser application, and (ii) from day 3, NO emissions decreased reaching minimum values after day 5.

Fertilised soils, as found by other authors (Slemr and Seiler, 1984; Shepherd *et al*., 1991; Harrison *et al*., 1995; Williams *et al.*, 1998; Venterea and Rolston, 2000; Akiyama and Tsuruta, 2003), showed greater NO emission rates than unfertilised soils.

Emission rates of up to 25.6 g NO-N ha^{-1} d^{-1} were measured from fertilised soils. These rates were greater than those reported by some studies (i.e. Meixner *et al.,* 1997: 4.3 g NO-N ha^{-1} d^{-1}; Cárdenas *et al.,* 1993: 10.3 g NO-N ha^{-1} d^{-1}; Skiba *et al*., 1992: 16 g NO-N ha^{-1} d^{-1}; Williams *et al.,* 1996: 16.8 g NO-N ha^{-1} d^{-1}), but smaller than those reported by other studies (i.e. Meixner *et al.,* 1997: 33.6 g NO-N ha^{-1} d^{-1}; Harrison *et al.,* 1995: 55.3 g NO-N ha^{-1} d^{-1}).

The fact that in NH_4^+ fertilised soils NH_4^+ (nitrifiable N) content was significantly greater than the NO_3^- (denitrifiable N) content throughout the experiment and NO_3^- -N accumulated suggests that nitrification, and not denitrification, was the main process of NO formation (Slemr and Seiler, 1984). The ammonium oxidising bacteria may have used the NO_2^- coming from the nitrification process as the alternative electron acceptor when O_2 had been limited during the nitrification process.

In contrast, the content of NO_3^- (denitrifiable N) in NO_3^- fertilised soils was significantly greater than the content of NH_4^+ (nitrifiable N) and NH_4^+ level was as low as that found in unfertilised soils. Therefore, we suggest that denitrification was the main process of NO formation (Cárdenas *et al.,* 1993; Bisson, 1994).

Correlations between NO emissions and the main factors measured (WFPS %, NO_3^- content, NH_4^+ content and soil temperature) were obtained for each treatment and this included: (i) combined soils of a N treatment or (ii) dry soils of a N treatment (<60 % WFPS) or (iii) wet soils of a N treatment (>60 %WFPS). Many other studies have used these coefficients as a tool to correlate soil factors and NO emission rates. These results are in good agreement with those of Williams *et al.* (1992) who found that due to high variability NO was weakly correlated with most of the measured soil factors (Table 5).

Table 5. Correlation coefficients (r) of NO emission rates with: WFPS %, soil temperature, NO_3^- content and NH_4^+ content for all the soils and for the dry and wet range of soils. (α= 0.05).

	WFPS (%)			**Soil Temperature**			**NO_3^- content**			**NH_4^+ content**		
	*a	*b	*c	*a	*b	*c	*a	*b	*c	*a	*b	*c
All soils	-0.31	-0.41	-0.36	-0.28	-0.24	-0.22	-0.50	0.61	-0.29	-0.07	-0.12	-0.23
Soils (WFPS<60%)	-0.18	-0.35	-0.34	-0.39	-0.24	-0.30	-0.75	0.58	-0.22	0.35	-0.31	-0.49
Soils (WFPS>60%)	-0.36	-0.43	-0.16	-0.12	-0.31	-0.19	-0.32	0.61	-0.14	0.36	0.24	0.36

*Soils fertilised with: (a) $(NH_4)_2SO_4$, (b) K NO_3 and (c) unfertilised.

Nitrate content was the best variable in the correlation (Thornton *et al.,* 1996). In fact, NO_3^- was correlated in most of the fertilised soils with NO emissions and showed coefficients greater than 0.5. A negative and a positive correlation between NO_3^- and NO emissions were found for soils fertilised with NH_4^+ and with NO_3^-, respectively. Although the sign of these coefficients may suggest that in NH_4^+ fertilised soils NO production decreased with increasing nitrified NH_4^+ and, in NO_3^- fertilised soils NO production decreased as NO_3^- was denitrified, correlation coefficients between NO and NH_4^+ content in the soil were too weak to support this suggestion. Contrary to what we have found on N_2O emission rates, soil moisture (% WFPS) was negatively correlated with NO emissions. Moreover, by plotting the average NO emissions against their corresponding soil moisture contents (Fig 3), we could fit the data to an equation involving a negative exponential function (r = 0.7 and S.E = 1.5, 95 % confidence). This function was represented as follows:

$$NO\ (g\ NO\text{-}N\ ha^{-1}\ d^{-1}) = 28.13 \cdot \exp^{(-0.05 \cdot \%WFPS)} \quad \textbf{(4)}$$

This function shows that the rate of NO emissions slows down as the soil moisture content approaches field capacity. Soil atmosphere becomes more O_2-limited and, subsequently, N_2O and N_2 increase while NO decreases. Optimum soil % WFPS values for maximum NO emissions were between 30% and 40% WFPS (Fig 3). This range of values lies between the observed ranges in other studies (Saxton *et al*., 1986: 47 % WFPS; Yang and Meixner, 1997: 20 % WFPS).

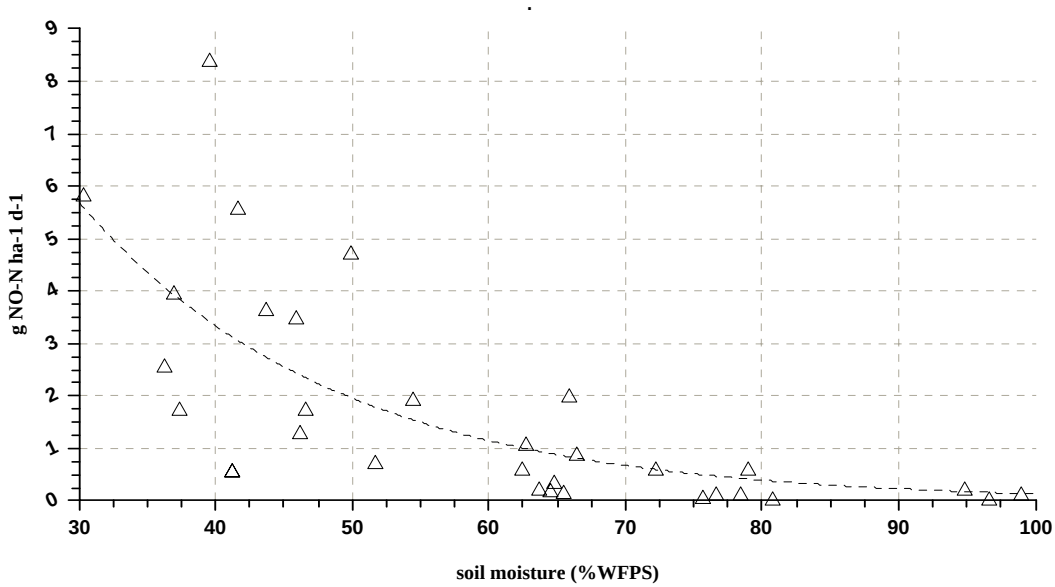


Figure 3. Average NO emissions related to soil moisture content (% WFPS).

Multiple regression analyses, in an analogous way to N_2O, were also carried out. We could only produce statistically significant regressions when we included the whole dataset in the analysis. The best multiple regression was represented with the equation as follows:

$$NO\ (g\ NO\text{-}N\ ha^{-1}d^{-1}) = 1.63+2.07\cdot10^{-4}\cdot A^2\cdot T-4.36\cdot10^{-5}W\cdot A^2 \quad \textbf{(5)}$$

where W= WFPS (%), T = Temperature in the soil (º) and A= ammonium content in the soil (kg NH_4^+-N ha^{-1}).

This equation explained 48% of the variation and the correlation was statistically significant at $p<0.0038$. More complex equations were tested but none of them improved

upon this one. Ammonium content and water content appeared to account best for the variation of NO emission rates. Although soil temperature as a single factor did not show a substantial correlation with NO emission rates, the multiple regression analysis, through including temperature in the best regression, showed that soil temperature had also had an effect on NO emission rates. Skiba *et al.* (1994), in a similar study, obtained a multiple regression that explained 60 % of the variation of the NO emissions by using NO_3^- content and temperature in the soil.

5.4.3. NO vs N_2O

The ratio of NO: N_2O emission was plotted against time as this ratio has been shown to provide some indication of the relative importance of nitrification and denitrification in producing NO and N_2O (Fig 4). Emission ratios > 1 are normally associated with active populations of nitrifiers and soil conditions favourable for nitrification, whereas emission ratios <0.01 are associated with denitrification and restricted aeration (Lipschulz *et al*., 1981; Skiba *et al.,* 1992).

Although NO: N_2O emission ratios ranged from 0 to 17, which explains, as previously observed, that both processes, nitrification and denitrification, could have occurred in the formation of N_2O and NO, ratios > 1 were only found during the first 2 days of the experiment (Fig 4), suggesting that nitrification may have been the main process of gaseous production only at the beginning of the experiment. This conclusion was also reached by Harrison *et al.* (1995).

Although NO: N_2O ratio as an indicator of nitrification and denitrification seemed to be reasonable for soils with large contents of NH_4^+ as it necessarily implies that NO is only formed through nitrification, in soils fertilised with NO_3^- where denitrification is the main process and where NO can be a free intermediate precursor (Ye *et al.,* 1994), ratios >1 can be misleading as they may indicate nitrification instead of denitrification.

The ratio of Ln NO: N_2O was plotted against soil moisture (Fig 5) and an equation involving a linear regression was fit. The negative slope of this equation demonstrates that NO emissions as previously observed and contrary to N_2O, increase as the soil moisture content decreases. This equation explained 24 % of the variation. We also investigated the

possibility to improve this correlation by omitting very small emissions (Davidson and Verchot, 2000). However, this value was not improved.

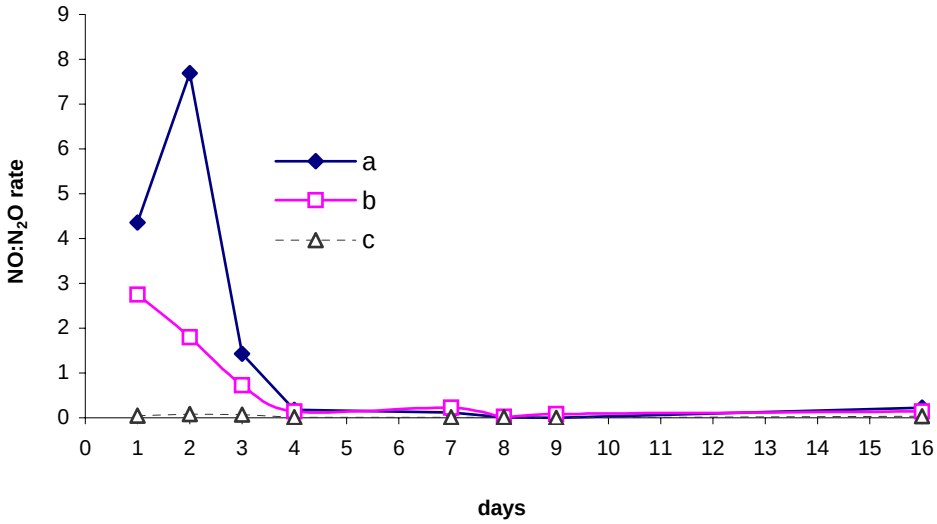


Figure 4. Temporal behaviour of the NO: N_2O averaged ratio during the days of the trial. (**a**= $(NH_4)_2SO_4$, **b**=KNO_3, **c**=Control).

The slope of the regression between WFPS % and the logarithm of the ratio of NO: N_2O emissions were $-6.5 \cdot 10^{-2}$ with the standard error of ± 1.4 (95 % confidence). Other studies have also found smaller slopes and standard errors. For instance, Davidson and Verchot (2000) and Davidson *et al*. (2000) found slopes of $-2.6 \cdot 10^{-2}$ and $-3.8 \cdot 10^{-2}$ with standard errors of ±0.7 and ±0.3, respectively, at the same confidence interval.

Comparing the behaviour of the N_2O and NO emission from soils fertilised with NH_4^+ during the first 3 days of the experiment, we can see that while N_2O emissions were small and increased with time, NO emissions were large. From this pattern, we could hypothesize that the enzymes responsible for the conversion of NO to N_2O (NO reductase) needed some time to become active.

Comparing the behaviour of the N_2O and NO emission from the soils fertilised with NO_3^- during the experiment, we can see that N_2O emissions were similar to those found different from the unfertilised soils until day 7. Again, we could hypothesize that the enzyme NO reductase needed some time to become active. The nitrate reductase and the nitrite reductase appeared to be active during the first days and the NO reductase was inhibited.

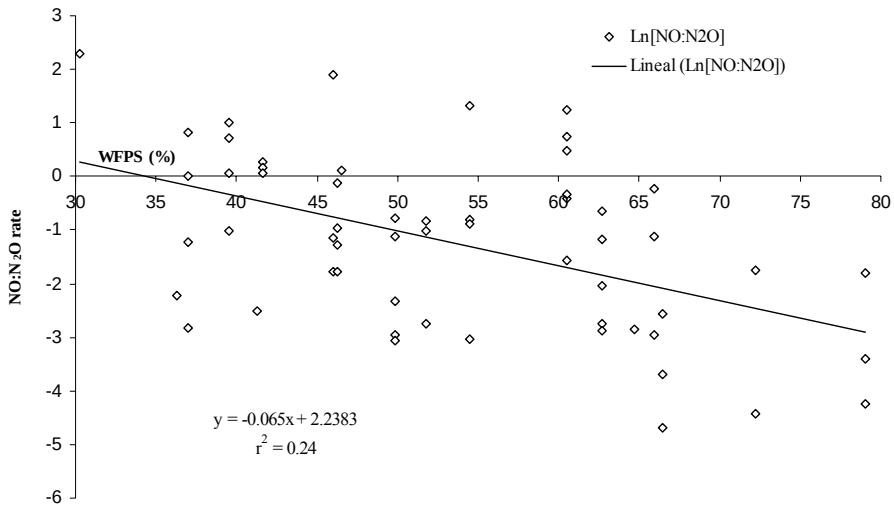


Figure 5. Relationship between averaged ratio of NO: N_2O emissions and soil water content (% WFPS).

5.4.4. N balances

Both NH_3 and N_2 estimated values were similar to values observed in other studies: NH_3 emissions were estimated to be about 4 % of the NH_4^+-N applied, which is similar to the value estimated by Webb *et al.* (1999). Denitrified N losses (measured N_2O + estimated N_2) from soils fertilised with NO_3^- and under wet conditions resulted in similar losses than those found by Scholefield *et al.* (1997) after application of 150 kg N ha^{-1} of KNO_3 on a similar type of soil (dystric gleysol).

The estimated N mass balances could be different from those found in a real field as in our experiment no plant shoots and drainage was allowed. Soils fertilised with NH_4^+ and under wet conditions resulted in greater apparent nitrification rates than under dry conditions (less soil NH_4^+ content). However, the fact that at the end of the experiment the increase of NO_3^- content under wet conditions was smaller than that found in soils under dry conditions may be indicating a great denitrification activity in wet soils during the last days of the experiment (which is explained by large N_2 losses in wet soils). The high positive value of $N_{immo\text{-}root}$ indicates that either NH_4^+ immobilisation and/or NH_4^+ root uptake (Watson, 1986) might have occurred.

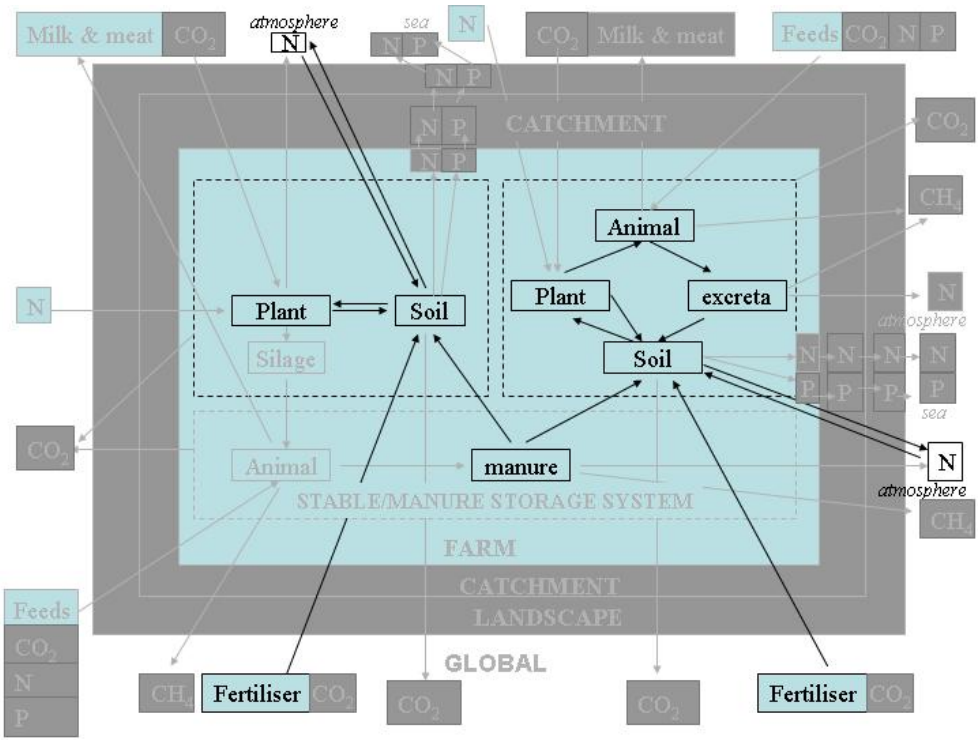
Soils fertilised with NO_3^- showed small mineralisation and nitrification rates (similar to those in the unfertilised soils) as no increase in NH_4^+ content was found during the experiment. Soils fertilised with NO_3^- and under wet conditions resulted in great N losses from denitrification and, thus, the decrease in NO_3^- content in this wet soil was greater than that found in dry soils. Nitrate root uptake and/or in a lesser way, NO_3^- microbes' immobilisation (Lægreid *et al.*, 1999) might have occurred to account for the high value of $N_{immo\text{-}root}$.

5.5. Conclusions

Our results have shown that N type in the soil has an important effect on the temporal behaviour of N_2O but not NO emissions. Nitrous oxide and NO can be produced by nitrification and denitrification in soils fertilised with NH_4^+ and denitrification in soils fertilised with NO_3^-. A long lag phase may be expected for the N_2O emitted from soils fertilised with NO_3^- (denitrification) with low temperatures. Soil moisture content was the most important factor governing N_2O and NO when soil mineral N was limiting. Total N losses from wet soils, particularly from N_2, are expected to be greater than those from dry soils. The N mass balance indicated that in soils fertilised with NH_4^+ and soils fertilised with NO_3^-, in all cases, a large amount of soil N was either immobilised by microorganisms or/and taken up by plant roots.

Chapter 6

N_2O gaseous losses in an intensively managed dairy farm receiving pig slurry.



6. N_2O gaseous losses in an intensively managed dairy farm receiving pig slurry.

Abstract

In this paper we present results from an experiment where we assessed the effect of management factors on nitrous oxide (N_2O) losses from an intensive commercial dairy farm in the Basque Country (Spain). In order to do so, we monitored N_2O fluxes from soil in 3 plots in the farm (grazed grassland on flat ground, grazed grassland on steep-sloped ground and a maize land). Results showed that N_2O emissions were remarkably affected by the combination of mineral and organic fertiliser management and climatic factors (i.e. rainfall).

Results of N_2O from grazed grasslands showed large spatial variability, thus resulting in poor statistical relationships between measured factors (soil % water-filled pore space (WFPS), soil temperature, soil ammonium (NH_4^+) and nitrate (NO_3^-) concentration) and fluxes of N_2O. The poor statistical significance of the N_2O results from the grazed fields supports the idea that there is a need to improve techniques to overcome the large spatial variability of grazed grass soils.

Emissions from the maize plot resulted in significant statistical relationships between N_2O fluxes and %WFPS, soil temperature and NO_3^- and NH_4^+ concentration in the soil. The relationship between N_2O emissions and %WFPS was fitted to a quadratic equation, allowing us to adapt an emission factor for this kind of soil management in our conditions. Although no significant statistical relationship could be established for grazed grass plots, the remarkable N_2O seasonal differences indicate that incorporation of seasonality as a factor for inventories of N_2O emissions from grazed grass is needed to improve the estimates of N_2O.

6.1. Introduction

Nitrous oxide (N_2O) is an important greenhouse gas (GHG) and it is also involved in the destruction of stratospheric ozone. Agricultural soils greatly contribute about 50 % of the global anthropogenic N_2O flux (IPCC, 2001), which is equivalent to a global warming

potential of 1 Pg C yr^{-1} (Robertson, 2004). Current IPCC protocols estimate agriculture contribution to atmospheric N_2O loading by simple Emission Factors (Efs), which generally have been empirically derived from a limited number of countries and hence soil and climatic conditions. For instance, 1.25± 1% of applied N to the soil is estimated to be lost as N_2O fluxes from fertilised *vs.* unfertilised field plots (Mosier *et al*., 1998). This approach has also the limitation that these Efs have been derived from controlled experiments; generally reflecting non-intensive and ideal managements such as supposing that manure is evenly spread in the surface land and its distribution in time is optimal.

So far, there have been controlled studies which have investigated the effect of different variables and management practices on annual N_2O emissions but this has seldom been studied on a commercial dairy farm. In this sense, in Europe significant amounts of manure being spread daily on the fields is reported to occur in six countries only, that is in France (5%), Czech Republic (7%), Belgium (8%), Norway (9%), the United Kingdom (12%) and Spain (13%) (Leip, 2005).

The aim of this work was hence to quantify annual N_2O emissions at a commercial farm scale and study the relationship between the main factors and N_2O emissions. By doing so, no replication or control was implemented and results analysis was inferred out of the monitored results.

6.2. Farm and site characteristics

The study was established in a very intensive mixed farm (dairy and pig) situated in the Cantabrico mountains and within the Urrunaga catchment (Basque Country, Northern Spain). Annual average rainfall from five years (2000-2005) in this area is around 1322 mm being half of the precipitation recorded from October to February and the weather is Atlantic with an annual average temperature of 10.5ºC.

The farm land comprises 200 ha and 12 ha of grass and maize, respectively. Both grass and maize are used to feed the dairy cows; grass undergoes grazing and cutting for silage, and maize is only cut for silage. The number of dairy cows in the farm is about 800 and the number of swines is around 5400. The average annual milk yield per dairy cow is about

10000 L milk yr^{-1}. Whereas the dairy cows spend around 7 months of the year grazing during most of the day, the swines are kept housed.

The soil is a poorly drained coarse clay and some of the plots often undergo compaction and flooding mainly due to high rainfall and intense grazing periods, enhancing denitrification losses (Estavillo *et al*., 1994).

The grass area is divided into 12 plots in which different manure and fertiliser amounts are applied. The application of manure in time is substantially affected by the volume of manure stored in the farm. The period in which this volume is largest is generally the winter period as the dairy cows spend most of the day indoors. The farm has as an open and impermeable lagoon (volume= 45000 m^3) to store the manure. During the year of the study 35000 m^3 of slurry from cows and 10000 of slurry from swines were surface-applied to maize and grass. Concentration of the applied manure total N ranged from 0.45 to 3.42 kg N m^{-3}.

6.3. Materials and methods

Two long-term grasslands plots (G1, G2) and a maize land plot (M) were selected for our study. Each plot was subject to different fertiliser management (Table 1 and Fig 1e-3e) and different physical characteristics: G1 was situated on a steep-sloped ground (10-20 % slope) and both G2 and M were on a flat ground.

Table 1. Fertiliser management (mineral and manure) in plots G1, G2 and M during the monitoring period.

	G1		**G2**		**M**	
Period	kg N ha^{-1}					
	mineral	manure	mineral	manure	mineral	manure
Autumn		62		205		
Winter		107		51		
Spring	75	280	61	106	85	967
Summer		60		65	149	
Total (annual)	75	509	61	427	234	967

Nitrous oxide fluxes were generally determined on a weekly and fortnightly basis at the same time of the day in order to minimise the impact of diurnal variation (Yamulki *et al.* 2001). Nitrous oxide was measured following the closed flux chamber technique (Velthof

and Oenema, 1995). The concentration of N_2O in the headspace was determined using a photo-acoustic infra-red gas analyser (Brüel and Kjaer 1302 Multi-Gas Monitor) after closing the flux chamber (internal diameter: 20cm, height: 15cm) at 0, 8, 16 and 24 minutes, N_2O emission rate was calculated from the change in concentration in the chamber over this time. The gas analyser was fitted with optical filters to selectively measure concentrations of N_2O, CO_2 and water vapour. Concentration of N_2O was compensated for interferences of CO_2 and water vapour. Six chambers per plot and sampling day were used for this purpose.

Subsequently, 6 soil samples from the chambers' locations were collected for mineral N content and moisture determination (expressed as % water-filled pore space: % WFPS) using 2.5 cm diameter x 10 cm length cores. Extractable soil NH_4^+ and NO_3^- were analysed as follows: 100 g moist soil for each sample was extracted with 200 cm^3 1M KCl and the soil suspension was then filtered (Whatman N° 1). The extracts were frozen until ready for analysis for NO_3^--N and NH_4^+-N using a segmented flow injection analyser (Alpkem 501).

Ammonium-N was determined by the Berthelot reaction, adapted for automated methods (Alpkem 1986, 1987). Nitrate-N was determined from a diazo-based colour reaction with nitrite, after passing the sample through a cadmium column, which reduced the nitrate to nitrite. Soil and atmospheric temperature was also recorded each sampling day. In order to minimize spatial variability among core-sets, the three soil samples were taken within a 10 cm distance of each other.

6.4. Results and discussion

The N_2O fluxes varied widely throughout the year at each plot. Nitrous oxide fluxes from individual chambers (data not shown) ranged from 0 to 585, 430 and 849 g N_2O-N ha^{-1} d^{-1} for G1, G2 and M plots, respectively. Seasonally these fluxes ranged from 0 to:

(i) 585, 430 and 623 g N_2O-N ha^{-1} d^{-1} for G1, G2 and M plots, respectively (autumn).

(ii) 48, 147 and 6 g N_2O-N ha^{-1} d^{-1} for G1, G2 and M plots, respectively (winter).

(iii) 37, 328 and 172 g N_2O-N ha^{-1} d^{-1} for G1, G2 and M plots, respectively (spring).

(iv) 58, 170 and 849 g N_2O-N ha^{-1} d^{-1} for G1, G2 and M plots, respectively (summer).

Variability in daily N_2O emission rates (mean of 6 chambers) was generally large in the 3 plots as shown by the standard error bars in Fig 1a, Fig 2a and Fig 3a.

Each plot had different seasonal response to N_2O emissions and hence showed peaks (> 50 g N_2O-N ha^{-1} d^{-1}) at different times of the seasons. In plot G1 N_2O fluxes peaked at the end of summer to end of autumn period; in plot G2 the largest N_2O emission rates occurred at autumn but peaks also occurred during spring, summer and winter; in plot M, however, the largest N_2O emission rates were measured during Summer time. Peaks, though smaller than that found in summer, were also found in spring and autumn.

Mean daily N_2O emissions from the 3 plots were firstly integrated over the 4 seasons (seasonal cumulative emissions) and subsequently, over the whole year (annual cumulative emissions). Results are shown in table 2. The maize plot (M) resulted in greater annual N_2O cumulative emissions (21.7 kg N_2O-N ha^{-1}) than any of the grassland plots (18.4 and 7.4 kg N_2O-N ha^{-1} from G2 and G1, respectively). This would represent 1.3%, 3.8% and 1.8% of the total fertiliser N applied in G1, G2 and M, respectively. Seasonally, although in autumn and winter the greatest N_2O emissions occurred in the grassland plots, in spring and summer the greatest N_2O emissions were found in the maize plot. Measured soil parameters (i.e. temperature, % WFPS, NO_3^- and NH_4^+) varied seasonally and were affected, as expected, by rainfall events, air temperature and fertiliser management (inorganic and manure).

Table 2. Cumulative N_2O emissions per plot and per each season of the year.

	G1	**G2**	**M**
Period		kg N_2O-N ha^{-1}	
Autumn	3.6	7.5	1.6
Winter	1.0	2.4	0.7
Spring	1.1	3.9	5.8
Summer	1.6	4.5	13.6
Total (annual)	7.4	18.4	21.7

Soil temperature ranged from 4 ºC to 22.4 ºC in the three plots (Fig 1c, 2c and 3c). Plot G1 generally showed lower soil temperatures than G2. This fact is probably due to the North and South orientation for G1 and G2, respectively. Soil temperature remained below 15 ºC all along the year except from end of spring to beginning of autumn.

Values from 14 to about 100 % WFPS were recorded in the first 15 cm of the soils (Fig 1c, 2c and 3c). Plots G1, G2 and M ranged from 14 % to 76 %, 22 % to 68 % and 45% to 100 % WFPS, respectively (Fig 1c-3c). In plot G1 while soil moisture content from mid autumn to

mid spring ranged between 60-80 % WFPS, it, however, never exceeded 40 % WFPS during the rest of the year, being particularly dry (<33 % WFPS) during summer time (Fig 1c). Plot G2 showed similar seasonal soil % WFPS patterns than G1 but soil was generally drier (i.e. soil moisture from mid autumn to mid spring ranged between 55 and 65 % WFPS) than in G1 (Fig 2c), which may be partially explained by the greater soil temperatures found in G2 compared to G1. Plot M (Fig 3c), however, showed waterlogged soil during autumn and winter (>80 % WFPS), wet soil (60-70 % WFPS) during spring to mid summer and moderately wet soil (50-60 % WFPS) due to the application of dirty water from mid summer to autumn.

Nitrate concentration in chamber soil samples had large variability during the year, ranging from 1 to 336 kg NO_3^--N ha^{-1}. Mean NO_3^- concentration in the soil (average of 6 chambers per plot) ranged from 2 to 29, from 2 to 71 and 3 to 276 kg NO_3^--N ha^{-1} for G1, G2 and M, respectively (Fig 1d, 2d and 3d). Variation within plots was generally large as shown by the standard error (SE) bars in Fig 1d, 2d and 3d. Seasonally, all plots (G1, G2 and M) showed small values of soil NO_3^- content (< 10 kg NO_3^--N ha^{-1}) from autumn (with exception of the beginning of autumn) to middle spring and generally values greater than 20 kg NO_3^--N ha^{-1} for the rest of the year (Fig 1d, 2d and 3d).

Largest soil NO_3^- values were found during the period middle spring-beginning of autumn and in the in the first summer half period for the grasslands (G1 and G2, Fig 1d and 2d) and maize (M, Fig 3d), respectively.

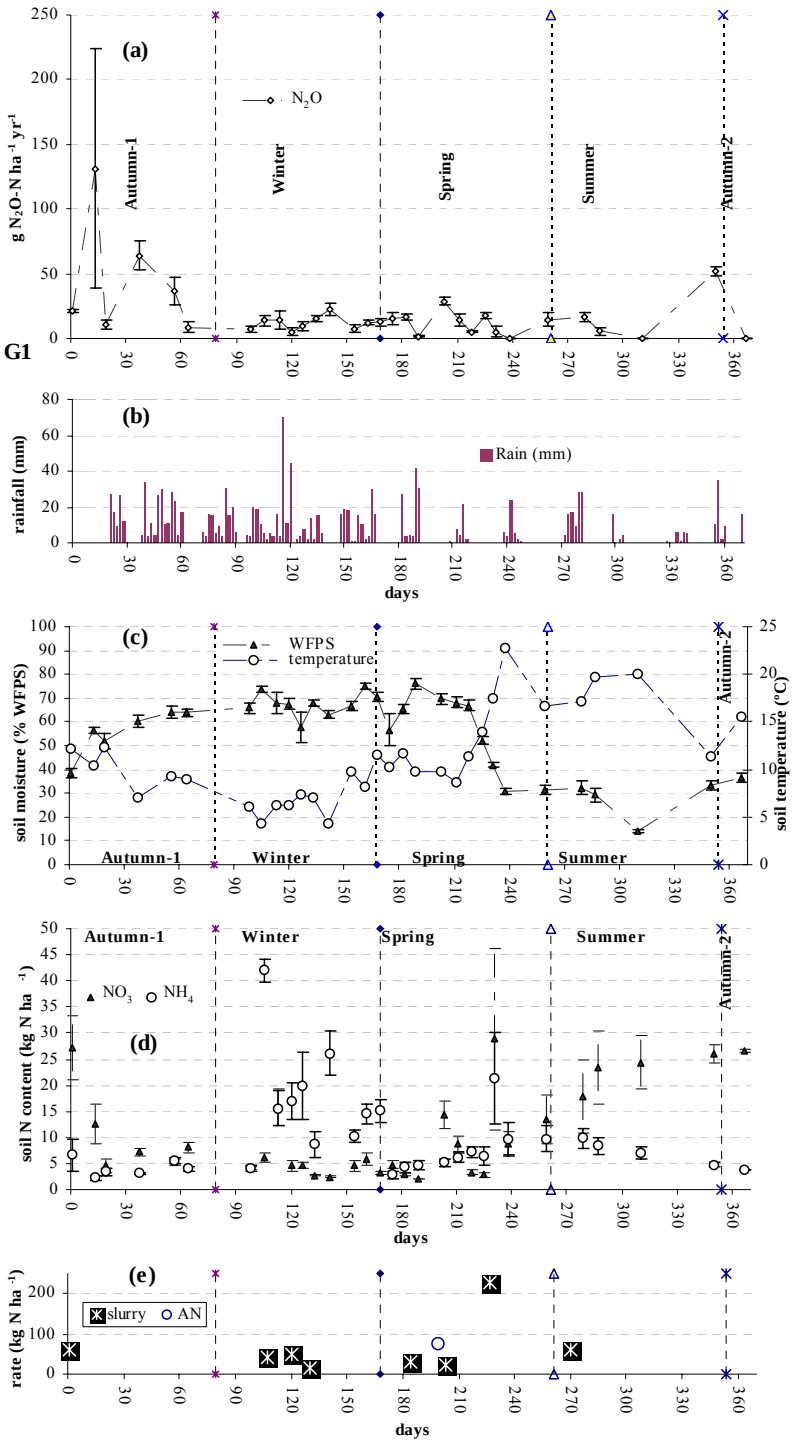


Figure 1. Seasonal evolution of mean N_2O fluxes (a), rainfall (b), soil %WFPS and temperature (c), NO_3 and NH_4 soil content (d) and fertiliser application rates (e) in G1. Vertical bars show standard errors (SE).

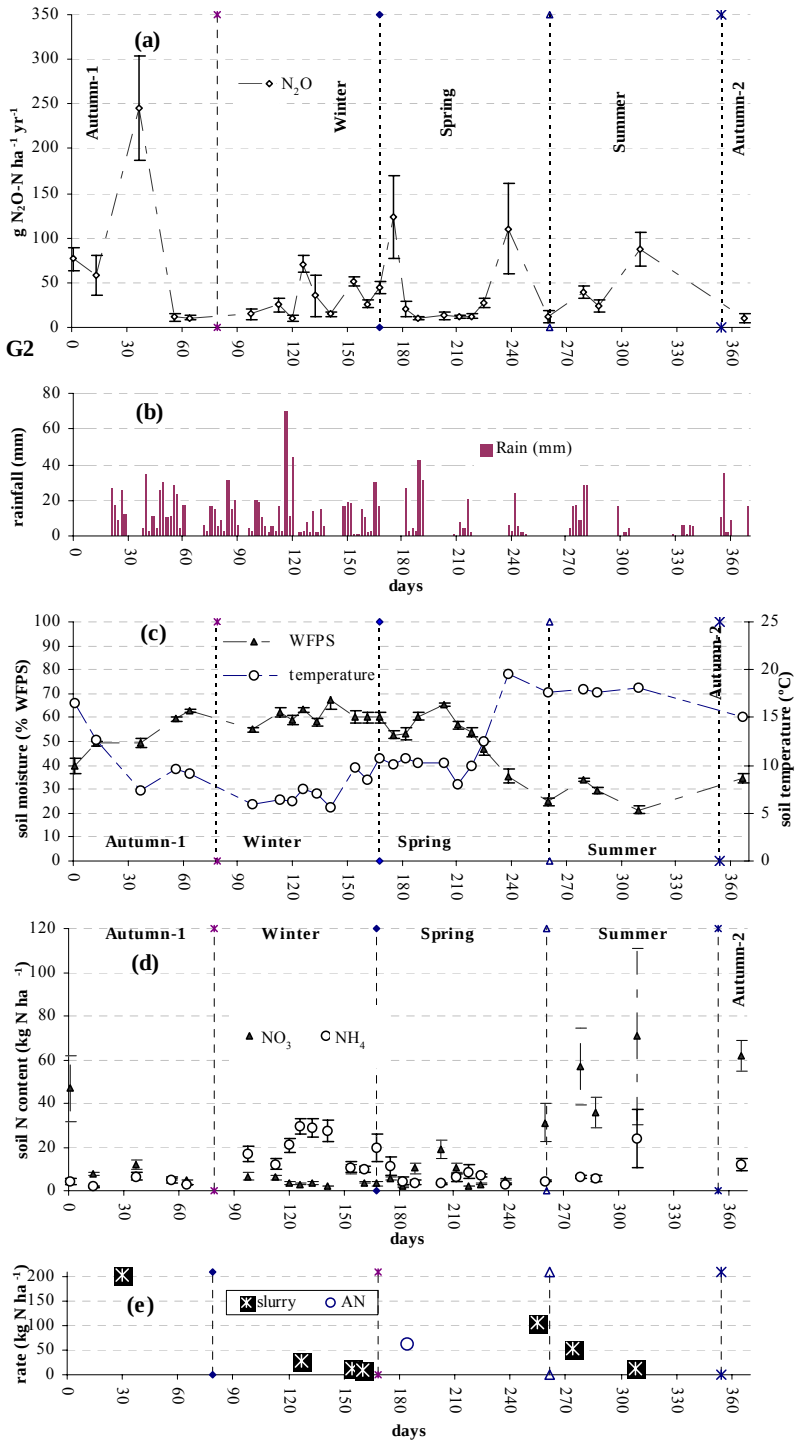


Figure 2. Seasonal evolution of mean N_2O fluxes (a), rainfall (b), soil %WFPS and temperature (c), NO_3 and NH_4 soil content (d) and fertiliser application rates (e) in G2. Vertical bars show standard errors (SE).

Ammonium concentration in soil samples had large variability during the year, ranging from

1 to 126 kg NH_4^+-N ha^{-1}. Mean NH_4^+ concentration in the soil ranged from 2 to 42, 2 to 30 and from 1 to 64 kg NH_4^+-N ha^{-1} for plots G1, G2 and M, respectively. Variation within plots, similarly to what we found for NO_3^-, was generally large as shown by the standard error (SE) bars in Fig 1d-3d. Seasonally, grassland plots (G1 and G2) showed small values of soil NH_4^+ content (< 10 kg NH_4^+-N ha^{-1}) from spring to winter time (with an exception of plot G2 in the middle of summer) and generally values greater than 15 kg NH_4^+-N ha^{-1} during the winter period (Fig 1d-2d). The maize plot (M), however, showed large values (> 15 kg NH_4^+-N ha^{-1}) of soil NH_4^+ content from half spring to half summer (Fig 3d).

As expected, N_2O emission rates from the different plots were greatly affected by fertiliser management and climatic conditions. In G1, the greatest N_2O emission rates (N_2O>50 g N_2O-N $ha^{-1}yr^{-1}$) occurred during the period end of summer-mid autumn (Fig 1a). During this period soil NO_3^- content (denitrifiable N) was the only measured factor which was consistently large. For instance, although large N_2O fluxes were measured during autumn-1 probably as a result of high NO_3^- values in the soil and prone-to-denitrification soil moisture content (60 % WFPS, Fig 1c), large fluxes were also measured in autumn-2 under much drier conditions (30 % WFPS) and with low values of NH_4^+, which rule out the possibility of these fluxes having been produced by nitrification. Moreover, large amounts of slurry and AN were applied in winter-spring and none resulted in large N_2O emissions.

In winter slurry contribution to the mineral N pool in the soil is reflected by the significantly (data not shown) high values of NH_4^+ content in the soil (Fig 1d). These values together with low temperatures and large soil moisture content (Fig 1c) resulted in small N_2O emissions (N_2O<25 g N_2O-N $ha^{-1}yr^{-1}$, Fig 1a) and the NH_4^+ content subsequently was depleted in early spring either by volatilisation, leaching or plant uptake.

In spring mineral fertilisation did not result in large fluxes, even though the soil was at a prone-to-denitrification soil moisture content (60 % WFPS, Fig 1c). Again, NO_3^- lost through leaching or taken up by the grass might have been the place sink of this N. The latest slurry application in summer resulted in a built-up of NO_3^- in the soil, possibly as a result of low emissions by denitrification, low NO_3^- leaching lost and a slow grass growth due to summer draught. In response to rainfall and thus higher WFPS, N_2O emissions increased at the end of summer (Figure 1a, b, c and d). In G2 whereas large NO_3^- content values (> 10 kg NO_3^--N ha^{-1}) in autumn and summer and large soil NH_4^+ content (> 20 kg NH_4^+-N ha^{-1}) in

winter resulted in peaks of N_2O fluxes (Fig 2a, Fig 2d), they did not appear to affect those peaks found in spring. Soil moisture content did not appear to consistently affect N_2O emissions throughout the study.

Autumn applications of slurry did not result in large amounts of measured NH_4^+ or NO_3^- in the soil. However, large N_2O fluxes were found during autumn-1 period after application of slurry. We may, therefore, think that partly soil NO_3^- and NH_4^+ was leached and partly denitrified, this denitrification occurring at a threshold of NO_3^- content around 10 kg NO_3^--N ha^{-1}.

Winter applications of slurry resulted in a build-up of NH_4^+ in the soil probably due to a slow nitrification process as temperatures were low during this time (Fig 2c). However, N_2O fluxes appeared to be a consequence of using these high values of NH_4^+ in the soil. Mineral fertiliser during spring did result in increased values of NO_3^- soil values but not on high N_2O values.

Summer slurry applications, in contrast, had a large effect on the build-up of both NO_3^- and NH_4^+ in the soil, which may be due to slow plant growth at summer draught conditions. However, an N_2O peak was found at very low soil moisture content, which does not fit the N_2O dependencies pattern. In plot M, large N_2O emission rates (N_2O>100 g N_2O-N $ha^{-1}yr^{-1}$) during half spring to half summer (Fig 3a) resulted from high levels of NO_3^- (> 70 kg NO_3-N ha^{-1}) and NH_4^+ (> 40 kg NH_4^+-N ha^{-1}) content in the soil (Fig 3d) and wet conditions (%WFPS= 50%-70%), (Fig 3c). Very large slurry and urea application rates (>1000 kg N/ha, Table 1) during this period resulted in an increased amount of NO_3^- and NH_4^+ build-up in the soil. Plant N requirements for maize growth were substantially exceeded and possibly, not only did that result in large N_2O losses but also great NH_3, N_2 and leaching losses.

Leaching (in G1 and G2) and run-off (only in G1) sampling was carried out at the same time that this N_2O monitorisation was taking place and although there are no sufficient data on the water balance to give total N loads lost weighted average of sample concentrations and estimated drainage may shed some light on the importance of these losses. Assuming that the estimated drainage volume could be in the range of 400-600 mm (del Hierro, *pers commun.*) and having measured concentrations of NO_3^--N in the leachate from 1 to 6 mg NO_3^--N l^{-1} and from 19 to 27 mg NO_3^--N l^{-1} in G1 and G2, respectively and 1 to 120 mg NH_4^+-N l^{-1} and 1 to 95 mg NO_3^--N l^{-1} in run-off in G1 (del Hierro, *pers commun.*) leaching

and run-off losses are likely to have been substantially large.

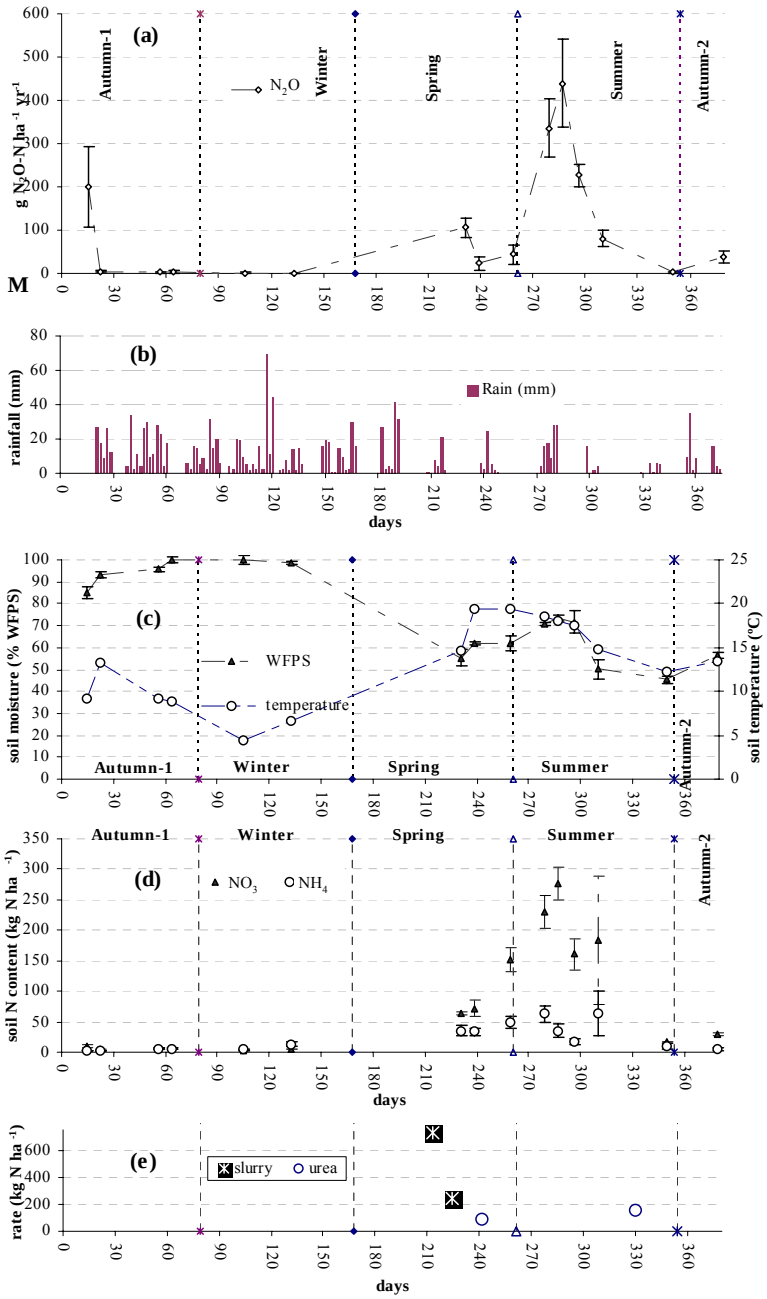


Figure 3. Seasonal evolution of mean N_2O fluxes (a), rainfall (b), soil %WFPS and temperature (c), NO_3 and NH_4 soil content (d) and fertiliser application rates (e) in M. Vertical bars show standard errors (SE).

For each plot and for the 3 plots as a total, coefficients of determination (R^2) (S.E = 1.1, 95 % confidence) were determined for the relationship between average N_2O emissions over soil water content (%WFPS), soil temperature, soil NO_3^- content and soil NH_4^+ content

(Table 3). We Ln-converted N_2O emissions as N_2O emissions have been described to follow Ln-normal distributions (Velthof *et al.,* 2000; De Klein *et al*., 1999).

Table 3. Determination coefficient values (R^2) of N_2O fluxes with: WFPS %, soil temperature, NO_3^- content and NH_4^+ content for all the soils and for the dry and wet range of soils. (α= 0.05)

		Plot		
Factor	**G1**	**G2**	**M**	**Total**
WFPS (%)$^{\partial}$	0.15	0.12	0.61	0.26
Soil Temperature	0.01	0.06	0.46	0.10
NO3- content	0.02	0.01	0.39	0.17
NH4+ content	0.04	0.01	0.19	0.06

$^{\partial}$Quadratic fit applied

Whereas the relationships between N_2O and soil temperature, NO_3^- and NH_4^+ were fitted to linear equations, that resulting between N_2O and %WFPS was fitted to quadratic equations (del Prado *et al.,* 2006b). Coefficients of determination were low (R^2<0.20) for G1 and G2 (Table 3) and thus, small ability to predict the effect of these factors on N_2O emission rates is expected. The grassland results are in line with literature values (Aulakh *et al.,* 1992; Bronson and Mosier, 1993; Thornton *et al*.,1996; del Prado *et al.,* 2006b).

The maize (M) plot, on the other hand, showed good fit between %WFPS (R^2>0.60) and soil temperature (R^2>0.45) and N_2O emission rates (Table 3). Graphs were drawn to show the fitted relationship between N_2O emissions and %WFPS (Fig 4a), soil temperature (Fig 4b), soil NO_3^- (Fig 4c) and soil NH_4^+ (Fig 4d).

Figure 4a showed that with increasing soil water content (% WFPS), N_2O emissions also increased until the soil water content reached approximately 70 % WFPS. Above this soil water content, N_2O emissions decreased with increasing soil water content. This response is similar to that found in other studies (i.e. Schmidt *et al.*, 2000; del Prado *et al*., 2006b). The most probable explanation in term of processes occurring is that N_2O emissions increased to a level where simultaneous denitrification and nitrification are at their maximum (75 %WFPS). Above this soil water content, denitrification was the main process producing N_2O and, as the soil became more anaerobic, emissions of N_2 became greater than those of N_2O. Increasing temperatures in the soil (Fig 4b) considerably increased the N_2O emission rates

(from 10 to 20 ºC, $Q_{10} \approx 5$) from a threshold temperature value (10 ºC). This relationship is stronger than that found by maize studies elsewhere (i.e. Meng *et al*., 2005).

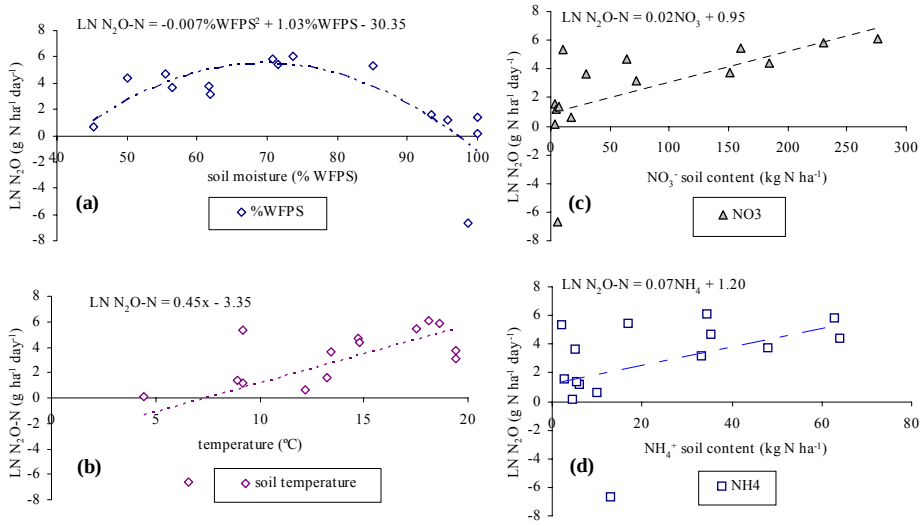


Figure 4. Fitted equations between average LN-N_2O emissions and (a) soil moisture content (% WFPS), (b) soil temperature, (c) NO_3^- soil content and (d) NH_4^+ soil content.

The fact that both NO_3^- and NH_4^+ in the soil showed weak correlation with N_2O emissions and the fact that large N_2O emissions did not necessarily occurred when mineral N pool was substantial suggest that NO_3^- and NH_4^+ in the soil thresholds values for denitrification to be produced may be smaller and thus less important controlling N_2O emissions than soil water content and temperature.

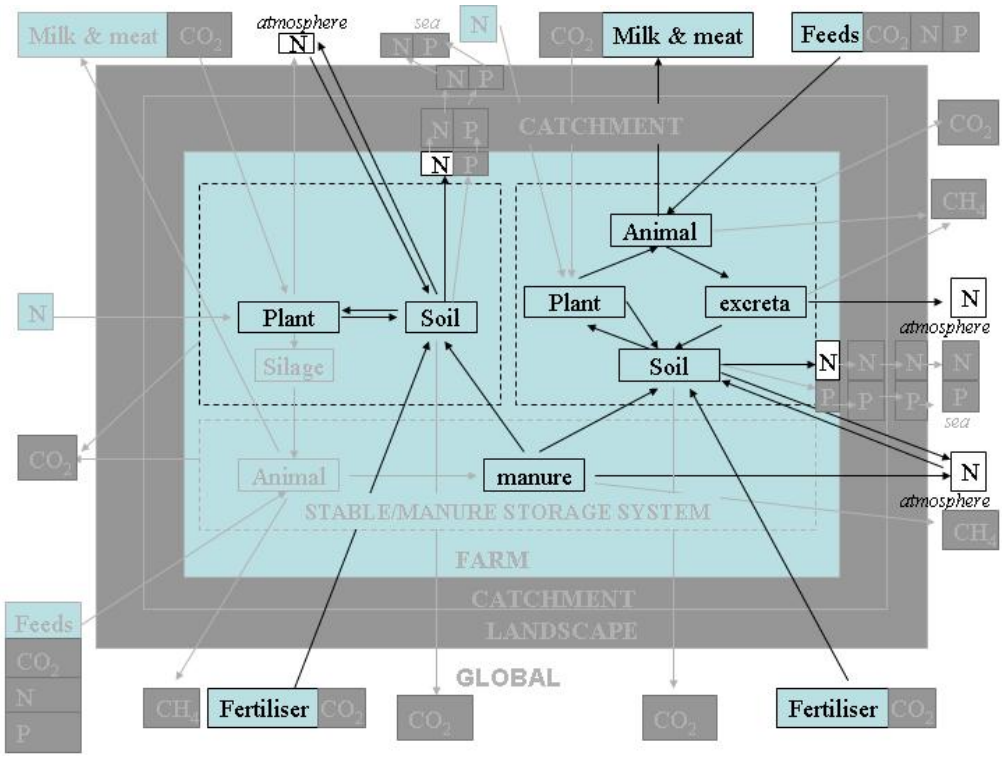
6.5. Conclusions

The poor statistical significance of these results from the grazed fields supports the idea that there is a need to improve techniques to overcome the large spatial variability of grazed grass soils. Results of N_2O emission from the maize plot, however, resulted in significant statistical relationships between N_2O emission and %WFPS, soil temperature and NO_3^- and NH_4^+ concentration in the soil. The relationship between N_2O emissions and %WFPS was fitted to a quadratic equation, allowing us to adapt an Ef for this kind of soil management in

our conditions. Although incorporation of seasonality as a factor to estimate N_2O emissions will account for part of the temporal variability of N_2O fluxes from grazed grass, there is still a need to address and quantify the effect of spatial variability on grazed fields.

Chapter 7

NGAUGE: a decision support system to optimise N fertilisation of British grassland for economic and/or environmental goals.



7. NGAUGE: a decision support system to optimise N fertilisation of British grassland for economic and/or environmental goals

Abstract

The poor efficiency with which nitrogen is often used on grassland farms is well-documented, as are the potential consequences of undesirable emissions of nitrogen. As fertiliser represents a major input of nitrogen to such systems, its improved management has good potential for increasing the efficiency of nitrogen use and enhancing environmental and economic performance. This paper describes the development, structure and potential application of a new Decision Support System for fertiliser management for British grassland. The underlying empirically-based model simulates monthly nitrogen flows within and between the main components of the livestock production system according to user inputs describing site conditions and farm management characteristics. The user-friendly Decision Support System ('NGAUGE') has a user interface that was produced in collaboration with livestock farmers to ensure availability of all required inputs. NGAUGE is an improvement on existing nitrogen fertiliser recommendation systems in that it relates production to environmental impact and is therefore potentially valuable to policy makers and researchers for identifying pollution mitigation strategies and blueprints for novel, more sustainable systems of livestock production. One possible application is the simulation of the phenomenon of pollution swapping, whereby, for example, the adoption of strategies for the reduction of nitrate leaching may exacerbate emissions of ammonia and nitrous oxide. Outputs of the Decision Support System include a field- and target-specific N fertiliser recommendation together with farm- and field-based N budgets, comprising amounts of N in both production and loss components of the system. Recommendations may be updated on a monthly basis to take account of deviations of weather conditions from the 30-year mean. The optimisation procedure within NGAUGE enables user-specified targets of herbage production, N loss or fertiliser use to be achieved while maximising efficiency of N use. Examples of model output for a typical grassland management scenario demonstrate the effect on model predictions of site and management properties such as soil texture, weather zone, grazing and manure applications. Depending on existing management and site

characteristics, simulations with NGAUGE suggest that it is possible to reduce nitrate leaching by up to 46%, (compared with a fertiliser distribution from existing fertiliser recommendations), and fertiliser by 33%, without sacrificing herbage yield. The greatest improvements in efficiency are possible on sandy-textured soils, with moderate N inputs.

7.1. Introduction

Experimental evidence, collected over the last 3 decades, of nitrogen (N) emissions from grassland (Ryden, 1981, 1984; Scholefield *et al*., 1993) has demonstrated the inefficiency with which N is frequently used. The loss of N has both economic and environmental consequences. The N loss pathways of primary concern to society are nitrate leaching and emission of the gases nitrous oxide (N_2O) and ammonia (NH_3). The increase in nitrate concentration in water bodies in recent decades has been a cause of concern because of the perceived potential threat to human health and because of the ecological and aesthetic consequences of eutrophication. In the UK, agriculture is the main source of nitrate in most UK rivers and groundwaters (Powlson, 2000) and is estimated to account for 69% of the emission of N_2O (Salway *et al.,* 2001), which contributes both to global warming and to the depletion of the stratospheric ozone layer. Ammonia emission and subsequent deposition may contribute to water and soil acidification (van Breemen *et al*., 1982) and is one of the main sources of the increased N supply to natural areas that may cause eutrophication of terrestrial and aquatic ecosystems (Isermann, 1990).

It has been shown (Scholefield *et al.,* 1991) that there is a strong linear relationship between total annual inorganic N input to a grassland system and percentage recovery of that N by plants, such that in systems of low N flux, a larger proportion of the total N is recovered by the plant than in systems of higher N flux. Agricultural systems can be manipulated to changed efficiency simply by increasing or decreasing N input. Additionally, efficiency of plant uptake of N changes seasonally with weather and soil conditions and with physiological traits of the plant. Nitrogen fertilisers are the major N input to a typical dairy farm in the UK, comprising as much as 74% of the total N input (Jarvis, 1993), and are the input to the grassland N cycle that is most easily managed. It appears that there is much

potential, therefore, to manipulate the efficiency of the system by appropriate management of fertilisers. However, simply reducing the fertiliser N input moves the system along the established efficiency relationship, and although losses can be reduced, production is also compromised. The challenge lies in the development and implementation of a system which lies above this line, i.e. is genuinely of greater N efficiency for the same total flux of N. This will involve both temporal and quantitative adjustment to fertiliser patterns.

Fertiliser recommendations for N have been produced in a similar format for England and Wales since 1973. With the exception of the most recent edition, recommendations have given little or no consideration to the potential environmental impacts of N application and have been rather generalised in relation to site variables. In the current version (RB209, MAFF, 2000), there is more site-specificity, in terms of soil types (3 classes), rainfall (3 classes) and previous management and N use. Although the publication points out the importance of achieving the right balance between profitable agricultural production and environmental protection, it also states that *'the primary aim of the recommendations is to maximise the economic return from the use of fertilisers'*. Improvement of the current UK recommendation system to effect improvements in efficiency would necessitate a change in emphasis from production/economic targets to a system driven, to a greater degree, by limitation of the undesirable exports: nitrate lost to surface water and N_2O and NH_3 emitted to the atmosphere. The application of such an approach would be especially beneficial in areas of particular sensitivity such as Nitrate Vulnerable Zones (NVZs, implemented under the Nitrates Directive, 91/676/EC), where the nitrate concentration of water draining from farmland is a fundamental consideration in the selection of agricultural management. The improved recommendation would seek to strike a compromise between production and environmental impact since the farmer still needs to achieve an acceptable level of income.

The objective of the research presented in this paper was to produce a recommendation system which would enable the efficiency of N use in grassland fields to be improved, by calculating the optimal temporal distribution of N fertiliser for a given field. In order to achieve this aim, a decision support system (DSS), NGAUGE, was developed, to provide field-specific monthly N fertiliser recommendations, which improve the efficiency with which N is used, for user-specified targets. This necessitates simulating flows of N on a site-specific basis, with sensitivity to climate, soil properties, sward management and on-going

weather, and the development of the means of determining the best distribution of fertiliser N through the year to improve the efficiency of N use.

7.2. Model development

An existing empirically-based model of N cycling in grassland soils, NCYCLE, (Scholefield *et al.*, 1991) was taken as the basis for the new model and DSS. NCYCLE is an annual, empirical model, based on published multi-site grassland data sets and has, since its creation, been validated for many of its key components (Rodda *et al*., 1995). NCYCLE simulates N flows through the major processes of N transformation in the soil and therefore links the input, production and loss components of the system. Sensitivity to soil properties, sward management and weather already exist within NCYCLE, although the latter is not sufficiently detailed for the purposes of the DSS development. NCYCLE is an annual model and therefore does not have the appropriate temporal resolution for prescribing fertiliser recommendations. The submodels within NGAUGE therefore calculate N cycling through N components and processes on a monthly basis. In addition, there are 5 main areas in which NGAUGE extends the capabilities of the original NCYCLE model:

(1) Inclusion of an optimisation procedure to recommend a fertiliser amount and distribution according to criteria of herbage production and N losses to the environment.
(2) Increased detail of average weather, and sensitivity to within-year ongoing weather
(3) Simulation of losses of NH_3 from, and mineralisation of applied organic manures, and consideration of the magnitude and timing of this source of N in calculating fertiliser recommendations.
(4) Provision of farm-gate N budgets (excluding import and export of animals).
(5) More detailed simulation of nitrification and denitrification to enable prediction of N_2O emissions separately from dinitrogen (N_2) and nitric oxide (NO).

7.2.1. Model components

7.2.1.1. Plant uptake

At different times in the growing season soil inorganic N is recovered by harvested herbage with contrasting efficiency. This was demonstrated in experiments such as those of Morrison *et al.* (1980) and Hopkins *et al.* (1990), in which equal amounts of fertiliser were applied in each time period (i.e. 'month'), giving a range of annual amounts of N of e.g. 0-750 kg N ha^{-1} $year^{-1}$. Plots were cut on a 4-weekly basis and N in herbage determined. These multi-site trials provide a source of information on N recovery at different rates of fertiliser N and at sites with different soil types and land-use histories. Data from these experiments were used to derive a set of curves (Fig 1), which describe the relationship between inorganic N flux (the sum of all the inputs to the soil) and plant N flux (including N in roots) for each month. Inorganic N includes N in fertiliser, N mineralised from soil organic matter and manures, N in urine (if grazed), N input from the atmosphere and 'carried–over' leachable N that was not leached in the previous month.

In order to calculate total N in plant from published data on N in herbage, assumptions were made about the *u* factor (defined in Scholefield *et al*., 1991 as the proportion of N in the whole plant that is harvested by the animal or by cutting).

There are few data to act as a guide to what the value of this factor may be. Parsons *et al*. (1983) report a value of 0.63 from measurements of carbon on continuously grazed pastures in south west England, which is similar to the value of 0.62 assumed for the NCYCLE model (Scholefield *et al*., 1991). Hanssen and Pettersson (1989), on perennial grassland leys, report values of 0.71 and 0.77, and Ourry *et al*. (1988) report values between 0.45 and 0.49.

In order for the criterion of annual mass balance to be satisfied, internal consistency between mineralisation, plant N uptake and losses must be observed. By assuming a monthly distribution for mineralisation (see section 2.1.3 below), the value of *u* and plant N in each month can be fixed from the herbage data. Existing datasets and systems simulations of NCYCLE were used to quantify *u* at a range of N input values. These data were then used to provide relationships between herbage N and *u* for each month.

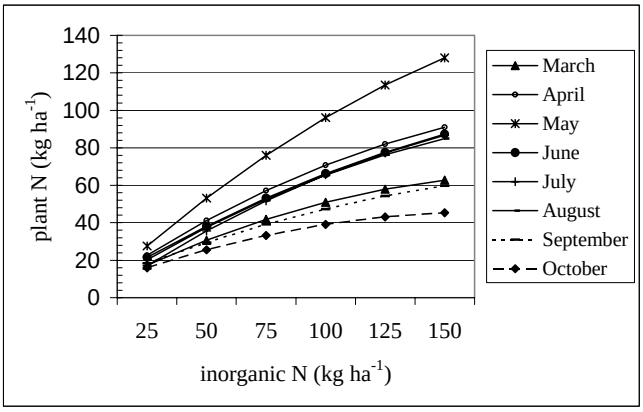


Figure 1. Monthly N uptake ('h') factors used in the optimisation process.

The values of *u* lie, for example in a 300 kg N ha^{-1} system between 0.2 (December) and 0.67 (June), with smaller values in winter months, when growth of the lamina region of the grass plant is limited, and large values in May and June, a time in which partitioning of N to the lamina and reproductive regions would be expected. From an N balance perspective, the lag between peak in herbage production (usually observed in May, particularly for cut systems) and mineralisation (frequently peaking in July or later) requires that a large proportion of the N taken up by the plant must be recovered in harvested material in the early summer months. The N uptake curves define the efficiency of the plant in recovering N in each month and are analogous to the annual '*h*' factor relationship used in NCYCLE. The comparison of these relationships between months is fundamental to the prediction of losses at each level of N input, and therefore to the operation of the optimisation procedure, described below.

The concentration of N in cut herbage was calculated using relationships between fertiliser N and %N in herbage, derived from Morrison *et al.* (1980). In the absence of better data for grazed herbage, the annual relationship used in NCYCLE was modified to produce a monthly relationship.

7.2.1.2. N cycling through the grazing animal

The amount of herbage N ingested by the animal is determined by the *u* factor for each month, as discussed above. The relationships used to calculate the partitioning of N within the animal into urine, dung and product were taken directly from Scholefield *et al.* (1991), and were based on empirical relationships describing the influence of herbage %N on N

partitioning. As with NCYCLE, it was considered that most of the urine N is mineralised within a few days, and therefore enters the inorganic N pool within the month of excretion. Twenty two % of the N in dung mineralises in each month (i.e. passes into the soil inorganic N pool), as discussed in Scholefield *et al.* (1991).

7.2.1.3. Mineralisation

Mineralised N was considered to be derived from 4 components: (i) the previous land use, (ii) the herbage production in the current year (iii) dung and (iv) applied manures. As in NCYCLE, the previous land use was categorised as long-term grassland, mixed ley and arable or long term arable. Annual starting values for each of these were determined from the zero N fertiliser plots of cut-plot experiments of Morrison *et al.* (1980) and Hopkins *et al.* (1990), assuming no N loss and that, on an annual basis, 0.62 of the N in the whole plant is harvested by cutting (as NCYCLE). The starting values were 134, 76 and 27 kg N ha^{-1} for long-term grassland, mixed ley-arable and long-term arable, respectively. These were then moderated by factors describing the effect of sward age, soil texture and drainage status. This annual total mineralised N was allocated to different months according to relationships describing the effect of soil moisture and temperature on mineralisation. For the former, it was assumed that mineralisation increases linearly between the soil's permanent wilting point and field capacity. This is supported by the work of Stanford and Epstein (1974), who found the highest N mineralisation between matric suctions of 0.3 and 0.1 bar (equivalent to 80-90% water-filled pore space), and that between this optimum range and 15 bars, there was a near linear relationship between mineralisation and soil water content. Reichman *et al*. (1966) report that ammonification and nitrification were almost directly proportional to soil moisture content at suctions of 0.2-15 bars.

For the effect of temperature on mineralisation, a factor was calculated based on a linear increase of mineralisation rate with temperature, between a minimum (zero) at $2^{o}C$ and a maximum (1) at $20^{o}C$. Macduff and White (1985) and Blantern (1991) support a linear relationship between mineralisation and temperature between 2 and $20^{o}C$ and 4 and $13^{o}C$, respectively. For each month, soil moisture content was calculated from soil moisture deficit (30 year average data for each zone and each month, see section 2.1.9), using algorithms supplied by the National Soil Resources Institute, which assume for each of the 5 textural

classes an effective depth of operation of the deficit, moisture content at field capacity and permanent wilting point, porosity and bulk density (C. Brown, *pers. comm*). Mineralisation from the current year's residues was calculated using empirically-derived functions, which relate monthly plant N to observed or estimated mineralisation. These values were then modified by factors which account for the effect of soil texture, drainage status, sward age and weather zone (using relationships with temperature and moisture as described above).

7.2.1.4. Denitrification

Denitrification was modelled as a function of soil inorganic N, water-filled pore space (WFPS) and temperature. WFPS was related to monthly denitrification using a relationship derived from the controlled laboratory experiments of Scholefield *et al.* (1997). Denitrification rate was assumed to increase linearly with temperature from 2 to 20°C. The relationship between temperature and denitrification rate has been found to be linear by Cho *et al.* (1979), between 2.7 and 20°C, and by Blantern (1991) between 7 and 16°C, although at higher temperatures (e.g. 15-35°C) a Q_{10} of 2 (i.e. a doubling in reaction rate for an increased temperature of 10° K) has been reported (Stanford *et al*., 1975). A rapid decrease in denitrification below 5°C has been observed (Bailey and Beauchamp, 1973), but minimum temperatures for denitrification may vary widely (Aulakh *et al*., 1992). Initially, the annual denitrification totals of NCYCLE were used together with weighting factors for soil texture, drainage status, temperature zone and rainfall zone to predict denitrification in each month. In order that denitrification could be calculated dynamically during the optimisation process (i.e. without recourse to annual totals) relationships were derived from these meta-data to predict denitrification from inorganic N in each month, retaining sensitivity to climate using the temperature and WFPS weighting factors described above .

In a monthly time-step model it is not possible to account for the effects of individual rainfall events, although it is widely recognised (Jarvis *et al*., 1991; Li *et al*., 1992ab) that the occurrence of rain events, and time since a rainfall event, may be major determining factors of denitrification rate, and that good relationships between denitrification rates and controlling variables may be obscured by the considerable temporal variation that occurs with denitrification.

7.2.1.5. N oxides sub-models

(i) N_2 and N_2O from denitrification

This sub-model was conceptually based on the "hole-in-the-pipe" model described by Firestone and Davidson (1989). This scheme postulates two levels of regulation for trace N-gas production: factors that control the rate of the overall process dictate the movement of N through the "process pipe" (denitrification and nitrification processes); and factors that control the partitioning of the reacting N species to NO, N_2O or N_2 (i.e. control the size of the holes in the pipe through which the different N-gases "leak").

In NGAUGE, N_2O and N_2 were assumed to be the only gaseous products of the denitrification process. Although NO has been proved to be produced during the microbial process of nitrification and denitrification (Firestone and Davidson, 1989), many studies have indicated that the NO gas does not constitute a major denitrification product (e.g. Anderson and Levine, 1986; Skiba *et al*.,1992; Neff *et al*., 1995; Parsons and Keller, 1995).

In order to predict N_2 and N_2O, the monthly values for denitrification were divided according to 3 factors: soil moisture content (WFPS), mineral N flux and mineralised N in the soil, using three functions to represent the effect of these factors on the N_2:N_2O ratio as proposed by Parton *et al*. (1996). The level of nitrate was expressed as mineral N in order to be compatible with the main model. Thus, the N_2:N_2O ratio was calculated as follows:

$$N_2 : N_2O = \min(Fr(\text{Min N}), Fr(\text{Mineralis})) * Fr(\text{WFPS}) \quad \textbf{(1)}$$

Where Fr(WFPS) is the effect of soil WFPS on the ratio, Fr(Mineralis) is the effect of mineralisation rate on the ratio and Fr(Min N) is the effect of mineral N level in the soil on the ratio.

(ii) N_2O and NO from nitrification

The monthly nitrification rate within NGAUGE was developed on the basis that the main substrates to be nitrified would be originated from the pools of ammonium (NH_4^+) mineralised from the organic matter (including excreta) and NH_4^+ from the mineral fertiliser.

The zero-order kinetics approach described by Gilmour (1984) was implemented into the model with the nitrification rate constant being a function of temperature and soil moisture. The functions were as follows:

$$\text{NIT rate} = K*[NH_4^+]_i \qquad K: (\text{month}^{-1})$$

(2)

$$\text{NIT rate} = (K_{maxW} *K/K_{max})*[NH_4^+]_i$$

(3)

Where NIT rate is nitrification rate (kg N ha^{-1} $month^{-1}$), $[NH_4^+]_i$ is the level of NH_4^+ in the soil at the beginning of the month and K/K_{max} and K_{maxW} are the soil temperature and moisture content factors, respectively, which affected the nitrification rate. The effect of temperature was modelled according to the Arrhenius equation.

K_{maxW} was derived from Macduff and White (1985), who used three different functions for soils under permanent wilting point, between permanent wilting point and field capacity and over field capacity.

From the predicted net nitrification pool, NO emissions were simulated on a monthly basis, following the approach of Davidson *et al.* (1993), in which NO fluxes are governed by the total amount of NH_4^+-N nitrified (nitrification), a factor describing the potential maximum percentage nitrified as NO (Max%NIT) and a modifier accounting for the soil moisture ($WFPS_f$) . The functions were as follows:

$$WFPS_f = 0.0181 *WFPS + 0.0165 \ (WFPS<55)$$

(4)

$$WFPS_f = -0.0667 *WFPS + 4.6667 \ (WFPS>55)$$

(5)

$$\text{NO (g N-NO ha}^{-1}\text{ month}^{-1}) = \text{Max\%NIT}*WFPS_f* \textit{NIT rate}$$

(6)

Nitrous oxide emissions from nitrification were calculated in the model following the approach of Mosier *et al.* (1983) who designed a simple mechanistic model to predict daily N_2O loss from soils from nitrification and denitrification. According to this study, the total amount of N_2O emitted from the nitrification process (N_2O_{nit}) is governed by the maximum potential rate of N_2O from nitrification, assumed in NGAUGE to be 110 g N $ha^{-1}day^{-1}$, based on maximum recorded field values (Yamulki *pers. comm.*), a normalised (0 to 1) factor accounting for the amount of NH_4^+ nitrified (*En*) and a soil moisture normalised (0 to 1) modifier (Eψ) as follows:

$$N_2O_{nit}\,(\text{g N ha}^{-1}\text{day}^{-1}) = 110 * E\psi * En \quad \textbf{(7)}$$

$$E\psi = 0.1 \text{ if RWC (water content)} = [0\text{-}4] \quad \textbf{(8)}$$

$$\text{Else} \quad E\psi = [(3/2 * \text{RWC}) - 5] * 0.1 \quad \textbf{(9)}$$

$$En = 1/(1 + 1.335 * e^{-1.24} * \text{NIT rate}) \quad \textbf{(10)}$$

Where RWC is the soil relative water content, which is equal to the difference between measured soil water content and soil water content at wilting point divided by the difference between soil water content at field capacity and the soil water content at wilting point.

7.2.1.6. Nitrate leaching

Leachable nitrate, peak and average nitrate-N concentrations are presented by the model on an annual basis. For each month, soil inorganic N flux was calculated as the sum of atmospheric input, mineralisation of soil organic matter, mineralisation of dung and manures, fertiliser, urine and ‘leachable N’ carried over from the previous month. From this total, uptake of N by the plant, NH_3 volatilisation and N lost by denitrification were subtracted. The fate of the remaining ‘leachable N’ depends on the month in question; for

January, February and December it was assumed that 'leachable N' contributes to the total annual leaching, and for other months it was passed to the succeeding month as a component of the inorganic N pool. In the growing season months, 'leachable N' is that which would be measured in the field as soil mineral N at the end of each month.

Peak and average concentrations of nitrate-N in leachate were calculated on an annual basis using the relationships derived by Rodda *et al.* (1995), which predict peak concentration from leached N, according to soil drainage and textural class (Fig 2), and average concentration from leached N and drainage class.

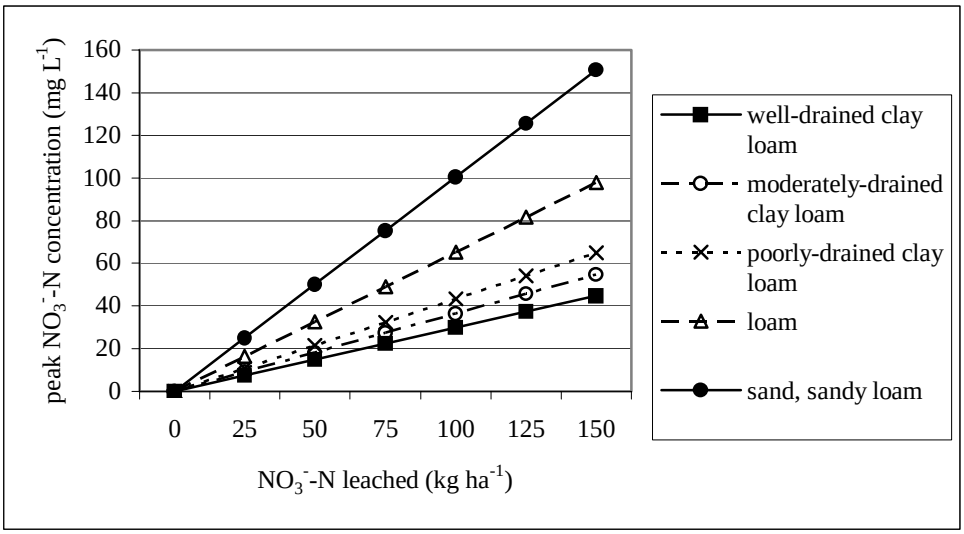


Figure 2. Relationships between nitrate leached and peak nitrate-N concentration (after Rodda *et al.* 1995).

7.2.1.7. Ammonia volatilisation

An NH_3 emission factor of 1.6% was suggested for ammonium nitrate (Van der Weerden and Jarvis, 1997), which is the most widely-used fertiliser N form in Great Britain. This factor is currently used in the UK ammonia emission inventory (Misselbrook *et al.*, 2000). It is generally the case that uniform emission factors are assumed across seasons (Pinder *et al.*, 2004) and there are insufficient data available to determine different empirical relationships describing ammonia emission in different months.

For NGAUGE, prediction of NH_3 volatilisation from fertiliser and its sensitivity to weather was achieved using the model of Misselbrook *et al.* (2004). In this model, it is assumed that

emission from ammonium nitrate fertiliser is moderated from a maximum value by temperature only. In NGAUGE, this gives emission factors ranging from 1.2% to 2.2% of applied N.

Emission of NH_3 from urine and dung deposited while grazing was calculated as 15% of urine and 2% of dung, as NCYCLE (Scholefield *et al*., 1991). Insufficient data were available with which to vary this factor by month or weather zone. For applied manures, emission factors for NH_3 volatilisation were determined according to the properties of the FYM or slurry, its application date and method of application (using data of Misselbrook *et al*., 2000). These emission factors range, for example, from 60% of applied N for dairy slurry with 10% dry matter, surface-applied in summer to 3% for dairy slurry with 2% dry matter, injected in winter.

7.2.1.8. Optimisation

The optimisation procedure is the means by which the best fertiliser distribution is calculated. There are two main concepts behind the operation of the optimisation procedure:

(i) Goal-seeking to a specified target

(ii) Satisfaction of optimisation criteria

The procedure was based on the set of monthly plant uptake (*h* factor) relationships, described above.

Initially, the average herbage N production of the farm is used as the target for the optimisation, but a field-specific target can be set by the user, and may be herbage N, N loss or fertiliser N. For one of these, the user selects the value desired (e.g. 300 kg herbage N ha^{-1}, 50 kg N ha^{-1} loss, or 300 kg N ha^{-1} fertiliser applied). The end point of the optimisation is achieved when the model reaches the target value, satisfying the optimisation criteria (Fig 3).

As the optimisation progresses towards its target, the optimisation criteria must be met in each iteration. The objective of the development of NGAUGE was to improve the efficiency with which N is used on grassland farms and the optimisation criteria were selected to reflect that. Three criteria are used, the one in operation in any given run is dependent on the target set by the user. All are a combination of maximising herbage and the efficiency ratio (ER), defined as kg N in herbage per kg N loss. These criteria may be combined in a number of ways that favour either one or the other, or treat them both almost equally, but their role in

the running of the model may be considered as outlined in Fig 3. While the optimisation criteria in run-time, and for the purposes of the ultimate end user, have been set, the procedure can be readily re-coded to enable other logical optimisation criteria to be met.

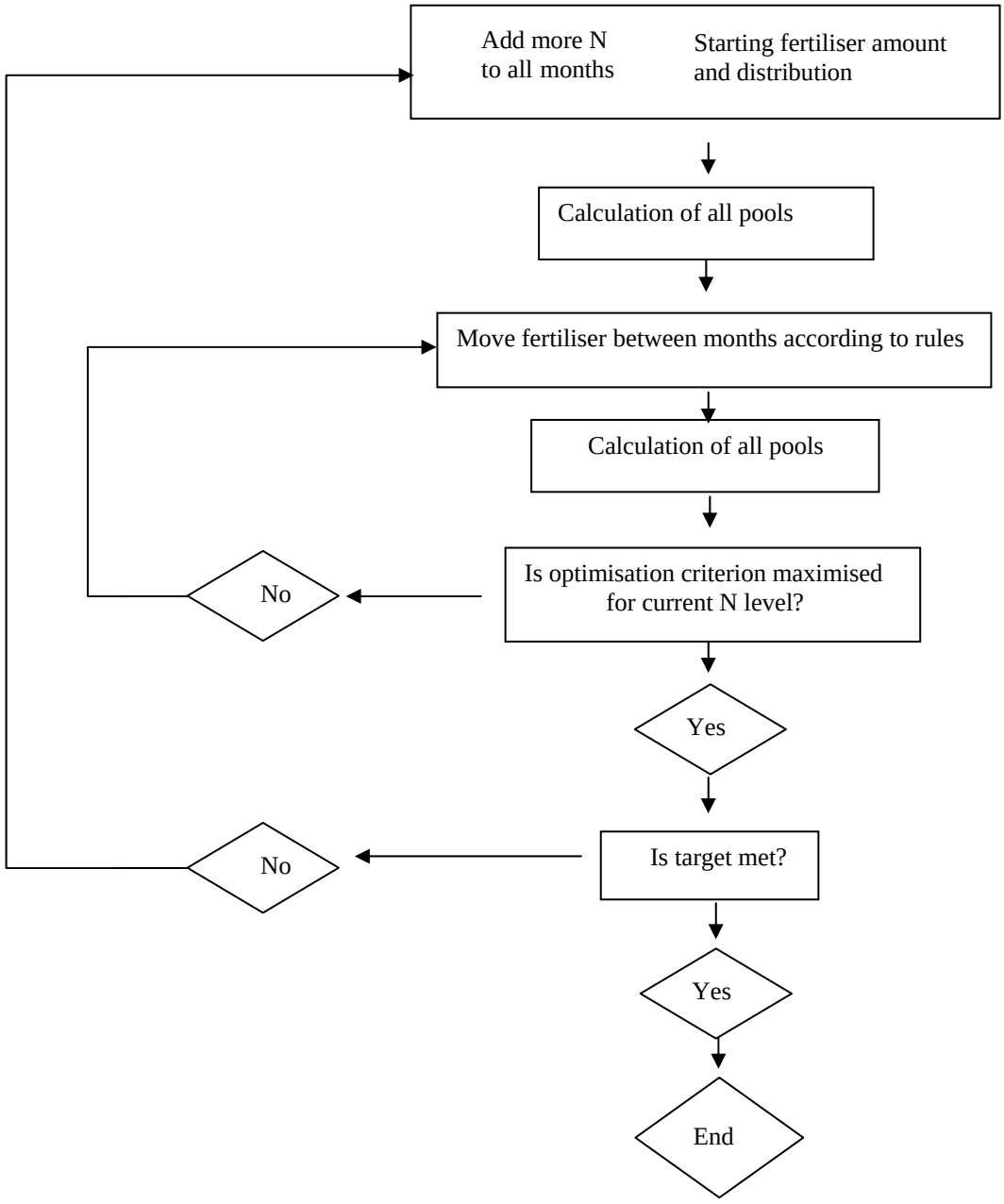


Figure 3. Outline of the operation of the optimisation process.

To begin the optimisation, an initial amount of fertiliser is allocated to all months and all pools are calculated (i.e. plant, herbage, product, mineralisation, denitrification,

volatilisation, leaching, urine, dung). Fertiliser is provisionally transferred between all combinations of months, the pools are re-calculated and the variables required for the optimisation criteria (currently herbage and ER) are compared. The pair of months (i.e. one donating and one receiving fertiliser) with the best combination of herbage and ER is identified and the transfer of N is effected. This new pattern of fertiliser is the 'optimal' distribution of fertiliser at this N level, but this fertiliser amount may be insufficient to achieve the specified target. If the target variable (e.g. herbage) has not yet met its target value, the procedure effectively returns to the top of Fig 3 and another unit of fertiliser is applied to all months.

7.2.1.9. Manure management

In order for N pools to be calculated, account must be taken of N supply from application of organic manures. Two slurry types and 2 farmyard manure (FYM) types are available for selection in NGAUGE, each associated with default values of ammoniacal N, organic N and total N following selection of dry matter content by the user. Following application of manure (with amount and month of application specified by the user), volatilisation of NH_3 is simulated. The remaining inorganic N from slurry or FYM (ammoniacal N – volatilised N) is assumed to enter the soil inorganic N pool in the month of application. The mineralisation of organic N in manure (transfer of N between the manure organic N and soil inorganic N pool) is simulated each month according to application date, C: N ratio (which is specified within the model according to manure type) and cumulative degree days above 5°C, according to the factors derived by Chadwick *et al.* (2000a).

NGAUGE has not been designed to optimise manure application dates and amounts because it is considered that this will be determined by fundamental constraints of the system, such as volume of slurry storage available and by legislation. However, the N from manure is taken into account when calculating an optimal fertiliser recommendation.

7.2.1.10. Weather

Location (i.e. weather) has a substantial effect on both the initial calculations of N pools and the outcome of optimisation for a particular target. In the initial run of NGAUGE, the weather is assumed to be 'average' for that location (rain and temperature zone). Thirty-year

average (1961-1990) weather data were obtained from 7 weather stations representing the range of agricultural weather conditions in Britain (Penecuik, High Mowthorpe, Waddington, Wattisham, Shawbury and Yeovilton). Data used were monthly total rainfall, monthly average daily temperature and soil moisture deficit, calculated for grass on a medium soil by the MORECS system (Thompson *et al.*, 1981). These data were allocated to zones so that rainfall, temperature and atmospheric input may be considered independently, thus increasing the complexity of the new model compared with NCYCLE. As with NCYCLE, there are 3 zones for atmospheric N input, setting values at 15, 25 and 35 kg N ha^{-1} but in the new model there are 6 zones for rainfall (based on average summer rainfall) and 6 zones for temperature, giving a total of 36 possible temperature/rainfall combinations.
Weather impacts on plant growth both directly and indirectly, through

(i) mineralisation (determining the supply of mineral N),
(ii) denitrification (influencing the amount of inorganic N in soil)
(iii) plant growth directly.

The effects of soil water and temperature on mineralisation and denitrification were described in section 2.1.3 above. For the effect of weather on plant growth, both temperature and soil moisture factors were considered. Plant N uptake was assumed to be limited by temperature according to a linear relationship between factors of zero at $5^{o}C$ and 1 at $20^{o}C$ (as Dowle and Armstrong, 1990). The effect of water availability was included by assuming that the growth factor was 1 at the moisture content at 2 bars of suction for each soil texture and 0 at the corresponding moisture content at 15 bars suction (permanent wilting point). Although water is considered available between suctions of 0.05 – 15 bars (Hall *et al.*, 1977), that held at suctions of less than 2 bars is generally considered easily available (Brady, 1984). Similar limitation factor approaches to the calculation of the effect of moisture on plant growth have previously been adopted. Dowle and Armstrong (1990), for example, assumed that maximum growth was possible between field capacity and wilting point, declining linearly outside this range to 0 at 100% soil moisture in the root zone and, at the opposite end of the range, at permanent wilting point.

Updating weather

Within an actual year of operation of the model, the observed N pools may be significantly affected by weather, and farmers may need to change their fertiliser management in the light of incident weather in order to achieve their specified targets. NGAUGE has sensitivity to on-going monthly weather in order to achieve these objectives, which impacts on 3 major sub-models: denitrification, mineralisation and plant uptake.

Using the 30-years' weather data described above, data were analysed for each rainfall and temperature zone, to produce 5 classes of data, representing the 10th, 30th, 50th , 70th and 90th centile. For the user, these centiles are accessed by the selection of weather categories for the preceding months (very wet, wet, average, dry and very dry for rainfall and very warm, warm, average, cold and very cold for temperature). These weather data, and denitrification and mineralisation factors derived from them are held in arrays and are used to recalculate pools from the beginning of the year to the end of the last full month before today's date. For example, for denitrification, arrays exist for temperature (of dimensions month, zone, centile) and water-filled pore space (of dimensions month, zone, centile, soil texture). To take an example of this, the 50th centile for a clay loam in zone 3 would give a water-filled pore space denitrification factor of 0.177, for the 10th centile this would be 0.02 and for the 90th centile 2.82.

Having re-calculated all pools according to the weather for the preceding months, the original recommendation (which was based on average weather) is updated to take account of the new weather information. This involves re-running the optimisation procedure. In this updating mode, although all months are included in the procedure and its calculations, movement of fertiliser can only take place between months that are forward of today's date (including the current month). Clearly, there are often cases in which it may no longer be possible to reach the user-specified target, particularly where this is related to loss. Achievement of the target may now be associated with different losses, different herbage total or different fertiliser totals, and it is necessary that the user is aware of this.

7.3. Model validation

The performance of NGAUGE was evaluated as assessment of the closeness of predictions and observations of N loss and transformation. Data from a purpose-built cut-plot experiment in mid Devon, UK were used to evaluate the predictions of NGAUGE against field measurements. The site was on an old sward (more than 20 years old) which had received moderate fertiliser additions for the past 13 years. The average annual rainfall was 1025 mm, 550 mm of which was in excess of evapotranspiration. The plots (each 10m x 3m) were laid out in a randomised design with their long axes aligned with the direction of slope (approximately 5°) and were hydrologically isolated to a depth of 30 cm with vinyl sheet. Drainage via runoff and lateral flow was channelled to tipping bucket flow monitors with flow proportional samplers (Scholefield and Stone, 1995). Half of the plots were re-seeded in the year prior to measurements, to provide a contrast in sward age. Three N treatments were applied, corresponding to approximately 230, 300 and 420 kg N ha^{-1} $year^{-1}$. Applications, as ammonium nitrate, were made monthly according to a pattern prescribed by the model. Mineralisation was determined on a monthly basis using the method of Hatch *et al.* (1990). Herbage was cut to 25 mm and weighed with a Haldrup forage harvester. Sub-samples were then dried in a forced draught oven at 85^oC for 18 hours and weighed. Goodness of fit of observed and predicted fluxes was assessed using the method of Whitmore (1991).

Measured mean values of net mineralisation were generally greater than those predicted by the model in both years, although due to the large variation in observations on each treatment, observed and predicted rates were not significantly different in 9 out of 12 treatment years. Dry matter yields were generally under-predicted in year 2, and over-predicted in year 1, suggesting that there is no systematic error in the model's predictions. Unusually low yields were observed in year 1 (e.g. less than 5 tonnes ha^{-1} $year^{-1}$ of dry matter from a fertiliser application of 350 kg N ha^{-1} $year^{-1}$) on the old sward, and the reason for this was not clear. Nitrate leaching was generally well predicted by NGAUGE: in 8 out of 12 cases, there was no significant difference between modelled and measured values. The good agreement between modelled and measured values is shown in Fig 4 (r^2 = 0.9). It appears (Fig 4) that NGAUGE may under-predict large values of leaching, but there are insufficient

points at the high end of the range to determine whether this is genuinely the case. Peak nitrate concentration was also well predicted, with no significant difference between modelled and measured values in 8 out of 12 treatment years.

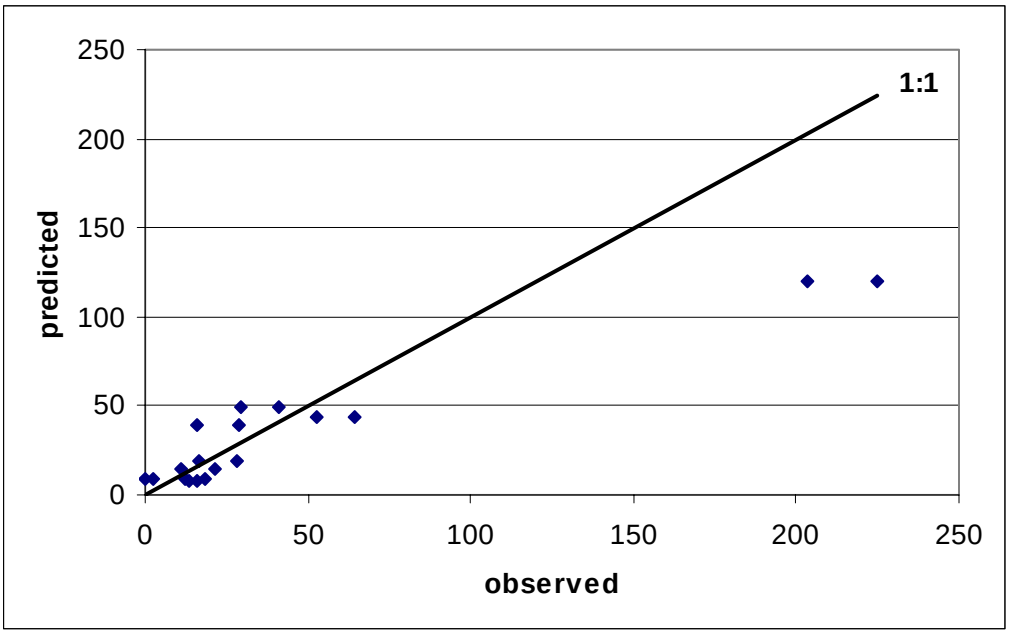


Figure 4. Comparison of observed and predicted annual nitrate leaching from a clay loam soil with six treatments of contrasting sward age and N input over two years.

7.4. User interface description

NGAUGE was programmed in Borland Delphi 5. This is an object-oriented language, which associates portions of code with 'events' that happen to objects (e.g. a click on the 'run' button). It was written in a modular structure, using procedures and functions that can be called from any part of the program.

The user-interface was designed and constructed in consultation with farmers, advisors, computer programmers and others with experience in DSS software development. User preferences suggested that a modular design with as few screens as possible should be aimed at. Thus, NGAUGE has 2 input and 3 output screens, each with logical positioning of check boxes, menus, edit boxes, tables and graphs. The first screen is used to enter generalised data about N use on the whole farm. From this, the model calculates the average N flows on the

farm and provides a target herbage yield as an initial basis for fertiliser optimisation on individual fields (output screen 1). It also calculates an N balance for the whole farm. This was included in order to give farmers a general appreciation of the magnitude of N inputs and losses on their farms, and the potential for improvement with optimisation. In the current stage of the DSS, it is based on the generalised data entered about the farm as a whole on input screen 1, and does not make calculations based on individual field inputs. The second input screen is used to enter data about individual fields for which optimised fertiliser patterns are required. Output screen 2 displays optimised and non-optimised N budgets according to target, with a facility to graph these, a histogram of the optimised fertiliser distribution and a means to alter the optimisation target (e.g. Fig 5). Output screen 3 is dedicated to updating the inputs and targets according to the weather experienced in each month in the year to date.

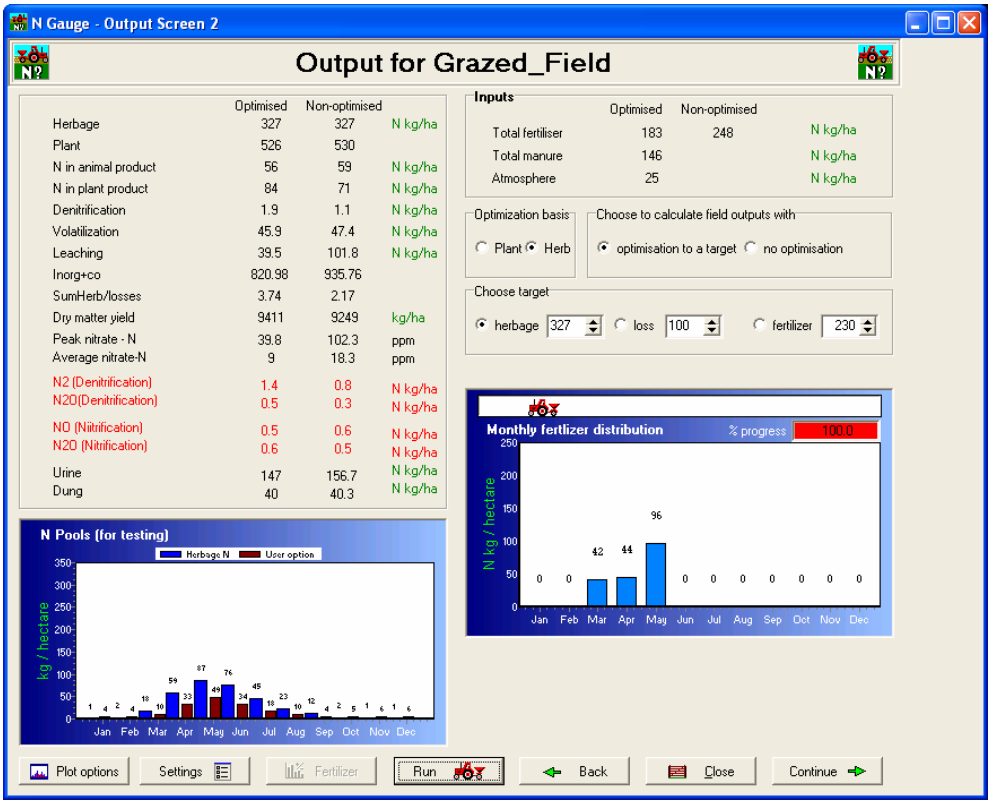


Figure 5. Example of NGAUGE output screen 2, showing output of a non-optimised field-based run at a fertiliser input of 248 kg N ha^{-1} and the corresponding optimised run using the same herbage N (327 kg N ha^{-1}) as a target.

7.5. Use of NGAUGE for prediction of existing and optimised N flows on livestock farms.

The degree to which optimisation is able to improve upon the predicted performance of a conventional system is dependent on the characteristics of the system (weather, soil type, fertiliser use etc.) and the optimisation performed. Some examples of NGAUGE runs are given below to exemplify its capability. For each scenario, the results from an optimised and non-optimised run are given. The conventional or non-optimised fertiliser distribution is based on MAFF (2000), for a fertiliser input of 300 kg N ha^{-1}.

7.5.1. Effect of soil texture

Soil texture exerts an important effect on N_2O, N_2 and NO losses by operating on both levels of regulation of N-gas products; it affects the process rate at which N is moving through the "pipe" (nitrification and denitrification net rates) and it controls the sizes of the holes through which the N-oxides "leak" (are transported to the atmosphere). In Table 1, non-optimised and optimised outputs are compared for a well-drained sandy loam and a poorly-drained clay loam soil, with the same management and climatic characteristics (11.5-12°C and 400-450 mm average growing season temperature and rainfall, respectively). The effect of soil texture may be seen by comparing Runs A and C, non-optimised runs for a sandy loam and clay loam, respectively.

Nitrous oxide and N_2 fluxes in the clay loam soil were much higher than in the sandy loam soil, reflecting the better diffusion of the gaseous N compounds with lower water-filled pore space. The simulated N_2O: N_2 from denitrification and NO: N_2O ratios in the sandy loam were greater (by factors of 1.6 and 63, respectively) than in the clay loam soil because of the enhanced water-filled pore space in the latter. Soil moisture governs whether nitrification or denitrification is the dominant process and strongly influences the corresponding turnover as well as the ratio of NO production over consumption rates. The slightly larger N_2O emission in optimised than non-optimised systems arises because the optimisation criteria are based on total N loss, rather than individual N loss processes. The effect is particularly apparent on well-drained soils, in which the largest component of loss is leached N.

For both soil textures, the efficiency with which the herbage yield was achieved (described

by ER) was improved by optimisation. For grazed systems (Table 1), greater reductions in losses were possible following optimisation on the sandy loam (Runs A and B) than clay loam (Runs C and D) systems (46% and 21% reduction in loss for the sandy loam and clay loam, respectively). On heavier-textured soils, denitrification is often the major route of N loss, and the period with greatest potential for denitrification coincides with the period for greatest potential for grass growth. The fertiliser distribution for maximum plant uptake is thus always compromised by the criterion that ER must increase when fertiliser is moved between months in the optimisation procedure.

In these grazed systems with higher N inputs and N returns from the grazing animals continuing into September, the recommended fertiliser distribution for the sandy loam soil at both locations becomes more polarised towards the beginning of the year (see Figure 6). The residual effects of these early applications will be carried through as soil mineral N into the later months. In the non-optimised system (Run A), leached N from the sandy loam site accounted for 33% of the fertiliser applied. This percentage was reduced to 19% for optimised systems on the sandy loam soil (Run B).

The fertiliser distribution from the optimisation was weighted more evenly through the growing season in the case of the clay loam soil, avoiding large applications in the period of maximum denitrification risk (March – May, Fig 6). For the sandy loam soil, the denitrification risk is smaller because of the relatively smaller retention of water within the soil. Fertiliser distribution can also be a major factor affecting the proportion of N_2 over N_2O that it is actually emitted to the air. Comparing two sandy loam soils with the same management characteristics in the same agroclimatic area but with a different fertiliser distribution (Runs A and B), NGAUGE predicted that a more temporally even fertiliser distribution (Run A) resulted in a lower N_2O: N_2 ratio (23 % smaller). This result agrees well with other studies (Firestone and Davidson, 1989). The optimisation process reduced the amount of fertiliser required to reach the herbage target by 9% and 18% for the grazed clay loam and sandy loam, respectively.

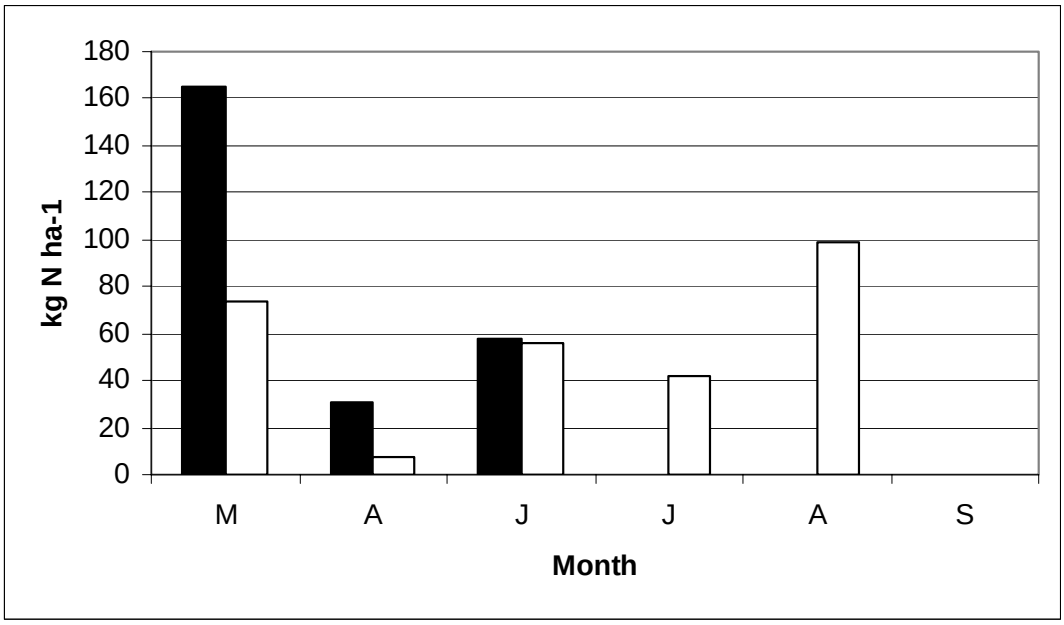


Figure 6. Fertiliser distributions from optimised runs for a grazed sandy loam (Run B, black bars) and grazed clay loam (Run D, white bars) at location 1.

Table 1. Predicted N outputs from non-optimised and optimised grazed systems on soils of contrasting texture at location 1.

Run	Soil Type	Location	Management	Run	Outputs (kg N ha^{-1} yr^{-1}) Herbage	Denitrification N_2	Denitrification N_2O	Nitrification N_2O	Nitrification NO	Leached N	NH_3	Fertiliser	Peak NO_3^--N (mg L^{-1})	ER	DM (t ha^{-1})
A	SL & WD	1	grazed	N	405	4.0	1.4	0.2	1.0	99.1	40.0	300	99.6	2.8	10.3
B		1	grazed	O	405	6.7	3.0	0.3	1.1	45.7	37.8	246	45.9	4.3	10.1
C	CL & PD	1	grazed	N	312	71.7	9.6	0.6	0.1	37.0	31.1	300	16.0	2.1	8.2
D		1	grazed	O	312	56.5	9.7	0.6	0.1	26.6	30.4	273	11.5	2.5	8.2

SL = sandy loam, CL = clay loam, WD = well-drained, PD = poorly-drained, N= non-optimised, O= optimised, ER = efficiency ratio (kg N in herbage/kg N lost), DM= herbage dry matter yield.

7.5.2. Effect of cutting/grazing management

The reduced efficiency of fields grazed by animals relative to cut-only fields can be seen for two contrasting soil textures in Location 1 by comparison of runs A and C (grazed management, Table 1) with E and G (cut-only, Table 2). The 'grazed' scenarios simulate the effect of grazing with dairy cows from April to September, inclusive. The reduced ER of grazed areas, relative to cut systems, (e.g. 2.8 for Run A, compared to 5.9 for Run E) is due to the greater total N in the system (as a result of animal excretion) and the addition of volatilised N to the total loss. Under the grazed system, all N losses (NO, N_2, N_2O, NH_3 and leaching) were greater than under cut systems, because of the greater total throughput of soil inorganic N. (To aid examination of the effects of grazing alone, this comparison does not address the potential applications of manure to cut fields, which may take place in reality. The effect of manure application is examined below).

The ER for both cut and grazed systems was improved by optimisation, compared with the non-optimised runs, with the improvement under cut systems being greater than that under grazed. The smaller effect in grazed systems is due to the fact that a larger proportion of the N input, i.e. that from returns of dung and urine from grazing animals, cannot directly be optimised, although it is affected by the optimisation procedure.

7.5.3. Effect of weather zone

Selection of different temperature and rainfall zones has a significant effect on both the simulated fluxes of N and the fertiliser recommendation resulting from optimisation. To demonstrate this, two locations were compared: location 1 has an average growing season temperature of 11.5 – 12°C (Temperature Zone 2) and an average growing season rainfall of 400-450 mm (Rainfall Zone 4), while location 2 has an average temperature of 9-10°C (Temperature Zone 5) and a rainfall of 300-350 mm (Rainfall Zone 2). The sites were identical in all other respects. For an non-optimised cut system with 300 kg N ha^{-1} fertiliser applied, the herbage dry matter yields from location 2 were 14% and 13% smaller for sandy loam (Table 3, Run M) and clay loam (O), respectively, than from location 1 (Table 2, E and G). Annual mineralisation calculated in a non-optimised run was 44% and 36% smaller at location 2 than location 1, for the sandy loam and clay loam soils, respectively. The cooler,

drier location 2 also had smaller N losses than location 1; denitrification was 65% smaller on clay loam soil at location 2 (Run O) than location 1 (Run G), for the non-optimised run.

Nitrous oxide and N_2 fluxes in the warmer and drier area were generally higher than in the colder and wetter area, due in part to the increased mineralization and greater inorganic N throughflow in the system. In drier areas, the N_2O: N_2 and NO: N_2O ratios were generally higher than in wetter areas.

Table 2. Predicted N outputs from non-optimised and optimised cut-only systems on soils of contrasting texture at location 1.

					Outputs (kg N ha^{-1} yr^{-1})										
Run	Soil Type	Location	Management	Run	Herbage	Denitrification		Nitrification		Leached N	NH_3	Fertiliser	Peak NO_3^-–N	ER	DM
						N_2	N_2O	N_2O	NO				(mg L^{-1})		(t ha^{-1})
E	SL & WD	1	cut	N	304	1.2	0.2	0.3	1.0	43.3	5.3	300	43.5	5.9	10.7
F		1	cut	O	304	1.2	0.2	0.3	0.8	14.6	4.5	251	14.7	14.1	11.0
G	CL & PD	1	cut	N	274	25.4	2.5	0.7	0.1	30.7	5.3	300	13.3	4.2	9.6
H		1	cut	O	274	16.7	2.8	0.6	0.1	6.2	5.2	286	2.7	8.7	9.9

SL = sandy loam, CL = clay loam, WD = well-drained, PD = poorly-drained, N= non-optimised, O= optimised, ER = efficiency ratio (kg N in herbage/kg N lost), DM= herbage dry matter yield.

Table 3. Predicted N outputs from non-optimised and optimised systems with contrasting grazing management and soil texture at location 2.

					Outputs (kg N ha^{-1} yr^{-1})										
Run	Soil Type	Location	Management	Run	Herbage	Denitrification		Nitrification		Leached N	NH_3	Fertiliser	Peak NO_3^--N	ER	DM
						N_2	N_2O	N_2O	NO				(mg L^{-1})		(t ha^{-1})
I	SL & WD	2	grazed	N	350	1.1	0.3	0.5	0.5	63.2	34.6	300	63.5	3.5	9.1
J		2	grazed	O	350	2.3	1.0	0.6	0.7	19.2	32.8	247	19.3	6.2	8.8
K	CL & PD	2	grazed	N	301	26.4	3.2	0.7	0.1	43.7	30.1	300	18.9	2.9	8.0
L		2	grazed	O	301	21.8	4.8	0.8	0.1	14.5	28.8	263	6.3	4.2	7.9
M	SL & WD	2	cut	N	260	0.4	0.1	0.5	0.5	32.4	5.3	300	32.5	6.7	9.2
N		2	cut	O	260	0.6	0.1	0.6	0.5	7.9	4.3	252	8.0	18.53	9.8
O	CL & PD	2	cut	N	239	8.9	1.0	0.7	0.1	27.6	5.3	300	11.9	5.5	8.4
P		2	cut	O	239	2.7	0.9	0.7	0.2	3.3	5.2	283	1.4	18.4	8.5

SL = sandy loam, CL = clay loam, WD = well-drained, PD = poorly-drained, N= non-optimised, O= optimised, ER = efficiency ratio (kg N in herbage/kg N lost), DM= herbage dry matter yield.

7.5.4. Accounting for manures

NGAUGE was used to investigate the effect of N from applied manures on N cycling in grassland systems and the degree to which fertiliser use may be reduced by taking account of this source. From a starting distribution of 300 kg N ha^{-1} fertiliser (based on RB209 as above) applied to a cut sward on a well-drained sandy loam soil (as Run E), the application of 30 tonnes ha^{-1} dairy slurry was simulated in February, May and November. This resulted in a significant increase in leached N (Run Q, Table 4), which was particularly due to the November application. Fertiliser use was then optimised to achieve the same herbage yield with more efficient N use, resulting in a 15% reduction in fertiliser use (Run R). The effect of optimisation on nitrate leaching is compromised in this run by the application of slurry, the timing and amount of which is not determined by the optimisation process but is considered as a fixed input. Injecting rather than surface spreading the slurry allowed a further 7 kg N ha^{-1} fertiliser to be saved (Run T), and NH_3 volatilisation to be substantially reduced (75%) demonstrating its effect as an NH_3 abatement strategy. However, nitrate leaching was predicted to increase (37%) with this application method. NGAUGE predicted an increase of 17 % in N_2O emissions when injecting slurry (run Q compared to Run S, Table 4). This effect of larger N_2O loss from injected than surface spread slurry has been reported in the literature (e.g. Dosch and Gutser, 1996).

7.6. Discussion

The simulation of existing fertiliser, manure and grazing practices in the non-optimised mode of NGAUGE enables the user to investigate the likely effects of changed management in any of these areas on both production and losses of N through the main processes of volatilisation, denitrification and leaching. The simulation of all of these processes also allows the potential effects of ‘pollution swapping’ to be monitored, as strategies for the abatement of individual loss processes are implemented. NGAUGE could, for example, be used to investigate the effect of the manure management changes associated with the recent NVZ guidelines on losses of N via both nitrate leaching, at which the legislation is aimed, and gaseous losses. This legislation affects both amount and timing of manure application to

grassland of particular characteristics. The effect on production of the constraints imposed by this legislation could also be assessed, for individual fields and farms.

A second potential application of NGAUGE in non-optimised mode to investigate the effect of management is the simulation of extending the grazing season into periods in which the animals would traditionally be housed. This is an increasingly popular practice in the grassland areas of the UK with milder climate, such as the south west and south Wales. The potential economic benefits of such grazing management have been demonstrated (Frame and Laidlaw, 2001), but debate continues about the potential environmental impacts of applying N, as fertiliser or grazing returns, outside the conventional grazing season. To assess the system fully, simulation would need to include the effects of the timing and amount of fertiliser application, the presence of grazing animals and the application of reduced amounts of animal manures during the traditional housed period. NGAUGE simulates the effects of all of these elements of the system and has usefully been applied to the assessment of extended grazing (Webb *et al.*, 2005).

Table 4. The effect of dairy slurry application on N outputs and optimisation from a cut system on a sandy loam soil at location 1.

					Outputs (kg N ha^{-1} yr^{-1})										
Run	Soil Type	Location	Management	Run	Herbage	Denitrification		Nitrification		Leached N	NH_3	Fertiliser	Peak NO_3^--N	ER	DM
						N_2	N_2O	N_2O	NO				(mg L^{-1})		(t ha^{-1})
Surface spread															
Q	SL & WD	1	cut	N	324	1.5	0.3	0.3	1.0	90.8	65.6	300	91.3	2.0	11.5
R		1	cut	O	324	1.8	0.3	0.3	0.9	60.3	64.8	255	60.6	2.5	12.4
Injected															
S	SL & WD	1	cut	N	332	1.9	0.5	0.2	1.0	113.9	17.3	300	114.5	2.5	11.9
T		1	cut	O	332	1.7	0.3	0.3	0.9	82.4	16.5	248	82.8	3.3	13.3

SL = sandy loam, CL = clay loam, WD = well-drained, PD = poorly-drained, N= non-optimised, O= optimised, ER = efficiency ratio (kg N in herbage/kg N lost), DM= herbage dry matter yield.

The facility to optimise fertiliser distribution within NGAUGE has a number of key advantages and applications. First, it allows N to be used more efficiently while still retaining the focus of the system on production targets. Secondly, and perhaps more importantly, it enables the focus to be shifted, and fertiliser plans to be developed for targets which reflect the changing, and multiple, objectives of modern agricultural systems. An example of this is the facility to use N loss, rather than production, as a target for optimisation. To make maximum use of this capability and to enable NGAUGE to contribute to an existing practical problem faced by the farming community, some changes to the operation of the DSS may be required, *viz* making peak nitrate concentration rather than 'N loss' the target of optimisation.

The scope for improvement in efficiency through optimisation is limited by site factors, but more importantly by the level of N input to the system. The latter is obvious from the shape of the N response curve in plants: there is greatest scope for improvement with steepest gradient of the curve. At low N inputs, N response is dominated by mineralization (largely unmanageable) while at high N inputs, response to incremental N input is very low.

While the model is capable of optimising the efficiency of N use for a particular grassland system, the optimised pattern of herbage production (high yields in early summer) may not be compatible with the farmer's preferred stock management. UK livestock management encompasses a range of degrees of reliance on grazed grass, with some farms operating zero grazing systems with indoor feeding of cut and conserved forage, and others utilising grazed grass throughout the year. The distribution of herbage production predicted by optimisation would benefit more the former, which reflects the basis for the popularity of silage-based grassland production.

The NGAUGE DSS provides site specific fertiliser recommendations for user-specified targets. In contrast to the existing UK fertiliser recommendation system (MAFF, 2000), the potential losses of N are taken into account in the production of this recommendation, both by ensuring that the target is achieved with the greatest ratio of herbage N to N lost, and by providing the facility for N losses to be entered as a target.

While there have been several other approaches to decision support for N fertiliser management, originating in the Netherlands (Dairy Farming Model: Van de Ven, 1996), France (AzoPât: Decau *et al*., 1997; Delaby *et al*., 1997) and New Zealand (NLE: Di and

Cameron, 2000, and Overseer: Wheeler *et al.*, 2003), NGAUGE is unique in its combination of farmer-friendly user interface, sophisticated description of process and optimisation capability, that enables both production and environmental losses to be quantified. In addition, NGAUGE is capable of interfacing with budget- and indicator-based systems of fertiliser management (e.g. Jarvis *et al*., 1996b, Shroeder *et al.*, 2003). Because of this combination of ease of use and complexity of simulation, the DSS should be of benefit to a variety of users. In addition to its use by farmers and their advisors, it could be used by policy makers to explore mitigation options for enabling compliance with N loss legislation (e.g. for NVZ regulation compliance, as mentioned above); and by researchers to explore impacts of novel farm managements on pollution swapping and fundamental controls on the efficiency of the system. To aid progress towards these objectives the model could be further developed to enable a wider range of forage crops to be considered and to explore the advantages of within- and between-farm optimisation.

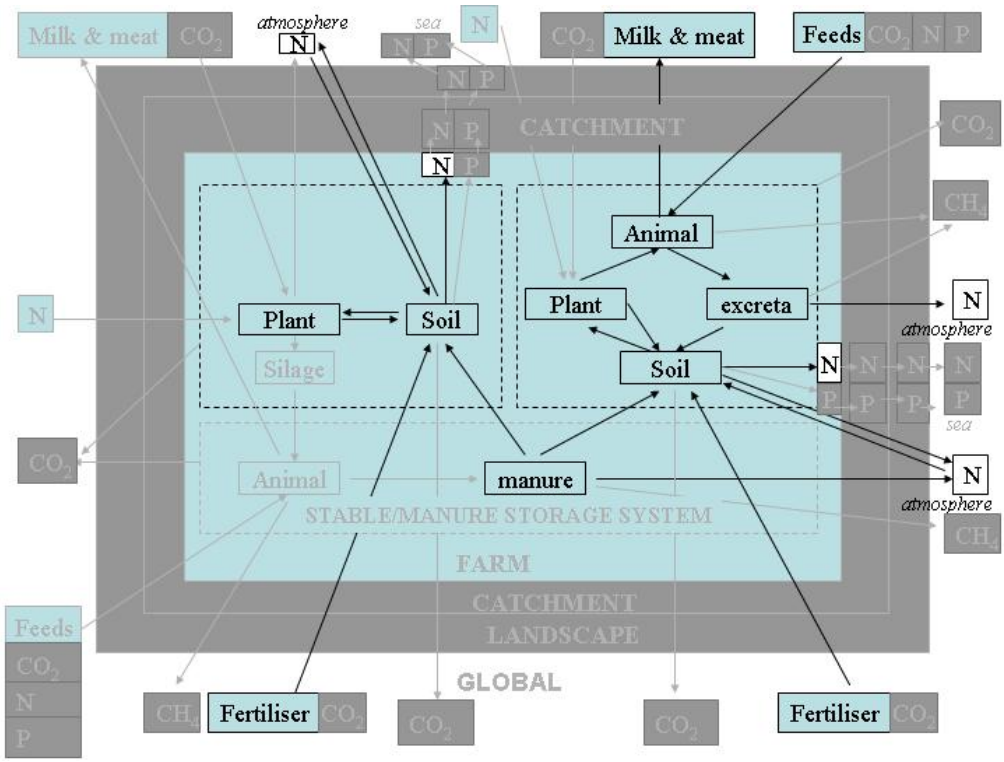
7.7. Conclusions

NGAUGE provides a basis for improved decision making about fertiliser management on grassland farms. It is a tool which enables users to be more aware of the magnitude of N losses and provides a means of improving the efficiency with which N used on grassland fields. The potential for improvement in efficiency was found to be dependent on site characteristics and existing management, with the greatest improvement possible on sandy-textured soils with moderate N inputs. It was possible to reduce nitrate leaching by up to 46% and annual fertiliser use by up to 33%, without compromising herbage yield. Field-specific fertiliser recommendations are provided, according to the user-specified target, soil texture and drainage status, weather, land-use history and manure use. The optimisation procedure was developed with dual criteria of increased herbage production and reduced losses for a given N input, enabling increased emphasis to be placed on limitation of undesirable losses compared to existing recommendation systems. There is potential for manipulation of these criteria in future applications, to further shift the emphasis of the

optimisation and resulting fertiliser recommendation, for example where limitation of a specific loss pathway is of particular importance.

Chapter 8

Use of the NGAUGE model to establish whether UK dairy farms can comply with the Nitrate Directive under current management, under NVZ rules and with alternative measures



8. Use of the NGAUGE model to establish whether UK dairy farms can comply with the Nitrate Directive under current management, under NVZ rules and with alternative measures

Abstract

The nitrate vulnerable zones (NVZ) measures in England aimed at reducing nitrate (NO_3^-) leaching from dairy farming were compared to some alternative abatement measures implemented on farms under English typical mineral fertiliser application rates. The measures were: (a) improving N fertiliser use, (b) improving manure timing strategy, (c) use of farm yard manure (FYM) instead of slurry and (d) exporting manure outside the dairy farm.

In order to carry out this study, we used the grassland simulation model NGAUGE. NGAUGE is a model that has been developed to optimise nitrogen (N) fertiliser distributions of grasslands in order to meet environmental and economical goals. The feasibility of these measures was analysed both in terms of environmental and herbage production performance using predictions of annual nitrate-nitrogen concentration in the leachate and dry matter herbage yields, respectively. The results indicate that by implementing one or the combination of some of the alternative measures on farms under average and low current fertiliser use, lower NO_3^- leaching losses compared to those resulting from applying the NVZ_{170} rules could be obtained with a significant economical benefit in herbage yield. Examples of possible negative effect of these measures on other pollutant forms of nitrogen and in other areas (i.e. by exporting manure) were studied. Those measures which involved mineral fertiliser optimisation resulted in substantially increasing N_2O emissions. It is however difficult to assess whether this increase was acceptable or not because of lack of N_2O emissions thresholds limits. The impact of exporting dairy farms manure to beef areas on NO_3^- leaching was acceptable and moreover, it could be ameliorated by implementing some of the alternative measures used for dairy farms. This study supports the contention that there could be significant scope for these measures to represent a real alternative to NVZ_{170} rules in England.

8.1. Introduction

Nitrate (NO_3^-) concentration in surface and ground-waters has increased in recent decades in many areas of Europe. In most European Union (EU) countries agricultural land has been regarded as the main diffuse source of NO_3^- pollution in rivers and groundwaters (i. e. in the UK: Powlson, 2000). Firstly, as a way to prevent the pollution of waters by NO_3^- from agricultural sources, the European Commission adopted the EU Nitrate Directive (Anon, 1991) and secondly, as a measure to reach good ecological status of all inland and coastal waters, they launched a more stringent directive: the EU Water Framework Directive (WFD) (EC, 2000). EU member states agreed that the EU Nitrate Directive and the EU WFD were to be fully implemented by 2003 and 2015, respectively. Unfortunately, the implementation of the EU Nitrate Directive has fallen seriously behind schedule (Goodchild, 1998) and most states are yet to accomplish the goals of this directive before even considering the EU WFD.

The EU Nitrate Directive required that each member state should: (i) either identify and designate catchments where the NO_3^- concentration either exceeded 11.3 mg NO_3^- -N l^{-1} or was at risk of doing so (i.e. UK), or select the whole territory as vulnerable (i.e. Ireland), (ii) establish action programs which contain mandatory measures concerning the land application and storage of manure and (iii) draw up at least one code of good agricultural practice which would be implemented on a voluntary basis throughout their territory.

In England and Wales, as well as already existing codes of Good Agricultural Practice (i.e. code of fertiliser recommendations: RB209), steps were taken to identify and designate catchments at risk and their influential Nitrate Vulnerable Zones (NVZ) and to implement effective controls over them (NVZ Action Program). By 2002 about 80 and 3 % of England and Wales, respectively, was designated as NVZ.

The NVZ Action Programme in England and Wales currently constrains farmers within the designated NVZ areas to follow specific manure management rules (Defra, 2002): it establishes closed periods for slurry application on sandy or shallow soils (between 1 September and 1 November to fields in grass) and provision of storage for slurry during this period must be ensured too. It also limits annual organic manure applications to 250 kg N ha^{-1} yr^{-1} of total N (NVZ_{250}) input averaged over the area of grass on the farm (this limit applies

to all organic manures, including that deposited by animals whilst grazing). However, this amount is still subject to EU agreement and it is likely to be reduced down to first 210 kg N ha^{-1} yr^{-1} and later to 170 kg N ha^{-1} yr^{-1} of total N (NVZ_{170}). If this threshold (250 kg N ha^{-1} yr^{-1}) is lowered the EU Commission will consider requests for derogation of this lowered level when based on objective criteria. Mineral fertiliser rules are less restrictive since although a close period for application is required (between 15 September and 1 February), there is no stipulated limit for levels of mineral fertilisation, except that crop requirement must not be exceeded.

The amount of total N from organic manure (including that deposited by animals) produced in a dairy farm is generally related to the number of dairy cows in the herd (reference). In a previous study (Scholefield, 2003) the current average conventional dairy farm was estimated to operate at a total N amount of organic manure of about 230 kg N ha^{-1} yr^{-1}. Because of the strong relationship between livestock density and net profitability of a dairy farm (reference), the economic and social implications of reducing from 230 to 170 kg N ha^{-1} yr^{-1} are likely to have considerable negative impacts on English dairy farmers.

Similar measures to decrease NO_3^- leaching losses from farming systems have been introduced in most of the rest of the EU-15 countries. A complete overview of the agri-environmental pressures and the nutrient management policies in the EU-15 members and in Norway and Switzerland was given in De Clercq *et al*. (2001).

Each EU-15 country, in an attempt to reduce the immediate negative impact of the EU Nitrate Directive measures, has proposed alternative measures to those explicitly indicated in the EU Nitrate Directive; The Netherlands, for instance, used a mineral accounting system (MINAS) in which all the farmers had to calculate an approximation of a complete N and P farm balance sheet and, subsequently and according to their N and P surpluses, they were subject to levies up to a certain N and P surplus threshold. The EU Commission, however, considered MINAS to be an addition to their policy rather than an alternative. Several European countries have also implemented processing of manure as an abatement option to reduce NO_3^- leaching although the effects of this measure have not always been reliable or sustainable. Many countries e.g. The Netherlands, Denmark and Sweden have also implemented ammonia (NH_3) reducing measures in their legislation, thus taking into account more integrated approaches to avoid pollution swapping.

In this paper we compare the effects of NO_3^- leaching abatement measures (English NVZ action plan *vs.* alternative measures) on losses of NO_3^- leaching, N_2O and NH_3 and herbage production per hectare in typical English grassland-based dairy systems. With this study we intended to assess whether there is scope for improving the current NVZ action plan through measures which result in reducing NO_3^- leaching losses and result in acceptable losses to the farm economy and/or other N pollutants. Although we recognise that farm profitability may be affected by numerous variables, we used predicted results of herbage yield as an indicator of farm economic performance. The alternative measures involved various mineral fertiliser and manure management strategies (i.e. optimising mineral fertiliser timing distribution so that the synchrony of inorganic N supply in the soil and grass N demand is improved).

In order to carry out this complex study a model was required to fulfil this role. Models are powerful tools for examining the effect of management / mitigation options, allowing the effect of other non-target pools of N to be considered and facilitating the investigation of changing efficacy of the strategies across contrasting environmental conditions. We used the empirically-based model NGAUGE (Brown *et al*., 2005) in this study as this model is capable of seeking the best fertiliser amount and distribution according to criteria of production and N losses to the environment (leaching, denitrification and ammonia volatilisation) and it can simulate the effect of monthly manure application within a wide range of environmental conditions and grassland managements.

8.2. Materials and methods

8.2.1. The tool: NGAUGE

NGAUGE (Brown *et al*., 2005) is an empirically-based mass-balance model which simulates monthly N flows within and between the main components of grazed or cut grassland system according to user inputs describing site conditions and farm management characteristics (i.e. monthly fertiliser and manure application).

NGAUGE is an improvement on existing N fertiliser recommendation systems in that it relates production to environmental impact and is therefore potentially valuable to policy makers and researchers for identifying pollution mitigation strategies and blueprints for novel, more sustainable systems of livestock production.,

NGAUGE prediction of plant N uptake is based on a set of empirically derived curves from multi-sites experiments (Morrison *et al*., 1980 and Hopkins *et al*., 1990) which describe the relationship between inorganic N flux (the sum of all the inputs to the soil) and plant N flux (including N in roots) for each month. In order to calculate total N in plant on N in herbage, assumptions based on existing studies and datasets were made about the proportion of N in the whole plant that is harvested by the animal or by cutting each month. The model predicts smaller values in winter months and large values in May and June. The concentration of N in cut herbage or grazed grass was calculated using relationships between fertiliser N and %N in herbage, derived from Morrison *et al*. (1980). The model subsequently calculates the partitioning of N within the animal into urine, dung and product. Urine is assumed to be hydrolysed to inorganic N within hours. Mineralised N is considered to be derived from 4 components: (i) the previous land use, (ii) the herbage production in the current year (iii) dung and (iv) applied manures and is very sensitive to climatic and soil conditions. Processes of denitrification, NH_3 volatilisation were modelled as a function of soil inorganic N, mineralised N, water-filled pore space (WFPS) and temperature. Leachable NO_3^-, peak (defined as the N concentration in the first 25 mm of leachate) and average nitrate-N concentrations are presented by the model on an annual basis.

For each month, soil inorganic N flux was calculated as the sum of atmospheric input, mineralisation of soil organic matter, mineralisation of dung and manures, fertiliser, urine and 'leachable N' carried over from the previous month. From this total, uptake of N by the plant, NH_3 volatilisation and N lost by denitrification were subtracted. The fate of the remaining 'leachable N' depends on the month in question; for January, February and December it was assumed that 'leachable N' contributes to the total annual leaching, and for other months it was passed to the succeeding month as a component of the inorganic N pool. Peak and average concentrations of nitrate-N in leachate were calculated on an annual basis using the relationships derived by Rodda *et al*. (1995).

A field-specific target can be set by the user for optimisation, and may be herbage N, N loss or fertiliser N. The end point of the optimisation is achieved when the model reaches the target value, satisfying the optimisation criteria. Three criteria are used, the one in operation in any given run is dependent on the target set by the user. All are a combination of maximising herbage and the efficiency ratio (ER), defined as kg N in herbage per kg N

loss. A comparison between modelled and measured data on herbage yield and NO_3^- leaching indicated that observed and predicted rates agreed reasonably well as they were not significantly different in 9 out of 12 treatment years and 8 out of 12 cases for dry matter yields and NO_3^- leaching, respectively. Further detailed information on the description of the NGAUGE optimisation procedure, validation and other principles of NGAUGE simulation of N flows are shown by Brown *et al*. (2005).

8.2. 2. Specification of typical conventional dairy farms in England (baselines)

We defined as baseline 3 typical dairy farms in England, each differing in mineral fertiliser use rate, using available data based on farm surveys (Jarvis, 1993). Although currently it is becoming increasingly popular to grow some arable crops (i.e. maize) within dairy farms, farm surveys, still support the idea that English dairy farms typically rely on grass production (and some bought-in feed) for sustaining animals (Jarvis, 1993). Grass silage for the housed period (generally in winter-autumn) and grazed grass during summer and spring. Dairy systems have a large variability on management practices. As a way to minimize this complex variability we simplified management in our farm simulated scenarios.

Consequently, we assumed that the farm was entirely based on in-farm produced grass and animals other than dairy cows were not taken into consideration. Grassland farm area was split into cut-only fields (3 cuts made for silage) and grazed-only fields (for 185 days from April to September), comprising 31 % and 69 % of the total grassland surface, respectively (after calculations based on data from Jarvis, 1993). Baseline farms mainly differed in their intensity of mineral fertiliser use (Low_{farm}, $Medium_{farm}$ and $High_{farm}$). Each baseline farm had mineral fertiliser application rates which comprised typical rates for each land use:130 (low), 175 (medium) and 250 (high) kg N ha^{-1} for grazed areas and 250 (low), 300 (medium) and 345 (high) kg N ha^{-1} for cut areas, (ADAS, pers. comm). The timing and percentage of annual total applied per month was designed to follow the UK fertiliser recommendations for agricultural crops (RB209), (MAFF, 2000).

We assumed that annual yield and proteins in milk per cow were the same in all the studied scenarios (baseline farms and NO_3^- abatement measures). The main differences, hence, are reflected as a per hectare basis and are intimately related to the amount of dairy cows that the

herbage production per hectare resulting from every scenario can actually support those cows.

8.2.3. Calculation of amount of manure produced during housing and applied to the fields

In order to calculate the amount of manure to be applied within the farm, we assumed that the number and type of livestock determined the quantity of N returned as manure, and indirectly, the N fertiliser input. Thus, total N excreted by the cows was calculated according to an empirical equation relating amount of mineral fertiliser N applied to the grass with livestock density (LU ha^{-1}) (Scholefield, *pers. comm*) and subsequently, using the typical value of N excreted by an adult average cow of 650 kg weight [annual N excretion of 116 kg N yr^{-1} cow^{-1}, after UK guidelines for farmers in NVZs (Defra, 2002)]. Total N inputs and livestock density for farms under typical fertiliser rates (low, medium and high) are shown in Table 1.

Total annual excreta were then split into N excreted during grazing and housing period. This split was calculated through various iterative steps: in the first step the model calculates the N excreted as urine and dung (grazed-only excreta) in grassland using mineral fertiliser as an input but not manure application (as this amount is not yet known). In subsequent steps the manure amount to be applied was calculated (subtracting the grazed-only excreta from the total annual excretion) and used as an input, together with the mineral fertiliser, in the grazed field by subtracting the grazed-only excreta (calculated in the previous iteration) from the total N excreta. The iterations stopped when a steady state for manure N amount was reached.

Table 1. Livestock density, annual mineral N and annual total N from organic manure per farm area for baseline farms (Low_{farm}, $Medium_{farm}$, $High_{farm}$).

Rate	Fertiliser	Livestock density	Organic manure
	kg N ha^{-1} yr^{-1}	*LU ha^{-1}*	*kg N ha^{-1} yr^{-1}*
Low_{farm}	167	1.66	193
$Medium_{farm}$	214	1.96	227
$High_{farm}$	279	2.37	275

All the calculations accounted for weighting the different proportion of grazed-only (69 %) and cut-only grassland area (31 %) and also for the fact that cut grasslands, on average, receive about 6 % more N from animal manure per unit of surface than grazed grasslands (based on calculations from Jarvis, 1993) .

The typical temporal patterns of distribution of the total manure applied followed the approach described by Smith *et al*. (2001b), in which, the year is divided into 4 quarters and the proportion of manure applied of the annual total is as follows: from February-April (40%), May-July (10%), August-October (25%) and November-January (25%).

As the baseline scenario for farms under typical application rates and no abatement measures, we spread slurry of 6 % dry matter in February, May, August and December.

8.2.4. Study areas, soil characteristics and past grassland conditions

This paper does not intend to study the sensitivity of our results to climatic conditions within England and therefore, we present results from only a typical dairy area in the south west of England (Devon). The Devon climate is a good example of a wet and mild Atlantic climate.

We focussed on soil textures with high potential for leaching and hence subject to NVZ rules application, therefore we simulated scenarios of farms on well-drained sandy loam textured soils. A history of more than 10 years of grassland leys and a sward age of 11-20 years was chosen to be typical. It must be noted that our results will not apply to the entire Devon area but only to that area under well drained sandy loam soils.

8.2.5. Abatement measures

For this study the measures resulting from the English NVZ action plan for England (NVZ_{farm}) focused on the limitations of: application of total N from organic manure at 170 kg N ha^{-1} yr^{-1} = (NVZ_{170}), closed periods for slurry application (between 1 September and 1 November to fields in grass) and mineral fertiliser applications following the RB209 guidelines of best fertiliser application.

We proposed the following farm strategies as alternative abatement measures for NO_3^- leaching and which were applied to farms under typical fertiliser rates (baseline farms under low, medium and high mineral fertiliser rates). The effect of a single alternative measure or combinations was simulated. Four alternative measures were used in this study:

Measure A ($ALow_{farm}$, $AMedium_{farm}$ and $AHigh_{farm}$): optimisation of mineral N fertiliser timing distribution by using NGAUGE optimisation and using the same amount of annual mineral fertiliser as the field-specific target.

Measure B ($BLow_{farm}$, $BMedium_{farm}$ and $BHigh_{farm}$): improving manure timing strategy by delaying application of first quarter manure (manure application in March instead of February).

Measure C ($CLow_{farm}$, $CMedium_{farm}$ and $CHigh_{farm}$): use of manure types with a slower release rate of inorganic N (FYM instead of slurry).

Measure D ($DLow_{farm}$, $DMedium_{farm}$ and $DHigh_{farm}$): decreasing manure N applied to land by exporting manure (that produced during the housing period) outside the boundaries of the dairy farm. It is important that this measure does not generate an unacceptable environmental impact on the receiving site. We therefore simulated the effect of exporting this amount of manure to a neighbour (same soil and climatic conditions as exporting manure dairy farm) typical finishing suckler beef farm ($Beef_{farm}$) as defined by Hopkins *et al*. (2003). This system has a stocking rate of 2.2 LU ha^{-1} (all the grassland area is grazed) and receiving 100 kg N ha^{-1} as mineral N fertiliser. We simulated this measure at different degrees of manure amounts to be exported (30, 50 and 100%).

In order to calculate the livestock density and annual mineral fertiliser application for farms under NVZ rules (NVZ_{farm}), we used the same principles described in section 2.3, by which NVZ_{farms} receive an annual mineral fertiliser of 136 kg N ha^{-1} yr^{-1}, have a livestock density of 1.47 and produce 170 kg N ha^{-1} yr^{-1} total N as organic manure (including excreta during grazing).

8.2.6. Criteria of comparison

The results obtained from the baseline farms (Low_{fam}, $Medium_{farm}$ and $High_{farm}$) were compared to those from the farms under NVZ rules (NVZ_{farm}) and those under typical mineral fertiliser rates plus the alternative measures ($ALow_{fam}$, $AMedium_{farm}$, $AHigh_{farm}$, $BLow_{fam}$, $BMedium_{farm}$, $BHigh_{farm}$, $CLow_{fam}$, $CMedium_{farm}$, $CHigh_{farm}$, $DLow_{fam}$, $DMedium_{farm}$ and $DHigh_{farm}$) in terms of NO_3^- leaching losses and herbage dry matter (DM) yield production (as an indicator of economic performance). Nitrate leaching results were shown as annual average and peak N concentration in the leachate (mg N l^{-1}) and the

threshold value proposed by the EU Nitrate Directive (11.3 mg N l^{-1}) was used as the basis to decide if the measures were successful in mitigating NO_3^- leaching impact on eutrophication of waters. In order to simplify, either average N concentrations or peak N concentrations were used in the results section.

The effect of a single or combinations of measures adopted by a farm under typical application rates was compared on % change basis. One of the main risks of targeting the reduction of one specific pollutant is the possibility that it might increase the undesirable effects of other forms of pollution (so-called "pollution swapping"). Mitigation strategies, hence, to be effective, should also minimize pollution swapping (Monteny *et al.,* 2006). Both NO_3^- leaching and nitrous oxide (N_2O) emission or NH_3 volatilisation and N_2O emission are often intimately linked and the reduction of one of them can increase the other. As an example, we evaluated the impact of applying measures A, B, C to Low_{fam}, $Medium_{farm}$ and $High_{farm}$ on N_2O and NH_3 losses.

8. 3. Results

8.3.1. Results from baseline farms, NVZ farms and farms under alternatives single measures

Table 2 shows the DM herbage yield per hectare and NO_3^- leaching (as average NO_3^- concentration in the leachate) total results for baseline farms and the effect on both herbage yield and NO_3^- leaching of applying the NVZ and the alternative single measures A, B, C and D (as % change towards baseline farms).

As expected, DM herbage yield and NO_3^- leaching losses increased with increasing applications of mineral fertiliser applications ($High_{farm}$>$Medium_{farm}$>Low_{farm}). All baseline farms, except for those under low mineral fertiliser application resulted in annual N average concentration in the leachate exceeding the Nitrate Directive threshold. The implementation of the NVZ rules enabled the dairy farm to decrease NO_3^- leaching under the Nitrate Directive threshold. However, it also represented a loss in herbage yield of 7- 26 % to that predicted from the baseline farms.

The alternative single measures had different effects on NO_3^- leaching losses. Whereas optimising mineral fertiliser distribution as a single option (measure A) resulted in

substantially decreasing NO_3^- in average N concentration in the leachate (32-39 %) and being these concentrations below (Low_{farm} and $Medium_{farm}$) or slightly over (average NO_3^--N concentration in the leachate in $High_{farm}$= 11.4 mg l^{-1}) the Nitrate Directive threshold, the rest of the alternative measures resulted in smaller reductions than measure A. These reductions were substantial enough to be below the Nitrate Directive threshold only in the case of farms under low mineral fertiliser rates (achievable in these farms even when no measures were implemented) and in farms under medium mineral fertiliser rates under measures of exporting 50 to 100% (D50% and D100%) of the manure generated during housing.

Measures A, B and C resulted in small increase (A and B) or no change (C) in herbage yield DM and measure D (exporting manure) lead to small decrease/no change in herbage yield (0-4 %). Farms under NVZ rules (NVZ_{farm}) had much greater penalties in herbage DM yield than any of the farms under alternative measures.

Table 2. Dry matter herbage yield per hectare and NO_3^- leaching (as average NO_3^- concentration in the leachate) total results for baseline farms and the effect on both herbage yield and NO_3^- leaching of applying the NVZ and the alternative single measures A, B, C and D (as % change towards baseline farms).

Baseline farms		**Alternative measures**						**NVZ**
		+A	**+B**	**+C**	**+D (30%)**	**+D (50%)**	**+D (100%)**	**NVZ_{farm}**
Herbage yield								
	(t DM/ha yr)				***% change (Herbage yield)***			
Low_{farm}	8.1	1	2	0	0	-1	-4	-7
$Medium_{farm}$	9	3	2	0	-1	-1	-4	-17
$High_{farm}$	10.1	5	2	0	0	-1	-3	-26
NO_3^- leaching								
	(mg/l)				***% change (NO_3^- leaching)***			
Low_{farm}	10.5	-39	-10	-6	-7	-12	-20	-13
$Medium_{farm}$	12.8	-37	-10	-5	-8	-13	-21	-28
$High_{farm}$	16.9	-32	-8	-4	-7	-12	-21	-46

As a single measure, optimisation of mineral fertiliser distribution (measure A) in farms under low and medium optimised mineral fertiliser rate lead to lower than those farms

following NVZ rules N concentration in the leachate and moreover, they showed no penalty on herbage yield as in fact they all increased herbage yield. The rest of the alternative measures generally failed to attain reductions in NO_3^- leaching losses down to the values of the NVZ farms. However, both exporting 50-100% of the manure (measures D50% and D100%) and applying manure in March instead of in February (measure B) generally resulted in reduction in N concentration in the leachate of over 10 %.

In data not shown, it must be noted that optimisation of mineral fertiliser (alternative abatement measure A) resulted in polarisation of N mineral fertiliser doses and herbage production in the period spring- early summer.

8.3.2. Results from combination of alternative measures

The results in herbage DM yields and NO_3^- leaching (peak N concentration in the leachate) of combining alternative measures (A, B and C) on farms under typical mineral fertiliser applications compared with those after application of NVZ rules (NVZ_{farm}) are presented in table 3. These results (combination of alternative measures) are expressed as a % change (in ranges of increase or decrease) towards those results from the NVZ_{farms}.

As expected, farms under any combination of 2 or more alternative measures resulted in larger herbage DM yields than NVZ_{farms}, ranging from about 5-15 % rise in farms under low typical mineral fertiliser practices (Low_{farm}) to more than 35% in farms under high typical mineral fertiliser practices ($High_{farm}$). Nitrate leaching results indicate, however, that not all the combination of alternative measures were efficient enough to result in lower peak N concentrations in the leachate than that from NVZ_{farm}.

Nitrate leaching from Low_{farm} and $Medium_{farm}$ + combination of almost any measures was smaller than that from NVZ_{farms}. In fact, any combination that included optimisation of mineral fertiliser (measure A) lowered the peak N concentration value from NVZ_{farm} by over 35 % and 5-15 % in Low_{farm} and $Medium_{farm}$, respectively. When the 3 measures were combined together on Low_{farm} and $Medium_{farm}$ peak N concentrations were 44% (Low_{farm}) and 22% ($Medium_{farm}$) smaller than those from NVZ_{farm} and herbage DM yields were about 10% (Low_{farm}) and 24 % ($Medium_{farm}$) greater than those from NVZ_{farm} (exact data not shown).

Table 3. Percentage change in predicted herbage dry matter yields and peak N concentration in the leachate in farms under typical mineral fertiliser application rates (Low_{farm}, $Medium_{farm}$ and $High_{farm}$) + combination of alternative measures (A: optimisation of application rates and/or B: spreading manure in March instead of February and/or C: using FYM manure instead of slurry) compared with farms under NVZ rules (NVZ_{farm}).

% change over NVZ_{farm} on	**Combination of alternative measures**			
	+AB	***+AC***	***+BC***	***+ABC***
	% change in herbage DM[b]			
Low_{farm}[a]	>5-15%	>5-15%	>5-15%	>5-15%
$Medium_{farm}$[a]	>35%	>15-25 %	>15-25 %	>15-25 %
$High_{farm}$[a]	>35%	>35%	>35%	>35%
	% change in peak N concentration in leachate[b]			
Low_{farm}[a]	<-35%	<-35%	≈	<-35%
$Medium_{farm}$[a]	<(-5)-(-15)%	<(-5)-(-15)%	>5%	<(-5)-(-15)%
$High_{farm}$[a]	>5%	>5%	>5%	>5%

[a] Farms under typical mineral fertiliser application rates (low, average and high) + A, B and/or C alternative measures.

[b] Percentage improvement in herbage dry matter yield (t/ha) and peak N in the leachate (mg/l) of farms under typical mineral fertiliser rates + abatement measures (A, B, C) compared with NVZ_{farm}.

Those combinations of abatement measures (A, B and/or C) which resulted in farms with smaller herbage yields or larger peak N concentrations in their leachate compared with farms under NVZ rules (NVZ_{farm}) were highlighted by grey colour in the table.

In contrast, Low_{farm} or $Medium_{farm}$ + combination of B and C alternative measures resulted in similar (compared with Low_{farm}) or greater (compared with $Medium_{farm}$) N peak concentration results with those N peak values from NVZ_{farm}.

No reduction in peak N concentration towards the NVZ_{farms} was observed when combination of A, B and/or C were used on $High_{farm}$.

The results in herbage DM yields and NO_3^- leaching (peak and average N concentration in the leachate) of single or combined alternative measures (A, B, C and D) and no measures on farms under typical mineral fertiliser applications compared with those after application of NVZ rules (NVZ_{farm}) are presented in Fig 1 (Low_{farm}:1.i, $Medium_{farm}$:1.ii and $High_{farm}$:1.iii).

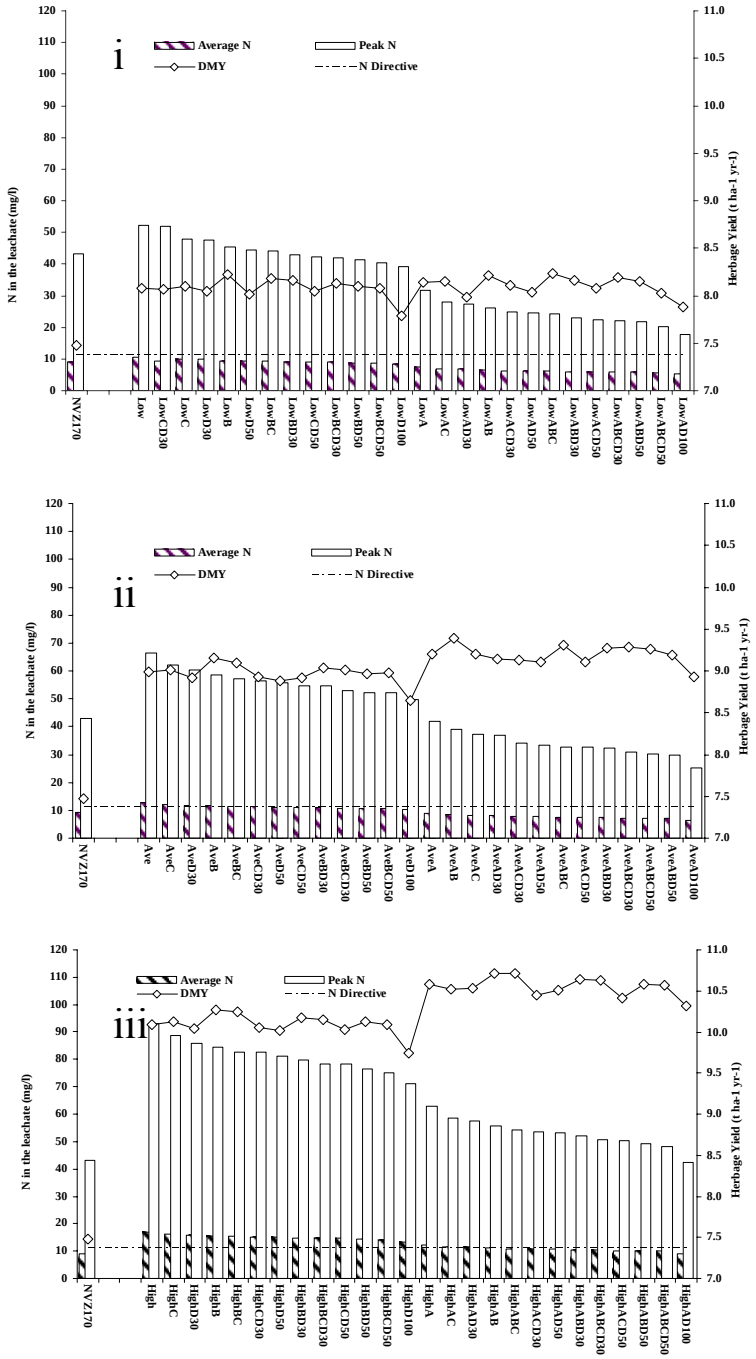


Figure 1. Simulated results of peak and average N concentration in the leachate and herbage dry matter yield (DMY) from farms following NVZ rules (NVZ_{170}) and under (i) low, (ii) medium (Ave) and (iii) High typical mineral fertiliser application rates + combinations of alternative abatement measures (A,B,C,D). Being: (A) optimisation of application rates and/or (B) spreading manure in March instead of February and/or (C) using FYM manure instead of slurry and/or (D30, D50, D100) exporting 30, 50 and 100 % of the manure, respectively. N Directive: EU Nitrate Directive concentration of 11.3 mg/l NO_3^--N in the leachate.

If we compare the effect of the combined measures on NO_3^- leaching to that of the NVZ_{farms}, about 72 (Low_{farm}), 52 ($Medium_{farm}$) and 4 % ($High_{farm}$) of those combinations were effective enough to reduce the NO_3^- leaching resulting from NVZ_{farm}. All the farms resulted in NO_3^- leaching losses exceeding the threshold of 11.3 mg N l^{-1} in peak N concentrations in the leachate and 100%, 77% and 35% of the combinations of alternative measures resulted in lowering the threshold of 11.3 mg N l^{-1} in average N concentrations in the leachate.

As expected, whereas farms under low typical mineral fertiliser rates needed to use a smaller number of measures or even just one to decrease the leaching values from NVZ_{farm}, farms under average and under high typical mineral fertiliser rates needed a greater number of measures (Fig 1.ii and Fig 1iii).

Some combinations of alternative measures on Low_{farm} resulted in small reductions in NO_3^- leaching compared with NVZ_{farm} but they were simple (i.e. LowBD30: application of slurry in March instead of February and export of 30 % of the manure) and resulted in about 1000 kg DM ha^{-1} yr^{-1} larger yields. Other combinations which involve a combination of a larger number of alternative measures (LowABD30: optimisation of mineral fertiliser, application of manure in March instead of February, FYM instead of slurry and export of 30 % of the manure) resulted in large reduction in NO_3^- leaching (about 3 and 15 mg l-^{1} in NO_3^--N average and peak concentration, respectively) and also about 1000 kg DM ha^{-1} yr^{-1} larger yields.

Combination of measures which include exporting manure, although decreased N leaching, they generally resulted in smaller herbage yields than those farms where manure was not exported.

On farms under high mineral fertiliser rates ($High_{farm}$), only when the mineral fertiliser is optimised (measure A) and when all the manure is exported (HighAD100), can the farm result in smaller NO_3^- leaching values than on NVZ_{farms}.

In some cases, after using some of the measures on farms under high typical mineral fertiliser rates ($High_{farm}$), NO_3^- leaching results were slightly greater than on the NVZ_{farms} but herbage yields were substantially larger (i.e. farms optimising fertiliser rate, using FYM instead of slurry and exporting 50 % of the manure to other areas (HighACD50) as herbage yield were increased about 3000 kg DM ha^{-1} with respect to that yield in NVZ_{farm}.

8.3.3. Possible impacts of exporting manures to beef farming systems.

As an example, we simulated that one of the dairy farms under typical mineral fertiliser application + combination of alternative measures which included manure export (LowAC30D: Fig 1) applied 30 % of its manure in an adjacent beef farming system (as defined in section 2.5). This beef system, which, in typical conditions (beef $_{baseline}$) resulted in predicted losses of NO_3^- leaching of 14.5 and 6.1 mg l^{-1} for peak N and average N concentration in the leachate, respectively and herbage DM grazed yield of 5400 kg DM ha^{-1} yr^{-1}; after application of the dairy farm manure, NO_3^- leaching increased up to 19 mg l^{-1} and 8 mg l^{-1} for peak N and average N concentration in the leachate, respectively and herbage yield was slightly increased about 200 kg DM ha^{-1} yr^{-1}.

Moreover, we tested the effect on herbage yield and NO_3^- leaching losses of applying to the beef system some of the dairy alternative abatement measures. As a matter of fact, if the dairy cow manure was applied in March instead of February (measure B), peak and average N concentration in the predicted leachate values of the beef farm were 12.6 and 5.3 mg l^{-1}, respectively, which actually was lower than the NO_3^- leaching results from $beef_{baseline}$ by about 13 %. This measure also led to increase herbage yield in the beef system by about 400 kg ha^{-1}.

As another measure which may decrease NO_3^- leaching after application of the dairy cow manure on the beef system, we tested the removal of the mineral fertiliser application + spreading the dairy cow manure in March instead of February (measure B). A large reduction in NO_3^- leaching was predicted to occur (up to 4.6 mg l^{-1} and 11 mg l^{-1} in average and peak N concentration in the leachate, respectively). However, this measure resulted in smaller herbage yields (<1300 kg DM $ha^{-1}yr^{-1}$) than those produced by $beef_{baseline}$ farm.

8. 3.4. Risks of reducing NO_3^- leaching on other N forms (pollution swapping).

The Effects of applying single abatement measures A, B or C to farms under typical mineral fertiliser rates on N_2O and NH_3 losses are shown in Fig 2. Results indicate that application of any of these measures affected N_2O and NH_3 losses in various degrees (Fig 2). Application of abatement measure A gave substantial N_2O emissions rise in the 3 farms under typical mineral fertiliser rates. Nitrous oxide emissions increased over 60 % in all cases and over 100% in $Medium_{farm}$ and $High_{farm}$, after application of abatement measure A.

Measure B and C lead to small N_2O emissions rise when they were applied to $Medium_{farm}$ and $High_{farm}$ (<13%) and similar N_2O emissions rise when they were applied to Low_{farm}. Seasonally (in data not shown), whereas N_2O emissions patterns following measure A changed from those patterns found in baseline farms, resulting in polarising N_2O losses during spring-early summer, no seasonal effect was found after application of abatement measure B or C.

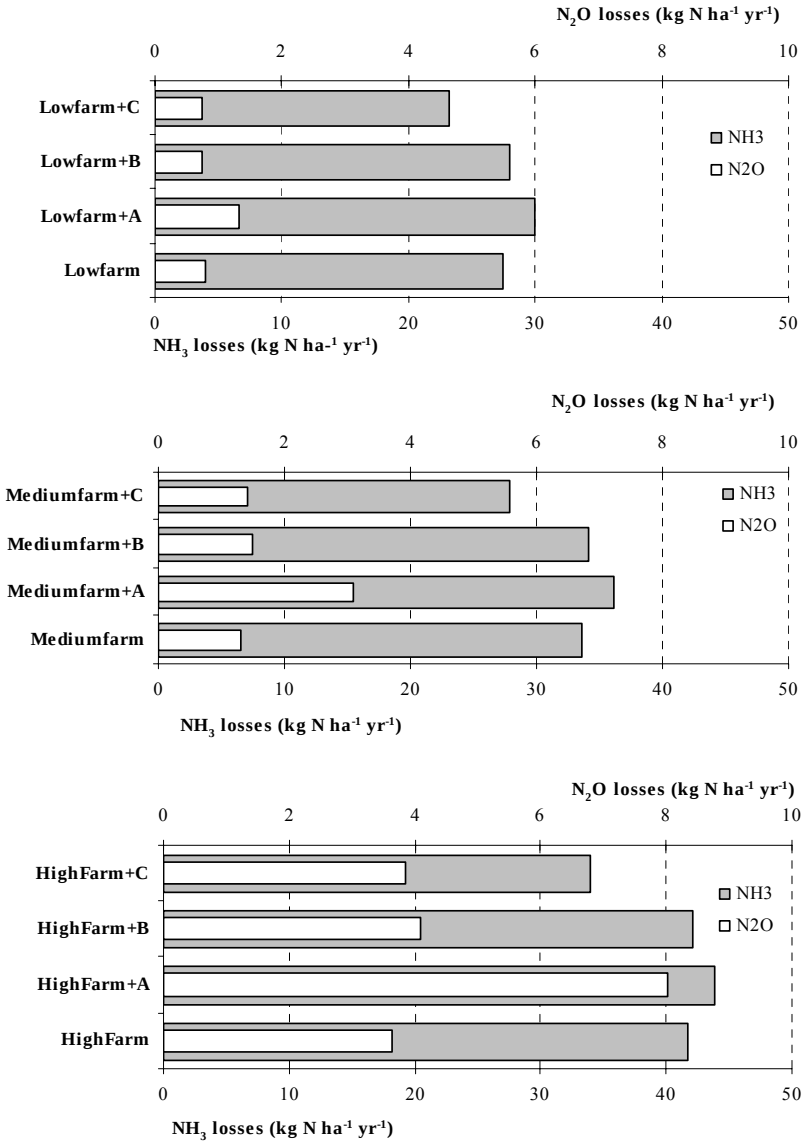


Figure 2. Comparison of NH_3 and N_2O losses between farms under typical mineral fertiliser rates (Low_{farm}, $Medium_{farm}$ and $High_{farm}$) and those farms plus A (optimisation of mineral fertiliser distribution), B (application of manure in March instead of February) and C (use of FYM instead of slurry) alternative abatement measures.

Although NH_3 emissions increased in the range of 5-9% after the abatement measure A was implemented, they remained similar after application of measure B and moreover, after application of measure C, emissions were reduced in the range of 15-20%.

8.4. Discussion

On one hand, a significant limitation for the application of the NVZ rules is their negative impact on herbage production. In Devon, we predicted a substantial herbage production decrease after application of NVZ rules compared with any baseline farm. Assuming that both NVZ_{farm} and baseline farms (Low_{farm}, $Medium_{farm}$ and $High_{farm}$) have the same total forage area, same type of dairy cows (in terms of milk yield and milk characteristics) and diet strategy, differences in herbage production would result in differences in farm herd size. Therefore, NVZ_{farms} would have fewer cows than baseline farms and, due to the strong positive impact of farm size on profitability (Gloy *et al.*, 2002; White *et al.*, 2002), reductions in their farm net income should be expected.

On the other hand, farms applying NVZ rules showed much smaller NO_3^- leaching losses than baseline farms. NVZ rules proved to be a good strategy to decrease NO_3^- leaching to values which would result in average NO_3^--N concentrations in the leachate< 11.3 mg l^{-1}, thus enabling Devon farmers to comply with the EU Nitrate Directive. It must be pointed out however that concentrations are very sensitive to different values of hydrologically effective rainfall (HER) values and therefore, drier and with similar temperatures' years than those simulated, for instance, would result in concentrations above the EU Nitrate Directive threshold. We also have to consider that there will be NO_3^- leaching variability once we consider scales broader than the farm unit. The catchment hydrology controls how the water from different sources is mixed and therefore, two identical farms under similar soil and weather conditions and the same load of N leached are also likely to result in different NO_3^- concentration levels.

Farmers utilising alternative abatement measures on farms under typical mineral fertiliser rates were at least if not more profitable than farmers following NVZ rules. Moreover, some

of these measures individually or in combination, proved to be effective enough to reduce NO_3^- leaching below the levels shown by farms following NVZ rules.

Optimisation of timing of mineral N fertiliser applications was the most successful alternative abatement measure acting singly to reduce NO_3^- leaching losses. Nitrate leaching losses from baseline farms were substantially reduced with no penalty on herbage production and moreover, in those farms using low and medium mineral fertiliser rates, NO_3^- average concentration values in the leachate were reduced to levels in compliance with the EU Nitrate Directive and these concentration values being smaller than those at farms following NVZ rules too.

Farms that did not optimise their mineral fertiliser were simulated to follow mineral fertiliser timing according to the last fertiliser recommendation system for England and Wales (RB209: MAFF, 2000). Our results suggest that the RB209 recommendation system, although it has been greatly improved from previous editions by being more site-specific and accounting for some balance between profitable agricultural production and environmental protection, it failed to be sufficiently tailored to agroclimatic areas and soil types in grasslands. Improvement of the current recommendation system would necessitate a more site-specific approach and a stronger emphasis from production/economic targets to a system driven, to a greater degree, by limitation of the undesirable N exports (Brown *et al*., 2005).

The criterion of mineral fertiliser optimisation used for this study is 'highest herbage with best N-use efficiency ratio'. This ratio is defined as 'total plant N/ total N losses'. The reduced N loss was mainly attributable to reduced leaching. However, there are two important consequences of optimisation. One is that the most efficient patterns of herbage production are not necessarily ones that are readily utilised on the farm through the farmer's normal stock management regimes – greatest herbage production is more polarised to the spring months (data not shown). The second is that the effects of such polarisation could be to increase N loss by the alternative route (leaching- denitrification and nitrification (N_2O)-volatilisation (NH_3) 'pollution swapping'). In fact, both N_2O and NH_3 losses increased after optimisation of mineral fertiliser. Ammonia volatilisation increase was much lower than that increase in N_2O emissions. NGAUGE simulates the effect that high NO_3^- concentrations inhibit N_2O reduction to N_2 (Bandibas *et al*., 1994) and thus, polarising larger mineral fertiliser rates (i.e. in spring) resulted in large denitrification losses as N_2O emissions and

small losses as N_2. The main question which still remains is, however, whether this level of pollution swapping is still acceptable. There are no explicit thresholds for NH_3 and N_2O as there is for NO_3^- concentrations in waters.

Dairy cows have different nutrient requirements depending on their lactation stage and thus the mismatch in time of the grazed grass which is on offer and the needs that the cow have must be effectively managed by either changing calving patterns and/or grazing intensity. For example, if we compare the temporal pattern of offered grazed grass per hectare in both baseline and mineral fertiliser-optimised farms (Fig 3) to that of required DM for a typical dairy cow which calves in spring (Fig 4), we can see that, irrespective of the farm type, this particular herbage pattern would maximise the match between grazed DM and DM requirements for a herd calving in March or April. However, differences in herbage DM on offer during the grazing season when comparing baseline farms with farms under optimised mineral fertiliser rates, although small, may drive herd management changes if the farmer wants to maintain the same level of milk production.

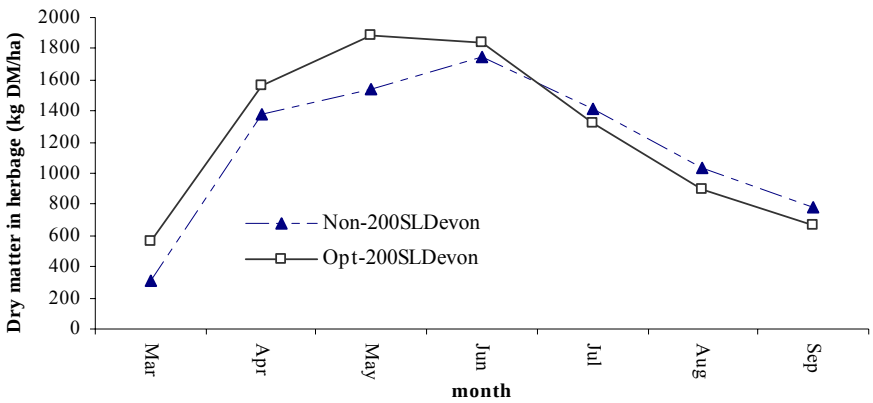


Figure 3. NGAUGE prediction of herbage dry matter on offer distribution during the grazing period of a grazed grass field annually receiving 200 kg N ha^{-1} as mineral fertiliser. This mineral fertiliser rate is distributed according to RB209 (---▲----) and according to optimised distribution by NGAUGE (---□----).

Changes in manure management other than those proposed by the NVZ rules, to a smaller extent and only in some cases, proved to be able to decrease substantially NO_3^- leaching losses resulting in gains or small penalties (i.e. exporting 100% of manure) in herbage production. As a single abatement measure exporting >50 % of the manure produced during housing or changing one winter slurry application from February to March allowed the

farmer to obtain average concentrations in the leachate <11.3 mg l^{-1} (EU Nitrate Directive threshold) using low and medium typical mineral fertiliser rates. Moreover, even though these 2 measures did not generally result in smaller NO_3^- leaching losses than the NVZ rules, they enabled the farmer to produce much more herbage than farms under NVZ rules and thus, support a larger herd. Farms, nevertheless, could be constrained if their manure storage systems do not have sufficient capacity to ensure the necessary flexibility in application dates or farmers may be discouraged if they consider that March manure applications compromise grass-silage quality (Chambers *et al*., 2000).

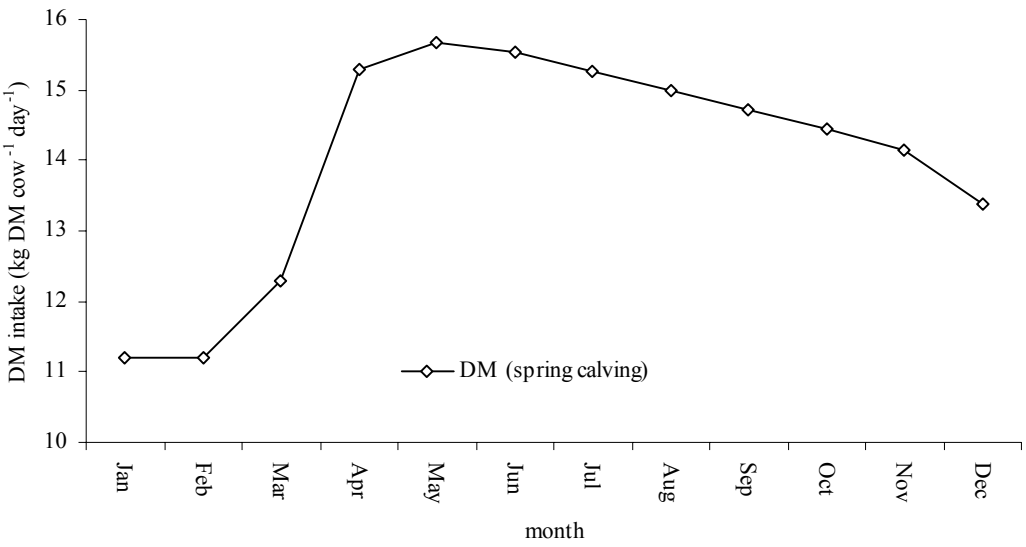


Figure 4. Dry matter requirements per day for the different weeks of lactation of a dairy cow calving in March with annual milk yield of 7300 L (After calculations using equations from Thomas, 2004).

Changing one winter slurry application from February to March generally resulted in small increase in N_2O and NH_3 losses compared with baseline farms. The use of FYM instead of slurry resulted in a small increase in N_2O emissions and small decrease in NH_3 losses. However, as a single measure, it did not substantially decrease NO_3^- leaching. Our results then suggest that even though the proportion of available N in FYM compared with slurry is lower, the application of FYM to grasslands during the closed period still leads to a substantial risk of NO_3^- leaching. Moreover, stored solid manure heaps can be a significant source of N_2O (Yamulki, 2006) and since our calculations did not consider losses during the

storage of manure we should expect much larger N_2O losses from FYM-based systems than those from slurry-based systems.

Other countries, such as the Netherlands, have imposed a ban on spreading any animal manure on agricultural land during the whole winter to reduce NO_3^- leaching.

Within a year, a simple approach to manure and mineral fertiliser management in order to decrease NO_3^- leaching could target replacing mineral fertiliser with slurry. Nevertheless, in a time-based more integrated strategy, the tactical N approach should take account of the effects of conserving available N over the long term of any enhanced build up of potentially mineralisable N (Jarvis *et al*., 1996b) and therefore, the goals should be focused on not so much replacing the mineral fertiliser N with corresponding amounts of slurry N, but on maintaining the levels of fertility in the soil throughout the years. Thus, reducing N losses of manure, prior to application, and avoiding uneven manure spreading could allow some fertiliser application reduction without altering the fertility level. Moreover, in the long term, when manure applications are continued, equilibrium is established between the annual organic inputs and the annual mineralisation and, should manuring be interrupted, residual N in the soil would be rapidly depleted (Schröder, 2005). The larger the ratio of (reactive) C and (reactive) N, the longer it may take to reach this equilibrium and hence, manure composition knowledge is a must to avoid the risk of underestimation of both the manure fertiliser value and the environmental impact. Uncertainties in herbage production results may also be a major discouragement for farmers to rely more on manure fertilisation. Schröder *et al*. (2005), for instance, indicated that the potential saving of 25 kg N ha^{-1} in mineral fertiliser by replacing it with manure N could imply a 20 kg N ha^{-1} risk of reduction in N yield (2-3 % in DM yield), which, in general, would be unacceptable for farmers.

Long-term impact of FYM is more difficult to be predicted (Schröder and Stevens, 2004). Some combination of alternative abatement measures resulted in large reductions in NO_3^- leaching and large increases in herbage production. For instance, in farms under low and medium typical mineral fertiliser rates more than half of the combination of measures resulted in lower NO_3^- leaching values than those at farms following NVZ rules.

Exporting manure to less intensive beef areas also proved to be an effective method in order to decrease NO_3^- leaching from dairy systems. However, if the beef system did not apply any abatement measure for NO_3^- leaching, some side-effects were observed. Nitrate

leaching increased in the beef system although it did not exceed the EU Nitrate Directive threshold. Exporting manure might not be the best choice where the amount to be transported off the farm is large and could pose environmental or health risks to another area or be economically undesirable. In one of our examples we propose as a possibility to transport 30 % of the total dairy manure to the beef system. If the manure receiving beef system is sufficiently close to the dairy farm system we should expect little impact in terms of pollution through transport. However, further studies should be carried out to evaluate health risks and economic risks.

Experiences such as in the Netherlands, which has developed the most sophisticated system for distribution, control and accounting of manures from the southern parts of the country to the northern part where there is less livestock and more arable crops, has evidenced disease concerns (Burton and Turner, 2003). To overcome this shortcoming, low-cost reliable manure decontamination should be used. Other, more subjective issues, such as the social acceptability of manure waste transport is also an issue that needs further analysis. The Danish derogation case (reference of commission 18-11-02), which allowed the application of livestock manure to a level of 230 kg N ha^{-1}, had a reference on denitrification stating that compliance with the maximum of 11.3 mg l^{-1} of NO_3^--N in groundwater was ensured considering denitrification. Nitrate leaching reduction through the NGAUGE fertiliser optimisation tool proved to be effective but it could be further improved by both implementing new algorithms that could target NO_3^- leaching + N_2O instead of total N losses and setting acceptable limits for N_2O values.

8. 5. Conclusions and policy implications

In the context of a change towards an NVZ_{170} Nitrate Directive, some European countries have already requested a derogation from this manure limit, postulating that the 11.3 mg N L^{-1} limit concentration may be met with higher manure application rates. For example, based on a high N-uptake of grass under Dutch conditions, the Netherlands government asked the EU to allow a manure input of 250 kg N ha^{-1} yr^{-1} in grasslands (Aarts, 2003). Our study shows that in England the NVZ_{170} rules would generally have a significant negative impact on the farmer economy and moreover, they would not be necessarily site-specific enough to

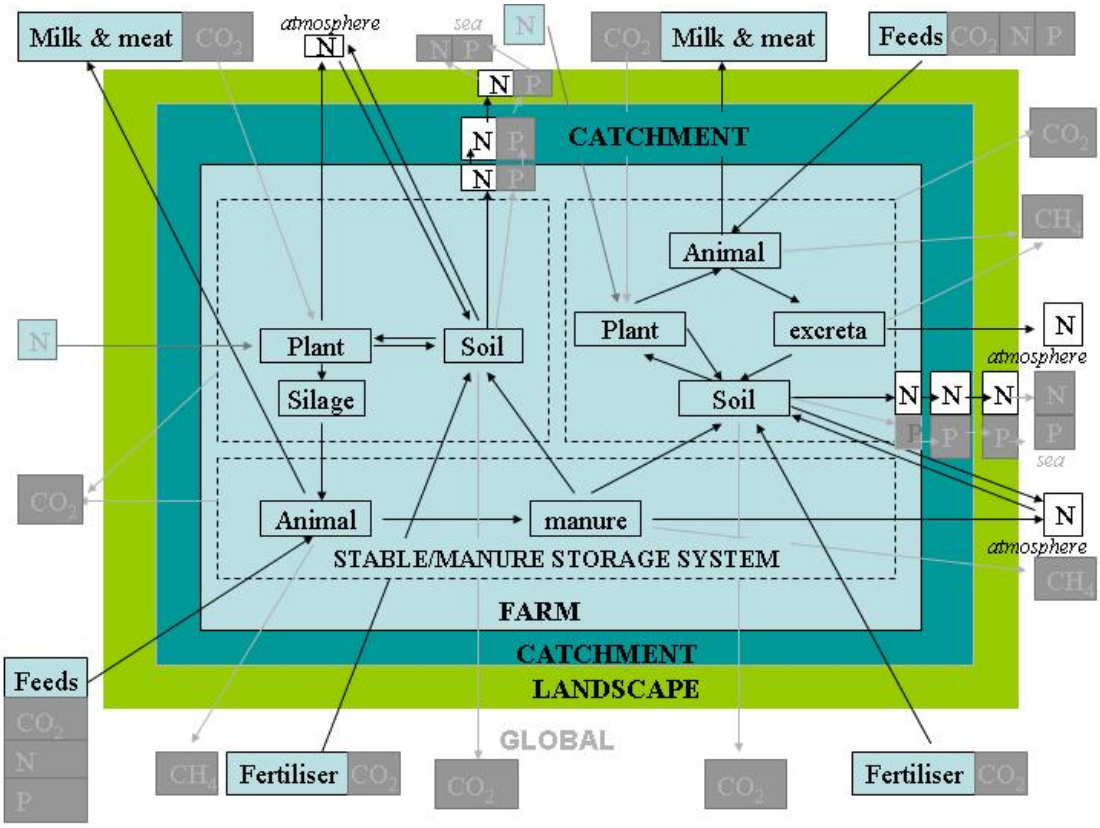
make farmers comply with the EU Nitrate Directive. We hence propose that alternative NO_3^- mitigation measures are considered as a way to both comply with the Nitrate Directive and enable farmers to remain viable. We also stress the importance of accounting for differences in climate, soil types and management when the policy is implemented. We showed that there is scope for improving management of fertiliser, both as mineral and/or manure, on farms under low and medium current fertiliser rates up to NO_3^- and herbage levels which result in an improvement against farms following NVZ_{170} rules. Some of the manure measures, however, may in some cases imply negative side-effects such as additional capital investment (larger manure storage pits) or compromise objectives of the new CAP reform (i.e. meet statutory animal welfare regulations: Oglethorpe, 2005) by transportation of manure.

NGAUGE proves to be a suitable tool to explore the effect of management, climate and soil not only on NO_3^- leaching and herbage yield, but also to account for other forms of N pollution without unacceptable pollution swapping. Other alternative measures (i.e. reseeding in spring against autumn, use of nitrification inhibitors and/or reduce grazing day length and season), not taken into account in this paper, could be explored in future studies.

Challenges to comply with the Nitrate Directive and still remain viable are considerable but still smaller to those compared to comply with the EU WFD. Although the EU WFD does not explicitly refer to NO_3^- concentrations but to the good ecological status of waters, this will necessarily imply even stricter threshold values of NO_3^- and very small threshold values of P. There is a need hence for new modelling tools which can study the effect of not only land use management on NO_3^- and P at different scales (from the farm to the regional scale) but are also capable of integrating other crucial issues (i.e. NH_3, greenhouse gases (GHG) emissions, animal welfare, socio-economic, biodiversity and soil erosion).

Chapter 9

Modelling N fluxes at the landscape scale



9. Modelling N fluxes at the landscape scale

Abstract

The distribution and impacts of different nitrogen pollutants are inextricably linked. To understand the problem fully, the interactions between the different pollutants need to be taken into account. This is particularly important when it comes to abatement techniques, since measures to reduce emissions of one nitrogen pollutant can often lead to an increase in another. This project represents a step towards greater understanding of these issues by linking together new and existing nitrogen flux models into a larger framework. The modelling framework has been constructed and some of the nitrogen flows between fields, farms and the atmosphere have been modelled for a UK study area for typical farm management scenarios.

9.1. Introduction

Processes within the nitrogen cycle interact and therefore factors affecting one process can have knock-on effects throughout the system (Erisman *et al*., 2003). Studying one process in isolation overlooks these interactions and, therefore, the behaviour of the system cannot be accurately assessed. One example of the problems this can cause is the effect of abatement techniques for reducing losses of nitrogen (N) to the environment, since there are several techniques that can reduce the loss of one N-containing pollutant, but increase the loss of another. An example of one of these trade-offs is the use of slurry injection techniques that reduce the losses of ammonia (NH_3) to the atmosphere, but can increase the potential for nitrate (NO_3^-) leaching and nitrous oxide (N_2O) emission. As well as considering the interactions between processes, it must be borne in mind that these processes and interactions occur in three dimensions and cover spatial scales ranging from the plot-scale to the catchment-scale and larger. To study these effects, a modelling framework has been set up incorporating different process-based models to simulate nitrogen flows at the landscape-

scale (i.e. at a scale that includes different types of land use). This paper documents the development of this modelling framework and presents the first results of the landscape level assessment.

9.2. The LANAS integrated model

The LANAS (Landscape Analysis of Nitrogen and Abatement Strategies) integrated model is designed to simulate the flows of N through an agricultural landscape, incorporating the flows between fields, farmyards, the atmosphere and groundwater. The LANAS model incorporates modifications of four existing N flow models and one process-based model developed specifically for the task. The four modified models are SUNDIAL (Simulation of Nitrogen Dynamics In Arable Land: Smith *et al*., 1996), NGAUGE (nitrogen flows in grassland field systems: Brown *et al*., 2005), LADD (Local Atmospheric Dispersion and Deposition model: Hill, 1998) and INCA (Integrated Nitrogen Catchment model: Whitehead *et al*., 1998). The newly developed model is the FYNE (Farm Yard Nitrogen Emissions) model, which simulates the N emissions from farmyards. The inputs and outputs of the component models are linked through a spatial database that holds and processes information on land use, farm management, nitrogen flows and meteorology. Fig 1 shows the linkages between the component models and the flows of N-containing pollutants between the fields, farmyards, atmosphere and groundwater.

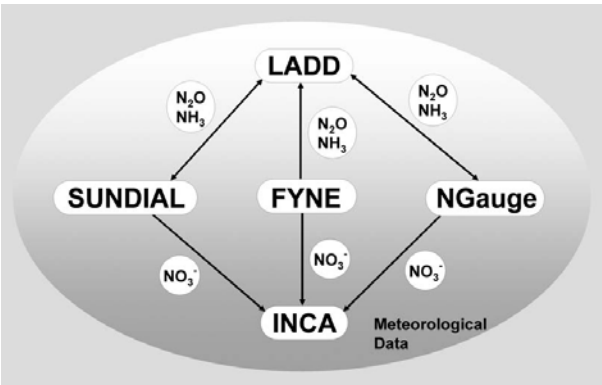


Figure 1 . Linkages between the component models of the LANAS integrated model and the flows of N-containing species between them.

The component models include additional N flows such as crop and animal N production. These are not shown in Figure 1 since they do not interact with the flows in the other models.

The component models run on differing time-steps ranging from daily to monthly. The LANAS integrated model operates on a monthly time-step in order to incorporate the N flows from all of the component models. Two study areas in the UK were chosen for the application of the LANAS model: one in western England, in an area of cattle and sheep farming and one in eastern England, in an area of pig, poultry and arable farming. Monthly mean NH concentration measurements were made using ALPHA samplers (Tang *et al*., 2001) throughout the study areas for a period of 13 months as a means of validating the LANAS model simulations. The integrated modelling framework is still being developed and currently contains the two models; the FYNE model and the LADD atmospheric dispersion model linked through the spatial database. The results presented in this paper are mean values for the 13-month measurement period for the eastern study area from this two-component model.

The FYNE model is a N mass flow model that estimates NH_3 losses to the atmosphere. The model traces the flow of nitrogen from the initial excretion by animals to the storage of the slurries and manures removed from the livestock housing and simulates NH_3 losses to the atmosphere using an emission factor approach. The emission factors have been based on the data from the UK Defra-funded project NARSES (National Ammonia Reduction Strategies Evaluation Systems: Webb *et al*., 2002) which has modified the emission factors of Misselbrook *et al*. (2000) to take into account additional experimental studies. The model takes inputs of livestock type/numbers, housing type/duration, manure/slurry storage methods and the import/export of manures and slurries. The outputs of the model are the NH_3 losses to the atmosphere from livestock housing, hard standings (solid surfaces used for livestock movements) and manure/slurry stores for all common livestock types.

The LADD model is described in detail by Hill (1998) and Dragosits *et al*. (2002) and therefore only a brief description follows. LADD is a Lagrangian model that simulates the atmospheric dispersion of NH_3 as well as the deposition to the surface using input data of wind statistics (mean wind speeds and wind direction probabilities), land use and background concentrations (taken from the FRAME national dispersion model of Singles

(1996)). The model can be run at various time-steps (typically a month or a year) and the outputs of the model are spatial concentration fields at several heights, NH_3-N deposition plus the budget of NH_3-N export. LADD was applied here at a grid resolution of 25 m.

9.3. Spatial Database and Geographical Information Systems

The component models of the LANAS model are linked through a MS Access database that is itself linked to a geographical information system (GIS). The resulting spatial database stores and processes four kinds of data: landcover, farm/field, nitrogen flow and meteorological data.

The component models of the LANAS model are linked through a MS Access database that is itself linked to a geographical information system (GIS). The resulting spatial database stores and processes four kinds of data: landcover, farm/field, nitrogen flow and meteorological data.

The landcover data were obtained by digitising landscape features (field boundaries, farmyards, roads, rivers etc.) from an orthophoto-mosaic (planimetrically corrected mosaic of 80 aerial photographs). Once the features were identified they were entered into the spatial database as a collection of polygons with a unique ID along with the landcover class for the polygon. Since the LADD model was applied on a 25 m grid, the attributes of each grid-square (land cover type and NH_3 emission flux) are also derived from the corresponding polygon. Farm and field data were obtained from farm survey questionnaires completed by farmers within the study area. Data include details of livestock (type, numbers, and housing), the fate and storage of manures/slurries and the management of the different fields (field use, animal numbers, crop type, amount of fertiliser applied, amount of manure applied and the dates of management activities). These data are linked to the respective polygons on the landcover map. The N flow data contain the amounts and form of nitrogen flowing between the different models for each month modelled. These data are a component of the input and output data for the models. The meteorological data stored in the spatial database contain information on the wind statistics (for the LADD model) and the temperature, rainfall, and potential evapotranspiration (for the field models).

9.4. Application of the LANAS integrated model

The execution of the LANAS model for the eastern study area with the linked FYNE and LADD models was conducted in 3 steps. Firstly, the FYNE model was run for all of the identified farms in the study area for each month. For the farmyards where survey data were not available, estimates of the type and number of livestock were made from interpretation of the aerial photographs. The total emissions from each farmyard were summed over the 13 months of the measurement period. The second stage involved the estimation of NH_3 emissions from non-farmyard sources. Since the LANAS model does not currently incorporate the field models (SUNDIAL and NGAUGE), the NH_3 emissions from the fields have been estimated using a variety of techniques. These techniques included using information obtained from the farm surveys, determination of field use from the aerial photographs and information on recommended fertiliser use (Defra, 2000). The third stage of the process was the execution of the LADD model with these emission rates.

The field and farmyard emissions were combined to give the total emission for each polygon of the landcover map (Fig 2) and the emissions for the corresponding 25 m grid-squares were used as input for the LADD model.

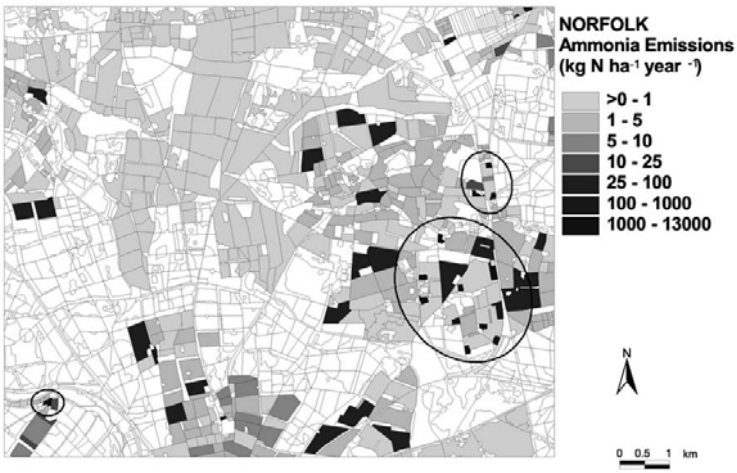


Figure 2. Annual ammonia emission fluxes in the LANAS integrated model. Selected intensively managed livestock farm systems are shown ringed.

Fig 2 shows that the largest estimated sources of NH_3 are the intensively managed farm systems such as livestock housing. Other significant sources are the fields where land spreading of slurries or manures takes place.

Fig 3 shows the modelled and measured mean NH_3 concentrations at a height of 1.5 m for the measurement period (February 2001-February 2002). The concentration map resembles the emission map in many respects reflecting the rapid dispersion of NH_3. The highest modelled concentrations are around the intensively managed farm systems and there are also significant concentrations in the vicinity of fields on which manure spreading occurred.

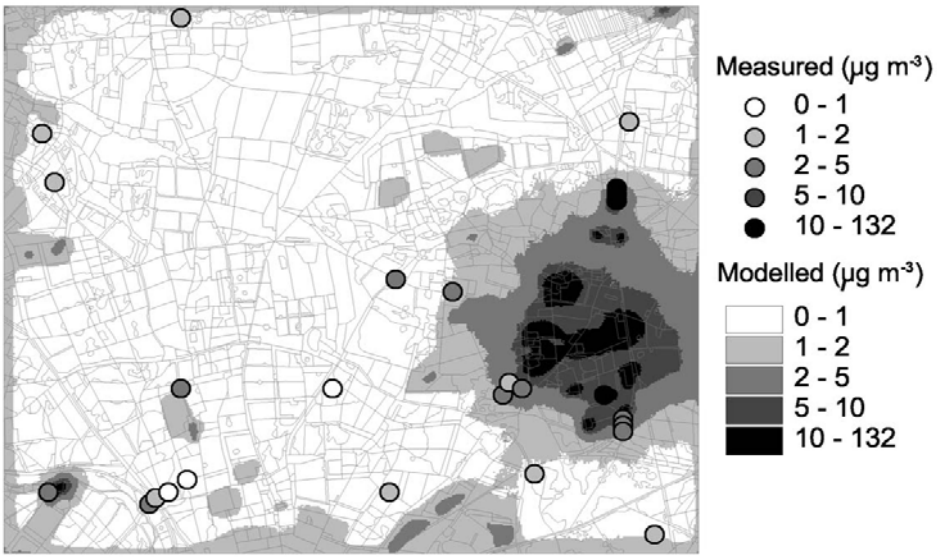


Figure 3. Spatial distribution of measured and modelled NH_3 concentrations for the eastern study area.

Figure 4 shows the modelled concentrations plotted against the measured values. This figure shows that the model is over-predicting the concentrations near sources (the highest concentrations) and under-predicting further away from sources, where the concentrations are lower. There are three possible reasons for this: i) an underestimation of the atmospheric dispersion, ii) uncertainty in the farm survey data, iii) uncertainty in the field emissions input to LADD due to the fact that the field models are not incorporated in the LANAS model or iv) uncertainty in the farmyard emissions due to uncertainties in the emission factors used. An underestimation of dispersion could be due to the lack of crosswind dispersion in the

model or the turbulence caused by buildings near sources (e.g. farmyards) which cannot be dealt with properly by the model.

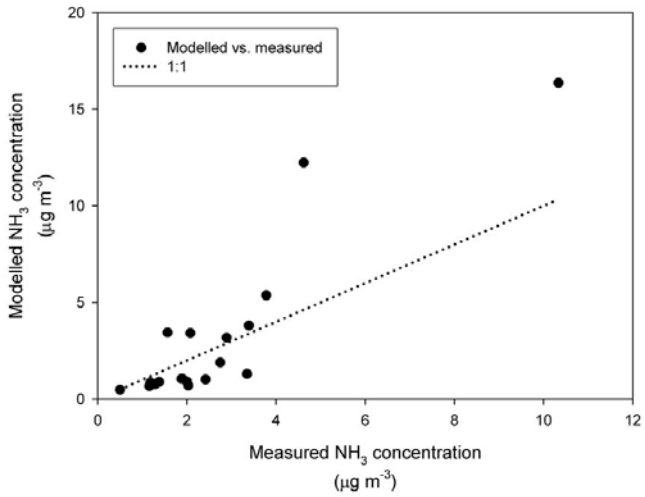


Figure 4. Modelled vs. measured NH_3 concentrations for the eastern study area.

The NH_3-N deposition estimates obtained from the model show that the highest predicted deposition occurs close to the farmyard sources, particularly in areas of semi-natural or woodland vegetation (due to the large surface roughness and small deposition resistance of these types of vegetation).

9.5. NH_3 abatement scenarios

The LANAS model has not yet been applied to simulate the abatement of NH_3-N deposition, but a parallel analysis by Dragosits *et al*. (2006) has shown that using buffer strips (areas of reduced NH_3-N emissions) and tree-belts around the perimeter of farms and nature reserves can reduce the transfer of nitrogen between the farm and nature reserve. Theobald *et al*. (2001) have also studied the potential of using tree belts to abate net NH_3 emissions from farms and estimate, from measurements at an ammonia release experiment, that the trees recaptured a few percent of the emitted ammonia. To assess the potential applicability of abatement techniques, the integrated model results can be combined with the socio-economic

study of abatement of nitrogen losses from poultry farms, which is currently being carried out by the University of Cambridge (Angus *et al.* 2003).

9.6. Model development

This paper reports the first stage of development of the LANAS integrated model. Current work is focussing on the incorporation of the two field models: SUNDIAL and NGAUGE. This will hopefully improve the predicted NH_3 concentrations. Following this development, the models will be modified to estimate the losses of other N-containing pollutants (N_2O and NO_3^-) and the INCA model will be applied to estimate the flows of NO_3^- in the catchment. The target is for the integrated model to be run on a monthly time-step to simulate the effect of different abatement scenarios on the flows of N.

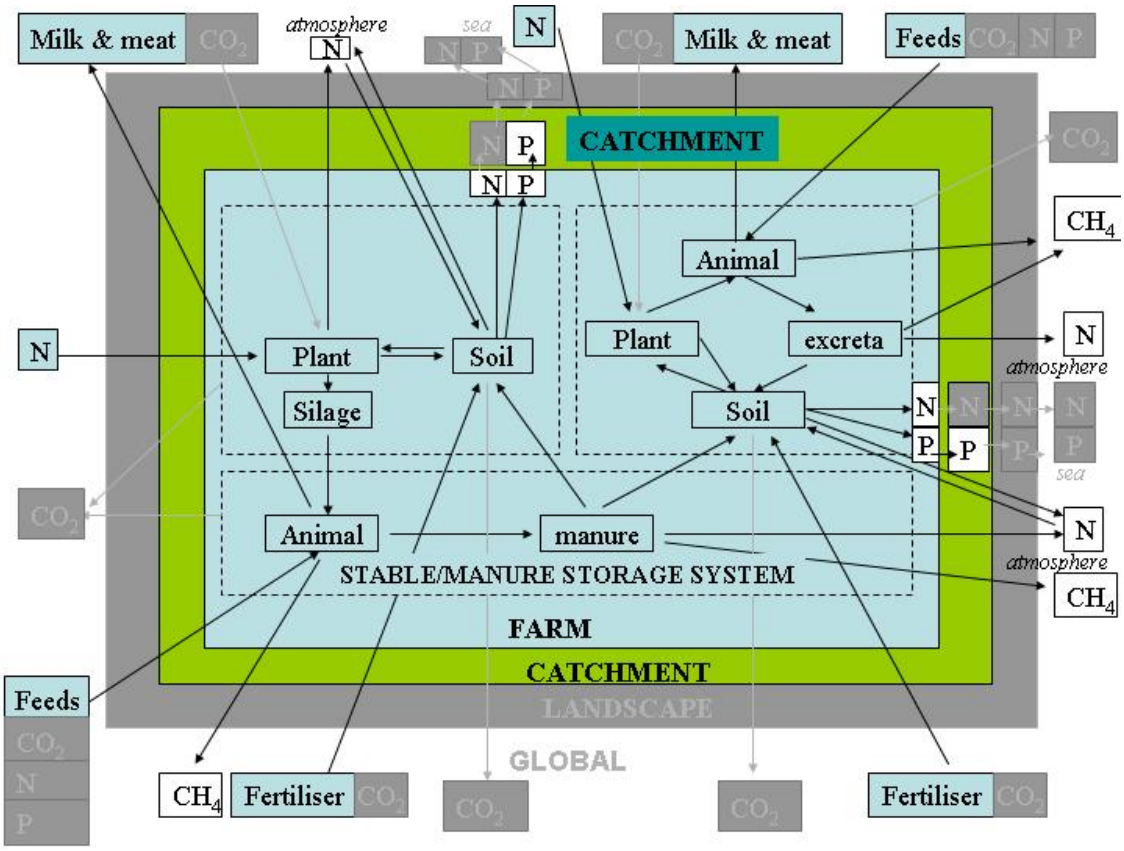
9.7. Conclusions

Due to the interactivity of landscape N flows, the whole nitrogen system needs to be studied to investigate the potential of scenarios to reduce N losses to the environment. Since N flows occur in 3 dimensions over distances greater than the farm or plot-scale, they should be studied at the landscape-scale or greater. This work has shown that the LANAS modelling framework can be used to study flows of N from the surface to the atmosphere and back to the surface. Model predictions can potentially be improved by the incorporation of the field models into the modelling framework.

Detailed farm management data are required to model all management activities and identify local sources. Concentrations and deposition of NH_3 in agricultural landscapes are highly localised so that the spatial interactions (including those with N_2O and NO_3^-) need to be considered. The effects of other pollutants such as N_2O and NO_3^- will have impacts over greater distances. Integrated N modelling at the landscape scale is a useful approach to study the potential of abatement techniques and trade-offs.

Chapter 10

$SIMS_{DAIRY}$: A modelling framework to identify new integrated dairy production systems.



10. $SIMS_{DAIRY}$: A modelling framework to identify new integrated dairy production systems.

Abstract

Sustainability in UK dairy farming is no longer secured by traditional management focused on production of commodities. Society awareness, legislations and consequently markets demand farming systems which can deliver attributes such as: clean environment, high biodiversity, picturesque landscapes, good animal welfare and high quality of product and soil. Not only are many of these attributes (i.e. EU Nitrate Directive) unachievable under existing systems and certain edapho-climatic circumstances (i.e. conventional UK dairy farm on sandy soils) but they are also interrelated to each other so that getting one of these goals may often compromise another and moreover, pose a high risk to the economic viability of the farm.

Farm level modelling is a useful tool in order to bring all of this complexity into an operational and scientific *modus operandi*. Nonetheless, appropriate models to objectively determine the sustainability of dairy farming systems are still lacking. In order to fill this gap, a new model ($SIMS_{DAIRY}$) has been developed. $SIMS_{DAIRY}$ integrates existing models for nitrogen (N) [ammonia (NH_3), nitrate (NO_3^-) leaching, nitrous oxide (N_2O), nitric oxide + nitrogen dioxide (NO_x)] and phosphorus (P), equations to predict methane (CH_4) losses and the cows' nutrient requirements, 'score matrices' for measuring attributes of biodiversity, landscape, product quality, soil quality and animal welfare and an economic model. $SIMS_{DAIRY}$ is capable of optimising dairy management factors in order to find more sustainable systems.

In this paper we describe the $SIMS_{DAIRY}$ modelling framework in terms of nutrient flows and transformations of a dairy farm system and the basis for the construction of the matrices to assess the less quantitative attributes that define sustainability. A sensitivity analysis was carried out with selected farm environmental/management (E/M) variables. This analysis showed that $SIMS_{DAIRY}$ predicted results (i.e. losses, net farm margin, and sustainable

attributes) with large sensitivity towards a vast number of farm E/M variables and thereby, it is a useful tool to study the complexity of the dairy farm systems.

10.1. Introduction

Western Europe dairy systems are facing numerous problems due to continuing intensification. It is fundamental to consider not only the productivity/economic aspect of dairy farming production but also other attributes which define farm sustainability as a whole. Dairy farming systems must hence: (i) ensure an adequate net farm income to support an acceptable standard of living for farmers, (ii) result in acceptable environmental impacts [i.e. satisfy pressures from EU Nitrate Directive, EU Water Framework Directive (WFD), Kyoto Protocol and Gothenburg Protocol], (iii) produce food that is safe, wholesome and nutritious, thereby promoting human health, (iv) promote a good level of animal welfare, (v) meet social expectations of picturesque landscapes (vi), enhance or maintain high biodiversity standards, (vii) improve or maintain the quality of the soil, and strike a reasonable balance among these key attributes (Bergström *et al.*, 2005).

Common Agricultural Policy (CAP) reforms in 1992 obliged EU member states to establish aid schemes (agri-environment measures) under which farmers obtain payments in return for complying with certain management practices. Designation of Environmentally Sensitive Areas is the oldest of a series of measures operating in the UK (Macadam *et al.*, 2001). The latest CAP reform (Directive 2003/1782/EC) focuses not on increased production, but rather on food quality and choice, environmental benefits and sustainable rural development. As a result, there is a window of opportunity to reconsider the balance between agricultural production and biodiversity management, to seek to redress the problems for biodiversity without reducing the capacity to meet the coming challenges of global change and population increase (Firbank, 2005).

Not only are many of these attributes unachievable under existing systems and certain edapho-climatic circumstances but they are also so interrelated that achieving any one of these goals may often compromise another and moreover, pose a high risk to the economic viability of the farm.

Farm level modelling is a useful tool in order to bring all this complexity into an operational and scientific *modus operandi*. Nonetheless, appropriate models to objectively determine the sustainability of dairy farming systems are still lacking. In order to fill this gap, a new model ($SIMS_{DAIRY}$) has been developed (del Prado *et al.,* 2006d). $SIMS_{DAIRY}$ integrates existing and new models, equations and 'score matrices' to optimise dairy management factors in order to find more sustainable systems.

Although linking these concepts to practical actions and decisions is not easy, mathematical models offer this capability. Different models have been produced to analyse economic and ecological sustainability on dairy farms (Hansen *et al*., 1992; Berentsen and Giesen, 1995; Osei *et al.,* 2003; Rotz *et al.,* 2005a) but have not dealt with the whole overall sustainability. Other approaches (MacNaeidhe and Culleton, 2000, van Calker *et al*., 2004; 2005, 2006), based on the use of indicators/parameters, have studied sustainability of dairy systems on a more holistic way. However, although they incorporate very useful sustainability functions and hence the criteria for sustainability are quite robust, their lack of mechanisms to simulate processes makes them too broad in most cases. Therefore, there is still a need for more flexible/robust modelling tools which can integrate knowledge (existing modelling approaches and new ones) leading to an understanding of a complex system such as the overall sustainability of a dairy farm.

The objective of this study is to describe and give example of use of a new modelling framework which is capable of: a) exploring combinations of farm attributes and nutrient managements that lead us to a sustainable farm and b) indicating ways/impacts to overcome lack of sustainability.

10.2. Model framework development

Sustainable and Integrated Management Systems for Dairy Production ($SIMS_{DAIRY}$) is a new modelling framework which integrates existing models for nitrogen (N) (NGAUGE: Brown *et al*., 2005; NARSES: Webb and Misselbrook, 2004), phosphorus (P) (PSYCHIC: Davison, *in press*) and farm economics (A. Butler, *pers. comm*), equations to simulate ammonia (NH_3) losses from manure application (Chambers *et al*., 1999), predict methane (CH_4) losses

(Chadwick and Pain, 1997; Giger-Reverdin *et al*., 2003) and cows' nutrient requirements [Feed into Milk (FiM) (Thomas, 2004)], 'score matrices' for measuring sustainability attributes of biodiversity, landscape, product quality, soil quality and animal welfare.

NGAUGE (Brown *et al*., 2005) is an empirically-based model which simulates monthly N flows within and between the main components of a grazed grass field according to user inputs describing site conditions and field management characteristics. Outputs of NGAUGE include a field and N fertiliser recommendation, comprising amounts of N in both production [N and dry matter (DM)] and loss components of the system [nitrate (NO_3^-) leaching, NH_3, dinitrogen (N_2), nitrous oxide (N_2O) and nitric oxide + nitrogen dioxide (NO_x)]. This optimisation enables user-specified targets of herbage, N loss or fertiliser use to be achieved while maximising efficiency of N use. NARSES (Webb and Misselbrook, 2004; Webb *et al*., 2006) is a model which estimates the magnitude, spatial distribution and time course of agricultural NH_3 emissions, together with the potential applicability of abatement measures and their associated costs. Phosphorus and Sediment Yield Characterisation In Catchments (PSYCHIC) is a model which predicts the risk of diffuse pollution from a source area by estimating source, mobilisation and delivery of P and sediment: phosphorus inputs in manure and fertilisers and soil residual P, the mobilisation of phosphorus and sediment through dissolution and soil detachment and the delivery of dissolved and particulate P, and associated sediment, to watercourses in surface and subsurface runoff (Davison *et al*., *in press*). PSYCHIC takes account of management practices as well as landscape factors and climate to predict the spatial and temporal distribution of flow, sediment and P, on a monthly time step.

$SIMS_{DAIRY}$ main components can be classified in 2 different hierarchical levels: modules and submodels. Modules represent the highest level of control and comprise the code in which the main general functions of $SIMS_{DAIRY}$ are represented ($MOD_{GENERATOR}$, $MOD_{SIMULATOR}$ and $MOD_{EVALUATOR}$). The submodels carry out specific tasks within $SIMS_{DAIRY}$ (i.e. predict N flows within a grazed grassland field) and are either modifications of existing models or new developments ($SIMS_{MANAGEMENT}$, $SIMS_{NGAUGE}$, $SIMS_{PSYCHIC}$, $SIMS_{ECONOMICS}$, $SIMS_{SCORE}$ and $SIMS_{RANK}$).

The whole framework operates automatically and, except for $SIMS_{PSYCHIC}$ submodel which is an external link through a Visual Basic (VB) Dynamic Linking Library (DLL) file,

has been coded into a program compiled with Borland Delphi 5.

10.2.1. Modules

MOD$_{GENERATOR}$ generates management options to be optimised. Management can be optimised as a single option or in combination through a matrix (Man i,j). The indices *i* and *j* represents different '*i*' management options and '*j*' values, respectively. For any given farm, existing management factors (i.e. manure application on different land use areas) and/or genetic traits (i.e. plants with enhanced ability to absorb N) can be optimised. The whole list of optimisable factors together with the main input environmental/management (E/M) variables data can be viewed in the input screen interface of SIMS$_{DAIRY}$ (Fig 1).

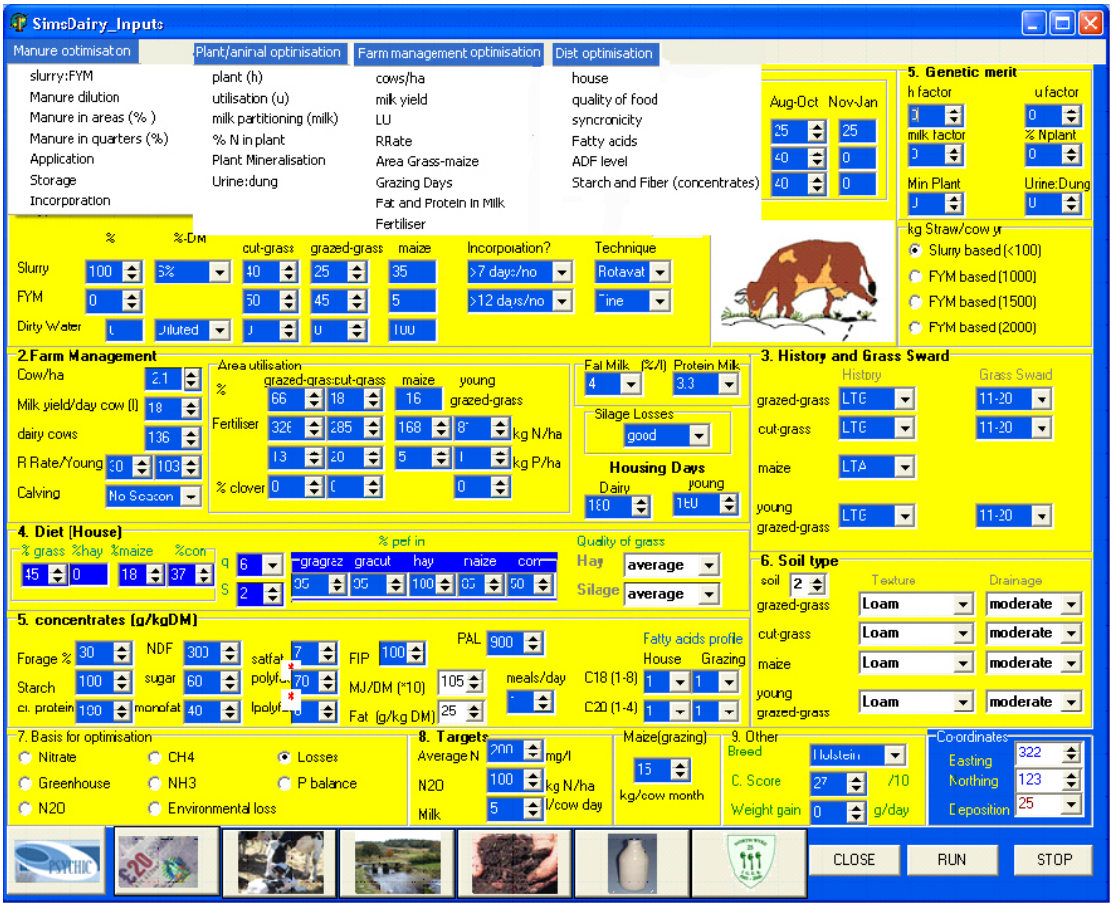


Figure 1. Input-screen of SIMS$_{DAIRY}$ with the main input data E/M variables used for the simulation of nutrient flows, transformations and losses and the whole list of optimisable farm factors (in white).

$MOD_{SIMULATOR}$ main tasks are to simulate within the farm: (i) the nutrient and energy flows, the impact of these flows on sustainability issues (i.e. milk quality) and the effect on farm profitability.

$MOD_{EVALUATOR}$ ranks farms management values by best match to a user-weighted multiple criteria result [i.e. Min CO_2 eq-GWP/L milk or max environmental index (Van Calker *et al.*, 2006)].

10.2.2. Submodels

$SIMS_{MANAGEMENT}$ is a new development which is used to enter the main data inputs, initialise E/M variables, calculate nutrient/energy flows at the herd level and link the main interactions among submodels.

$SIMS_{NGAUGE}$ is a modification of the NGAUGE model (Brown *et al.*, 2005) by which, DM and N plant yield and N losses (N_2, N_2O, NO_x, NH_3 and NO_3^- leaching) per unit of hectare are predicted for growing grass (grazed and/or conserved) and arable crops (maize). Modifications have been carried out to incorporate the simulation of flows of P (P losses are not calculated at this stage).

$SIMS_{PSYCHIC}$ is a Psychic (Davison *et al.*, *in press*) metamodel which has been developed for $SIMS_{DAIRY}$ and includes simple functions to represent the annual total loss of elemental P (dissolved and particulate P from soil and losses from fertiliser and manure) to watercourses.

$SIMS_{ECONOMICS}$ is a newly developed model (Butler, *pers. commun.*) which calculates the net farm margin by subtracting the total fixed costs and overheads from the gross margin.

$SIMS_{SCORE}$ is a new submodel which simulates the effect of both nutrient management variables (i.e. effect of unsaturation of fatty acids in the diet on milk yield) and non-nutrient management variables (i.e. available surface per cow during housing) on the sustainability of the farm in terms of biodiversity, landscape, milk quality, soil quality and animal welfare. The scores assigned reflect poor (0) to very satisfactory (6) sustainability. Subsequently, $SIMS_{ECONOMICS}$ calculates the net farm margin by subtracting the total fixed costs and overheads from the gross margin. Variables costs are calculated by the model as a function of management variables (i.e. £ per unit of applied manure volume). Some management strategies (i.e. those resulting in enhancing landscape), due to large cost variability, are user-proposed inputs and hence do not intend to reflect an accurate value.

The farm sustainability is then evaluated by the submodel $SIMS_{RANK}$, which ranks farms under different management strategies according to the user-defined criteria (i.e. minimising global environmental impacts over unit of milk).

10.3. Stream of calculations

Fig 2 gives a schematic representation of how the model works. The program starts by entering all the relevant user-inputs for the simulation. These are mainly the optimisable and/or basic (Fig 2) management inputs, site characteristics (Fig 2), inputs directly affecting $SIMS_{SCORE}$ (Fig 2) and the criteria which are used for optimisation (i.e. Min CO_2 eq-GWP/L).

One *j* value from an *i* optimisable management option is selected from the $MOD_{GENERATOR}$ matrix (Man i,j). $SIMS_{DAIRY}$ will evaluate the effect of different *i* x *j* farm scenarios until *i* and *j* indices reach their maximum value. Once Man i,j has entered its value, $MOD_{SIMULATOR}$ calculates the main flows in our farm system.

$SIMS_{MANAGEMENT}$ simulates flows of dry matter, energy, N and P at the animal level through calculations of feed requirements and supply (dry matter, energy, and N) under different diet profile strategies and for a given lactating herd defined by: (i) number and type (breed, condition score, calving season, total weight, weight gain/loss, average milk yield, milk protein % and butterfat milk % target) of dairy cows, (ii) number and type of followers, (iii) grazing days and (iv) diet profile (i.e. proportion of concentrates in the total dry matter housed ingestion). Calculations are based on the Feed into Milk (FiM) system (Thomas, 2004). $SIMS_{DAIRY}$ uses reference default values of feed characteristics and user-defined inputs (i.e. forage intake potential of concentrates).

In order to simplify the complexity of a dairy system, diet profile is defined in terms of concentrates: grass grazed: maize silage ratio, and concentrates: grass silage: maize silage ratio for the grazing and housing period, respectively. Prediction of feed voluntary DM intake during the housing and grazing period is calculated as a function of forage intake potential (FIP), concentrate dry matter intake (CDMI), animal condition score (CS), animal weight (W), milk energy output (MEO), week of lactation (WOL) and forage starch

concentration (FS).

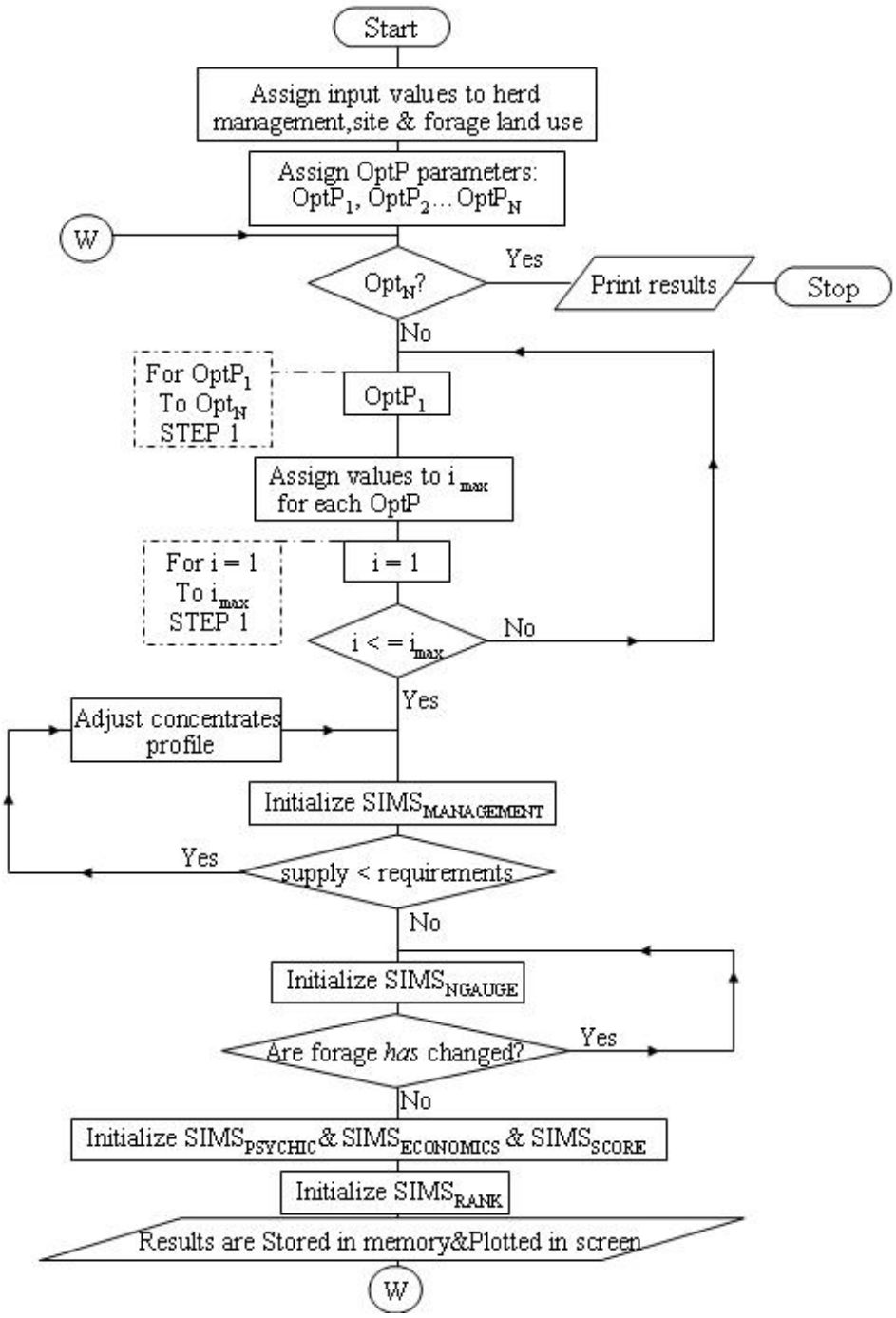


Figure. 2. General flowchart diagram of SIMS$_{DAIRY}$.

Total metabolisable energy (ME) and true protein (MP) requirements is defined as the energy/proteins needed for body weight change, pregnancy post 250 days, maintenance, milk

production and activity (i.e. grazing). For any given diet comprising silage (grass and/or maize) and concentrates, $SIMS_{DAIRY}$ optimises the concentrates characteristics in order to ensure that: (i) feed supply matches dairy cow requirements (DM, energy and N), (ii) rumen does not become acidic, (iii) amino acids in the diet are optimum for milk protein synthesis and (iv) the effect of diet composition on the composition of milk is predicted.

Total energy requirements in the herd are obtained by multiplying the number of dairy cattle and young cattle with their respective requirements per animal type. Depending on whether the requirements refer to either dairy or followers spending time during grazing or housing, they are divided into 4 main classes (Table 1): $ReqHouse_{LC}$ (lactating cows' requirements during housing period), $ReqGrazed_{LC}$ (lactating cows' requirements during grazing period), $ReqHouse_{YC}$ (young cows' requirements during housing period), $ReqGrazed_{YC}$ (young cows' requirements during grazing period).

Manure produced during housing and excreta deposited during grazing (N and P) is then calculated for each type of cow and subsequently in total (applying number of animals of each type) by subtracting N and P in milk from those ingested by both housing and grazing young and lactating cows. Manure (N and P) produced during housing is simulated to be applied to the different farm fields. Prior to application, gaseous N and CH_4 losses (house and storage) and straw N from bedding are calculated and computed with the total existing pool of N in manure. The remaining N and P in the manure is then applied at field rates given by $SIMS_{MANAGEMENT}$ submodel and used as inputs to the field-scale $SIMS_{NGAUGE}$ and $SIMS_{PSYCHIC}$ submodels, respectively. Flows of N and P are simulated within the fields and losses (P, NO_3^-, N_2O, NO_x, N_2 and NH_3 and CH_4) and products (milk N and N, P and DM plant yields) are calculated for the different fields (cut and cut & grazed grasslands and maize). Small concentration values of P in the soil may limit plant growth. $SIMS_{NGAUGE}$, using a simple mass balance approach, estimates Olsen P in the soil and subsequently applies a reduction in the DM prediction of the plant if the soil Olsen P is limiting (P_{index}<=2). Phosphorus in the harvestable part of cut and grazed grass and maize is estimated from standard values of P DM^{-1}.

$SIMS_{NGAUGE}$ can either use fertiliser application rates given by $SIMS_{MANAGEMENT}$ submodel or predict the best monthly N fertiliser distribution and amount according to

NGAUGE optimisation criteria (maximise N in herbage: N in loss) by using harvested kg N $_{hafield}^{-1}$ grass and maize as the target to achieve (Brown *et al.,* 2005).

Table 1. Requirements in the herd depending on the source feed source

Sources	ReqHouseLC	ReqGrazedLC	ReqHouseYC	ReqGrazedYC
grass silage from cut-only fields	GrassCutLC		GrassCutYC	
grass silage from cut&grazed fields	GrassGrazCutLC			
concentrates	ConHousedLC	ConGrazLC		
maize silage	MaizeCutLC			
grazed grass		GrassGrazLC		GrassGrazYC

Dairy systems produce both solid (FYM) and liquid wastes (slurry). Losses of N and CH_4 from manure management greatly depend on manure system chosen (FYM vs. slurry). SIMS$_{MANAGEMENT}$ submodel assumes that slurry-based and FYM-based systems operate at cubicle (slatted floor) and loose housing, respectively. Calves are assumed to operate in a straw-based system. The most important difference lies on the amount of bedding used. The amount and type of bedding material not only affects manure solids contents but also alters the physical, chemical, and biological composition of the manure (Sommer *et al.,* 2006). The most common bedding materials are sand, sawdust and straw. SIMS$_{MANAGEMENT}$ submodel assumes that straw is the only material used for bedding and that whereas FYM-based systems use an amount of 1500 kg straw dairy cow^{-1} (0.4 % N), slurry-based systems straw use is negligible.

Manure N losses are simulated according to a mass flow approach from Webb and Misselbrook (2004), by which NH_3, N_2O, NO_x and N_2 emissions are calculated from the pool of total ammonium nitrogen (TAN) in manure N according to different Emission factors (Efs) for different manure management stages.

Firstly, TAN in manure N (prior to housing NH_3 losses) is predicted by splitting manure N into urine and dung N according to the approaches described by Brown *et al.* (2005) and Kebreab *et al.* (2001) and subsequently calculated as the sum of readily mineralised N from urine and dung N. It is assumed that most of the urine N is mineralised within a few hours

and that 22 % of the dung N is readily mineralisable and will contribute to the TAN pool in the manure and to NH_3 volatilisation.

Increases in dietary protein or N intake leads to substantial increases in urinary loss (Van Soest, 1994) with almost all N ingested in excess of animal requirements excreted in urine (Peyraud *et al.,* 1995). Kebreab *et al*. (2001) proposed different relationships based, not only on the level of cow protein intake but also on the quality of forage (starch or fibre based diets). According to this study, starch-based diets make cows partition more of the ingested N into dung and less into urine than fibre-based diets do, which may well affect N losses as NH_3 and the composition of the manure produced. In straw-based systems, N from straw is added to the pool of manure (FYM) N and a proportion of the total TAN is predicted to be immobilised (0.0068 kg TAN kg straw^{-1} added). Ammonia losses from housing are calculated as a percentage loss from the TAN content of the manure (based on the 2004 inventory of NH_3 emissions from UK agriculture), being 31.4, 33.2 and 9 % for slurry, straw-based and calves manure, respectively. Generally, a straw-bedded cattle house is likely to emit less NH_3 than a slurry-based one. In comparisons between FYM and slurry based housing systems (Chambers *et al.,* 2003), the straw-based system resulted in significantly less NH_3 emission than the slurry system (33 and 49 g NH_3 cow^{-1}day^{-1}, respectively).

After subtracting NH_3 losses generated during housing from the initial TAN content in manure, NH_3, N_2O, NO_x and N_2 losses from storage are predicted as a percentage of the remaining TAN content in the manure. For FYM, a value for initial TAN immobilised during storage of 20 % is used (Webb and Misselbrook, 2004). The remaining TAN from young cows manure is at this stage assumed to result in slurry and consequently is added to the slurry TAN pool. $SIMS_{MANAGEMENT}$ submodel incorporates 8 types of slurry tanks and 2 types of FYM heaps with their respective Efs for NH_3, N_2O, NO_x and N_2 (EMEP/CORINAIR, 2005). The Efs values are shown in Table 2.

The manure N that is not lost through NH_3 losses during the housing or storage period is assumed to be applied in the soil. Both seasonal and forage field type distribution are initially provided by the $SIMS_{MANAGEMENT}$ submodel as a percentage of total applicable manure basis (i.e. 30, 40 and 30 % of total manure applied to cut & grazed grassland, only cut grassland and maize, respectively) and subsequently transformed into rates of kg N manure applied per hectare of field type as a function of the initial subdivision of forage type

areas. These forage type areas and hence manure rates will subsequently be adjusted once harvest yields per hectare for each type of forage area are calculated and compared with sources of nutrient requirements.

Table 2. Gaseous N Efs for dairy manure storage (EMEP/CORINAIR, 2005)

	Partial emission factor (kg kg^{-1} TAN)			
Store type	NH_3	N_2O	NO_x	N_2
slurry tank: open	0.15	0	0	0
slurry tank: rigid cover	0.03	0	0	0
slurry tank: floating cover	0.07	0.001	0.0001	0.003
slurry tank: crusted	0.07	0.003	0.0003	0.009
lagoon: open	0.35	0	0	0
lagoon: rigid cover	0.07	0	0	0
lagoon: floating cover	0.15	0.000	0	0
lagoon: crusted	0.15	0.003	0.000	0.009
FYM heap	0.3	0.1	0.01	0.3
FYM heap: cover	0.27	0.1	0.01	0.3

The remaining TAN and total N (after NH_3 losses from housing and storage) from slurry and FYM is subsequently associated to volume unit (m^3) by using default values of ammoniacal N, organic N and total N per m^3 according to the selected class and % DM of manure (Brown *et al.,* 2005). Although NH_3 emissions from manure application to the land are basically calculated as described in Brown *et al.* (2005), the original Efs were modified to be sensitive to more relevant manure management. New Efs for NH_3 volatilisation from slurry were determined for application on grassland and maize land according to: (i) properties of the slurry (% DM), (ii) its application date (for soil moisture content), (iii) incorporation timing after application, (iv) method of application and (v) method of incorporation. Equations from MANNER (Chambers *et al.,* 2000) were used for this purpose. Emission factors for NH_3 volatilisation from FYM were also incorporated from MANNER taking incorporation delay and technique as the main driving factors for controlling NH_3 losses from application.

As previously mentioned, the initial subdivision of forage type areas is recalculated so nutrient requirements (N and DM) from different sources match harvested and grazed N and DM plant yields (after allowing losses from grass and maize conservation). Total surface for forage (sum of cut & grazed grassland, cut-only grassland and maize) and number of lactating dairy cows per hectare of forage are calculated at this stage. Nitrogen losses from conservation are a mixture of NH_3 and N oxides (Maw *et al*., 2002). SIMS$_{DAIRY}$ incorporates

5 qualitative classes of silage management quality (very good, good, average, bad and very bad). Total losses from grass and maize conservation are split as: (i) gaseous losses of NH_3 and NO_x and (ii) other losses which may be attributed to surface waste and silage effluent. Nitrogen losses during conservation were assumed to be proportional to the loss of DM (Schils *et al.,* 2005). Total N and DM losses were calculated, depending on their management quality, as a proportion of the total N and DM ensiled grass and maize ($Silage_{Eff}$), these losses ranging from 6 to 30 % of the initial harvested crop (Bastiman and Altman, 1985). Total losses were split as (i) gaseous losses: 78 % and (ii) other losses: 22 % (from calculations derived from Mayne and Gordon, 1986ab). In the absence of sufficient quantitative data, gaseous losses were assumed to be split according to a 50: 50 ratio between NH_3 and NO_x losses.

Some environmental goals may be used as constraining targets. The model checks at this point if all of these targets are met; otherwise, $MOD_{EVALUATOR}$ makes $SIMS_{DAIRY}$ return to the beginning of the sequence of calculations and $MOD_{GENERATOR}$ generates a new '*i*' management option and/or '*j*' values (or value) to be simulated and evaluated. Should environmental goals be met; a full economic assessment is then carried out by $SIMS_{ECONOMICS}$, by which net income in the farm is calculated. $SIMS_{SCORE}$ calculates score indices of sustainability for milk quality, animal welfare, landscape, soil quality and biodiversity. $MOD_{EVALUATOR}$ classifies then the management options by best user-weighted multiple criteria result and stores all the results and inputs used in memory and in graphs in the $SIMS_{DAIRY}$ interface.

Subsequently, the model returns to $MOD_{GENERATOR}$, which makes the indices of the matrix (Man i,j) progress and $MOD_{SIMULATOR}$ simulates a new farm scenario. $SIMS_{DAIRY}$ stops when the $MOD_{EVALUATOR}$ evaluates the farm scenario corresponding to the last '*j*' values of the last '*i*' management option of the matrix Man i, j.

10.4. How does SIMS$_{SCORE}$ work?

10.4.1. Milk quality

An important pillar of sustainable dairying is production of higher-value milk and milk products that command a market premium: UK dairying can not longer compete in the world dairy commodity markets. There are a number of aspects of milk quality that can contribute to future differentiation and niche marketing- notably different types of fat [polyunsaturated fatty acids (PUFA) and conjugated linoleic acids (CLA)] and proteins that might benefit the health of consumers. This analysis also needs to consider the possibility that new management strategies might lead to problems such as off-flavours or reduced shelf-life of milk.

Polyunsaturated fatty acids in the milk has been described to have a positive effect on the health of the milk consumers (Parodi, 1997) but a negative effect on the oxidative stability (shelf life) of the milk [this can be ameliorated by the use of additional vitamin E in concentrates (Al-Mabruk *et al*., 2004)]. Evidently, there is a close relationship between PUFA profile in the diet and that found in the milk. Dewhurst *et al*. (2003 ab), for instance, indicates that the inclusion of fish oil in the diet of grazing dairy cows deeply affects the fatty acids profile of milk fat, resulting in an increase in concentrations of PUFA. Some PUFA in the milk, such as α-linolenic acid (18:3), have been described to be higher under fresh forage than under conserved diets (Dewhurst, 2005). Moreover, cows on pasture grazing and at a high herbage allowance produce milk with the highest concentrations of PUFA (Elgersma *et al*., 2006). This is not just due to the greater content of 18:3 fatty acids in fresh forage as opposed to conserved forage, but differences in CLA content in milk have been found with cows grazing different ryegrass cultivars (Loyola *et al*., 2002). Oxidation during field wilting and biohydrogenation in the rumen are the main sources of loss of herbage PUFA (Elgersma *et al*., 2006). Among the harmful components of milk, PUFA and taints are the most important elements. They both reduce the shelf-life of milk. The ingestion of red and white clover silage based diets has an increased risk for abnormal taste in the milk as a consequence of increased levels of PUFA in milk (Al-Mabruk *et al*., 2000). The higher the unsaturation of the fatty acids the lower melting point the milk has, which affects the spreading and processing attributes of milk products.

$SIMS_{SCORE}$ calculates a score index of sustainability for milk quality based on 4 milk properties: (i) Beneficial components for human health, (ii) shelf-life of milk, (iii) off-flavours and (iv) spreadability. These 4 milk properties, as previously commented are strongly related to diet management factors such as the concentration of PUFA and the ratio of fresh: conserved forage in the diet. In the absence of specific literature values, we constructed an equation in order to assess the qualitative PUFA concentration in the milk by relating it to concentration of long-chain PUFA from different diets and the ratio of fresh: conserved forage. High PUFA concentration in the milk can result in beneficial for human health (positive relationship) which can be scored up to 82 % of the total maximum value (6). The rest of the score weight is given for the shelf-life of milk (negative relationship with milk PUFA), off-flavours (negative relationship with milk PUFA) and spreadability (positive relationship with milk PUFA), each at 6 % of the total maximum value (6).

There is literature supporting other possibilities to enhance milk quality, For instance, selenoproteins in the milk can benefit both human and animal health (Walker *et al*., 2004). This factor and others could be incorporated into future versions of $SIMS_{DAIRY}$.

Although it is not part of the milk quality score per se, it is worth mentioning that total protein and butterfat milk content generally influence the price of milk. In $SIMS_{DAIRY}$ the fat and protein content, together with seasonality of production, the hygienic quality of milk and pattern/volume of milk supply control milk price. Protein and butterfat milk content are mainly calculated according to the Feed into Milk (FiM) system (Thomas, 2004). Studies have shown that butterfat concentration levels in milk can be largely related to the Physical effectiveness of Neutral Detergent Fibre (PeNDF) (Mertens, 1997) or undergo depression when the diet contains elevated levels of PUFA (Offer *et al*., 1999). Some modifications have been introduced to account for butterfat depression since the FiM system did not account for them (i.e. Fig 3 represents the effect of PeNDF on butterfat depression).

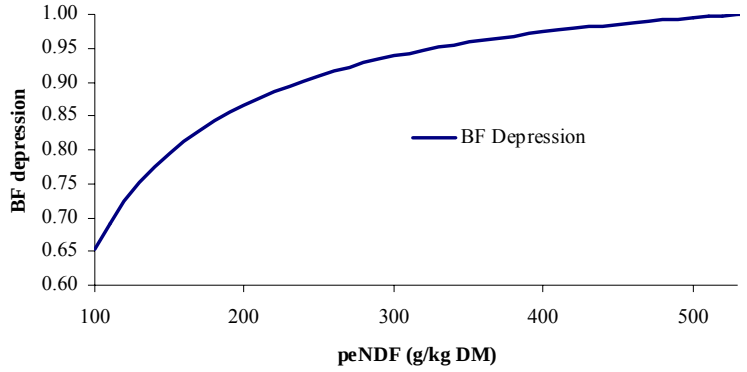


Figure 3. Relationship between Physical effectiveness of NDF (PeNDF) and butter fat (BF) milk depression (as a proportion of predicted BF milk). Equation derived from Mertens (1997).

10.4.2. Biodiversity and landscape.

Society awareness has driven to an increasing emphasis within agri-support measures throughout Western Europe to encourage biodiversity in farming systems. Intensification of grassland farming has no doubt resulted in the loss of biodiversity on grassland farms (Wilkins and Harvey, 1994). Reductions and, in some cases, extinctions of farmland bird species has been associated with agricultural intensification (Chamberlain *et al*., 2000) and dominance of landscape by agricultural grassland (Chamberlain and Fuller, 20001; Atkinson *et al*., 2002).

In terms of environmental consequences of high stocking rates, soil compaction and structural damage can be severe (Whitmore, 2001). Soil structural changes caused by intensive management are likely to have both direct and indirect consequences for grassland fauna and biodiversity generally. For example, ease of soil penetrability and availability of soil invertebrates are known to be key factors influencing the breeding of wading birds (Green *et al*., 1990; Ausden *et al*., 2001). Moreover, the challenge to revert this trend is substantial as studies suggest that changing to more extensive practices does not necessarily yield to restore grassland biodiversity in the short term and incorporation of patches for biodiversity within the farm are not as well developed for grassland fields as they are for arable systems (Smart *et al*., 2003).

Unless a farmer receives agri-environmental payments to manage a field to create structural heterogeneity, i.e. a mix of tall and short swards, then management will generally

aim at maximizing utilisation of the grass crop. Frequent grazing or cutting management creates sward structural uniformity and, particularly under grazing, dense swards with high tiller numbers can develop across a wide range of N inputs (Tallowin *et al*., 1995). Sward height and density are likely to be important factors that influence prey accessibility for grassland birds (Whittingham and Markland, 2002). Lack of spatial and structural heterogeneity in farmed landscapes is now widely recognised as a key factor influencing farmland birds and biodiversity generally (Siriwardena *et al*., 2000; Benton *et al*., 2003). Simplification of botanical composition and loss of structural variation within and between agricultural grassland fields through increased intensity of utilisation are perceived to have major influences on farmland biodiversity (Benton *et al*., 2003). However, the exact mechanisms through which grassland management influences the suitability of grassland as a foraging habitat for birds remain poorly understood (Barnett *et al*., 2004).

SIMS$_{SCORE}$ calculates a score index of sustainability for biodiversity based on 5 management factors: (i) grazing intensity, (ii) fertiliser rate, (iii) cutting management, (iv) reseeding management and (v) the inclusion of patches for biodiversity (margins, hedges and buffer-strips). A conceptual relationship between grazing pressure and species diversity (Grime, 1979) has been modified and incorporated into an equation in SIMS$_{SCORE}$.
According to this equation, vegetation can not maintain its integrity if grazing pressure is either too high or to low (Fig 4).

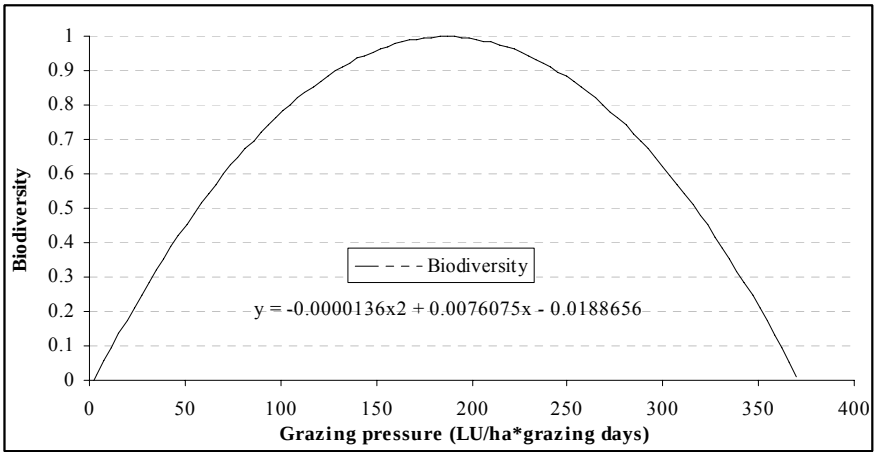


Figure 4. Relationship between grazing pressure and biodiversity (after Grime, 1979).

If we could separate the effect of grazing with the effect of, for instance, previous year management, the maximum biodiversity in a particular field would be achieved, for instance, at a combination of 185 grazing days and 1 LU/ha yr. Because there is still a lack of quantitative data on grazing effects on biodiversity it should be noted that this equation provides a qualitative assessment of the relationship between grazing and biodiversity rather than quantitative and therefore refinement is required once future scientific evidence is collected. Application of fertiliser has been a key factor in reducing floristic diversity in species rich grassland (Mountford *et al.,* 1993). Fertiliser addition encourages the growth of competitive species, usually resulting in the loss of many species which are of substantial ecological significance (Macadam *et al.,* 2001; Firbank, 2005). Studies conclude that while N remains the main element limiting plant diversity its availability is being controlled by P. Some negative effects produced by the excess of fertilisation are for instance: positive interactions between increased N and crop foliar diseases (McLaughlin and Mineau, 1995). The addition of animal wastes (i.e. manure) has similar effect on biodiversity than mineral fertiliser does.

A relationship by Herrmann *et al*. (2003) between nutrient input (mineral fertiliser and manure) and biodiversity has been incorporated into $SIMS_{SCORE}$. Six classes (a modification from Herrmann *et al*. 2003 classes) comprising ranges of nutrient inputs (mineral fertiliser + manures) relate the effect of N inputs to the soil and biodiversity: the classes are as follows: (i) class 1; nutrient inputs ≤ 50 kg N ha-1 yr-1 (score 1), (ii) class 2; nutrient inputs = 50-125 kg N ha-1 yr-1 (score 0.9), (iii) class 3; nutrient inputs = 125-200 kg N ha-1 yr-1 (score 0.8), (iv) class 4; nutrient inputs = 200-275 kg N ha-1 yr-1 (score 0.6), (v) class 5; nutrient inputs = 275-350 kg N ha-1 yr-1 (score 0.4) and (vi) class 6; nutrient inputs ≥ 350 kg N ha-1 yr-1 (score 0.2). Classes are scored as follows: class 1= 1, class 2= 0.9, class 3= 0.8, class 4= 0.6, class5= 0.4 and class6= 0.2. Five classes were also incorporated to simulate the effect of P inputs on biodiversity. The classes are as follows: (i) class 1; nutrient inputs ≤ 10 kg P ha-1 yr-1 (score 1), (ii) class 2; nutrient inputs = 10-20 kg P ha-1 yr-1 (score 0.9), (iii) class 3; nutrient inputs = 20-40 kg P ha-1 yr-1 (score 0.6), (iv) class 4; nutrient inputs = 40-60 kg P ha-1 yr-1 (score 0.4) and (v) class 5; nutrient inputs ≥ 60 kg P ha-1 yr-1 (score 0.2).

Positive scores are also given for cutting for hay as it has been described to have an advantage for biodiversity as it makes it suitable as a habitat for birds and insects whereas

negative score is given to reseeding, which generally will decrease biodiversity (McLaughlin and Mineau, 1995) and compaction of soil by cattle, which has been found to make habitat unsuitable for some invertebrates (Sanderson, 1989).

The model allows some capital investment on margins, hedges, buffer strips and wildlife strips, which generally will result in increased biodiversity and which also positively affects landscape quality. Landscape quality is assessed through partly E/M variables which are linked to nutrient management or biodiversity and E/M variables which can only be accounted in isolation (i.e. enhancement sense of mystery in the farm). The assessment is based on O'Leary *et al*., (2004), in which a semi-quantitative checklist for assessment of the landscape quality of farms is described.

10.4.3. Animal welfare

Although intensive dairy production may often be considered incompatible with animal welfare by ethologists (Stookey, 1994), there is no universal guide to the minimum level of conditions that is acceptable for the adequate welfare of the cattle. Although it is hard to find strong relationships between management factors and animal welfare there is evidence that some conditions pose an increased risk on cows' health or behaviour disorders. They can be tabulated in a qualitative manner in terms of relative risks (Thursfield, 1997). Breeding for higher yielding cows has improved the ability of the cow to partition nutrients into milk preferentially to maintenance and/or growth. This has undoubtedly resulted in increased efficiency and other benefits such as a cow's lifetime production can be achieved in less lactations (less maintenance costs). However, the management of these high genetic merit cows also has become more complex and has generated animal welfare implications. High genetic merit cows have been associated with increased problems with fertility and some diseases (i.e. mastitis: Ingvartsen *et al*., 2003).

Feeding cows mainly on fermented herbage (silage) also poses increased risks, which are principally generated by undesirable microorganisms (i.e. Listeria), undesirable chemicals (mycotoxins), and excess acidity (Wilkinson, 1999). Cows housed in cubicles systems seem to have an increased risk of suffering from lameness, which is generally associated to the cow walking on hard concrete covered in slurry (Phillips, 2002). Housing not only impacts on lameness but also, irrespective on the system, on the social structure of the cattle. Hence

the longer the cows are housed the largest the impact on their social structure. As opposed to cubicles, straw-based housing systems provide floor comfort and although weak, there is evidence that mortality appear higher among cattle kept on slatted floors (cubicles) than on straw yards (Tuyttens, 2005). High levels of some PUFA have also been described as having a positive effect on fertility (Robinson *et al*., 2002; Formigoni and Trevisi, 2003; Ambrose *et al*., 2006) or affect gestation length (Pickard *et al*., 2005), with implications for calf survival and the incidence of dystocia. In order to score animal welfare of the farm $SIMS_{DAIRY}$ incorporates the prototype of clinical welfare score for dairy cattle proposed by Noordhuizen and Metz (2005), in which information about: (i) general husbandry, (ii) pasturing, (iii) housing, (iv) milk harvesting and (v) dairy cows per se needed to be input.

The resulting score is weighted with a newly developed factor which took into account: housing period, livestock density, genetic merit of the cows, proportion of silage feed of the total diet and PUFA concentration in the diet.

10.4.4. Soil quality and definition of scores

The effect of different factors on soil compaction and N fertilisation effects on quality of organic matter in grasslands (Malhi *et al*., 2005) are incorporated into a scoring system to assess soil quality in the farm. The interactions between the effect of tillage, cow density in the grazing area, the grazing period, the soil texture (defined by apparent density), weather conditions (to asses water logging) and the amount of farm traffic are the factors that $SIMS_{DAIRY}$ uses to evaluate soil compaction.

Sustainability matrices are scored by the submodel $SIMS_{SCORE,}$ which simulates the effect of both nutrient management variables (i.e. effect of unsaturation of fatty acids in the diet on milk yield) and non-nutrient management variables (i.e. available surface per cow during housing) on the sustainability of the farm in terms of biodiversity, landscape, milk quality, soil quality and animal welfare. The scores assigned reflect poor (0) to very satisfactory (6) sustainability. Subsequently, the net farm margin is calculated by subtracting the total fixed costs and overheads from the gross margin. Variables costs are calculated by the model as a function of management variables (i.e. £ per unit of applied manure volume). Some

management strategies (i.e. those resulting in enhancing landscape), due to large cost variability, are user-proposed inputs and hence do not intend to reflect an accurate value.

10.5. Sensitivity analysis

The influence of a number of selected environmental/management (E/M) variables (Table 3) on state variables values (Table 4) was tested through sensitivity analysis.

Table 3. Selected environmental/management (E/M) variables to be changed. There are 2 types depending on their change properties/accountability: (a) numerically accountable and (b) numerically unaccountable.

Type of E/M variables to be changed	
(a) numerically accountable	**(b) numerically unaccountable**
Housing days	Increased PUFA in diet
Fertiliser N	Injection of slurry
Fertiliser P	Closed manure for storage
Herd size	Arable past (grass)
Milk yield/cow	4-6 years old (grass leys)
Milk protein	>2 years old (grass leys)
Milk fat	Very good silage making
Concentrates	Poor silage making
Fibre (NDF)	Loam soil
Starch	Clay loam soil
% DM in manure	Spring calving
Winter-autumn manure	Autumn calving
Manure to grazed grass	FYM-based system
h factor$^{\otimes\partial}$	
u factor$^{\oplus\partial}$	
N in plant (%)$^{\varnothing\partial}$	
Plant dead mineralised$^{\partial}$	
Urine: dung ratio$^{\partial}$	

$^{\otimes}$ 'h factor' represents the efficiency of the plants to absorb N and $^{\oplus}$ 'u factor' represents the efficiency of plant N harvesting by the farmer or animal and $^{\varnothing}$ 'N in plant' represents the concentration of N in the plants. $^{\partial}$Efficiency factors in the soil-plant-system which can be manipulated in SIMS$_{DAIRY}$ simulating different plant and animal traits.

The sensitivity of a number of state variables (Table 4) to E/M variables variation (those numerically accountable: Table 3) was calculated as the change in state value relative to the change in E/M variable value:

$$\text{Sensitivity} = [(S_1-S_2) / S_b] / [(P_1-P_2) / P_b] \times 100\ \% \quad \textbf{(1)}$$

In which S_1 and S_2 are the state variable values for the minimum (P_1) and maximum (P_2) E/M variable values, and S_b and P_b the state value for the basal E/M variable value.

For those E/M variables that their value changes are not easily accounted numerically (Table 3), the sensitivity test was carried out by a simple comparison of the % change on state values compared with those values resulting from the basal E/M variable values. Basal, maximum and minimum E/M variable values and changes to unaccountable E/M variables are shown in Table 5. Results of sensitivity analysis are shown in Fig 5 and 6, for accountable and unaccountable E/M variables, respectively.

Table 4. Selected state variables used for the sensitivity analysis.

Type of state variable and units				
Losses	**Units**		**Economical**	**Units**
NO_3^-	g/L of milk	kg/ha	Net margin	£/ha
CH_4	g/L of milk	kg/ha	Price of milk	£/L of milk
N_2O	g/L of milk	kg/ha	**Surface**	
NO_x	g/L of milk	kg/ha	Total	ha
NH_3	g/L of milk	kg/ha	Grazing	ha
P	g/L of milk	kg/ha	Maize	ha
Global warming potential (GWP)	kg/ha		Cut grass	ha
Manure	m^3/ha			
Sustainability attributes			**Dry matter in diet**	
Milk quality	dimensionless		Grass	tonnes
Biodiversity	dimensionless		Maize	tonnes
Animal welfare	dimensionless		Concentrates	tonnes
Landscape	dimensionless			
Soil quality	dimensionless			

To a certain extent, most of the state variables showed to be sensitive to changes in most of the E/M variables for both accountable and unaccountable E/M variables. However, as expected, a large degree of variability could be found on the levels of sensitivity.

Table 5. Basal E/M variable values and maximum and minimum parameter values and changes to unaccountable E/M variables.

numerically accountable				numerically unaccountable			
E/M variables	**Basal**	**Min**	**Max**	**E/M variables**	**Basal**	**change to**	
Housing days	180	100	260	Increased PUFA in diet	No	Yes	
Fertiliser N (kg/ha)	263	132	399	Injection of slurry	No	Yes	
Fertiliser P (kg/ha)	14	8	22	Closed manure for storage	No	Yes	
Herd size (dairy cows)	136	68	204	History of grassland	Grassland	Arable	
Milk yield (L/cow d)	17	10	25	Grass lay (years)	11-20	4-6	>2
Milk protein (%)	3.4	3.0	3.7	Silage making quality	Average	Very good	Poor
Milk fat (%)	4.3	3.9	4.8	soil texture	Sandy loam	Loam	Clay loam
Concentrates (kg)	150399	104225	200470	Calving pattern	All-year	Spring	Autumn
Fibre (NDF) (%)	48.8	45.9	51.7	Manure system	Slurry	FYM	
Starch (%)	4.5	3.6	5.5				
% DM in manure	6	2	10				
Winter-autumn manure	65	0	100				
Manure to grazed grass	25	0	50				
h factor	0.47	0.34	0.59				
u factor	0.60	0.51	0.70				
N in plant (%)	3.37	2.95	3.73				
Plant dead mineralised	0.56	0.45	0.65				
Urine: dung ratio	0.74	0.53	0.93				

Accountable variables (Fig 5): In terms of losses, for instance, those N losses from soil (NO_3^-, N_2O and NO_x) showed the largest levels of sensitivity. Increasing N fertiliser, % N in plant, % fat in milk, dead plant mineralised N, 'u factor' (proportion of harvested N of total plant) and the ratio of urine: dung increased NO_3^- and N_2O losses both per L of milk and per hectare of surface. Of these E/M variables, % fat in milk target, N fertiliser, 'u factor', dead plant mineralised N and the ratio of urine showed larger sensitive to the losses per hectare whereas the rest were more sensitive to the losses per L of milk. Increasing the efficiency of N absorption by the plant 'h factor' always led to reduction of NO_3^- leaching losses both per L of milk and per ha but whereas it decreased most losses per L of milk, it increased those losses per ha (except for NO_3^-).

Ammonia, P and CH_4 losses also showed sensitivity to some E/M variables. Whereas increasing N fertiliser, the ratio of urine: dung and % N in plant led to increasing NH_3

emissions both per L and per ha, increasing milk yield/cow and % protein in the milk led to smaller NH_3 losses. There was not any E/M variable that led to substantial sensitivity to CH_4 losses as both per L of milk and per ha. Whereas increasing fat content in milk and herd size led to increasing CH_4/L milk, increasing milk yield/cow and protein content in the milk led to decreasing CH_4/ L milk. Increasing housing days, 'h factor', 'u factor' and dead plant mineralised N led to increasing CH_4/ha and increasing % N in plant led to decreasing CH_4/ha. Phosphorus losses were very sensitive to housing days, winter-autumn manure, milk yield /cow, fat content in milk 'h factor'and 'u factor'. Increasing housing days and winter-autumn manure % led to smaller and greater P losses both per ha and per L of milk, respectively. Increasing of global warming potential as the CO_2 equivalents of N_2O+CH_4 (Fig 5d) showed to be positively influenced by fertiliser N, herd size, fat content in milk, %N in plant and the ratio urine: dung and negatively influenced by housing days, milk yield/cow and protein content in milk.

All of the sustainability attributes except landscape aesthetics showed sensitivity to changes in some of the studied E/M variables (Fig 5c). Biodiversity and animal welfare showed the largest levels of sensitivity. Increasing housing days, fertiliser N, herd size, 'h factor', 'u factor', dead plant mineralised N and the ratio urine: dung led to substantial negative biodiversity scores while increasing fat content in milk and %N in plant led to substantial positive ones. Increasing animal welfare was positively and sensitively related to decreasing housing days, concentrates ingestion, 'u factor', %N in plant and decreasing fat content in milk. Soil quality was positively affected by fat content in milk, %N in plant and milk yield/cow and negatively affected by increasing housing days, fertiliser, 'h factor', 'u factor', dead plant mineralised N and the ratio urine: dung. Milk quality was negatively affected by increasing the housing period.

The net margin showed large sensitivity to most factors (fig 5d). Net margin was positively affected by increasing herd size, milk yield/cow, fat and protein content in milk, 'h factor' and 'u factor' and negatively affected by housing period, concentrates in the diet and %N in plant. As expected, price of milk was sensitive to fat and protein content in the milk.

The area needed in the farm for forage (Fig 5d) was sensitive in a positive way to herd size, milk yield /cow and %N in plant and in a in a negative way to housing days, fertiliser, 'h factor', 'u factor', dead plant mineralised N and concentrates in diet. The areas needed for

maize and cut grass showed greater sensitivity to changes than the area needed for grazing (Fig 5f). Both maize and grass cut areas were substantially positively sensitive to housing days, 'u factor', fertiliser N, %N in plant and dead plant mineralised N and negatively sensitive to herd size, milk yield/cow and 'h factor'. Grazing grass surface was positively affected by fat content in milk and negatively affected by housing time, herd size, 'u factor' and %N in plant.

Production of manure volume per hectare (Fig 5e) was positively sensitive to housing time, fertiliser N, 'h factor', 'u factor', concentrates, % N in plant and dead plant mineralised N and negatively sensitive to % DM in manure, milk yield/cow and protein content in milk.

Unaccountable variables (Fig 6): All of the variable E/M variables studied except for seasonality of calving generally showed similar trends of % change in terms of losses per L of milk and per ha. Nitrous oxide and P losses were extremely sensitive to soil type (Fig 6a, 6b and 7), with heavier the texture the larger the losses. Farm Yard Manure-based compared with slurry-based systems also resulted in largely increasing N_2O losses and past arable slightly decreased P losses and young swards slightly increased P losses. Nitrate leaching was found to be much smaller in heavier soil textures, past arable, in FYM-based systems and using 4-6 years old swards and it was only increased when manure was injected or stored in closed systems and in young swards (<2 years old). Nitric oxide and nitrogen dioxide losses showed large sensitivity to the quality of silage making and soil type. The poorer the quality of the silage process and the heavier the soil texture the more NO_x emissions. Ammonia losses were reduced when manure was injected or stored in closed systems, under heavier soil textures (only per ha though), in FYM-based systems and where grasslands have an arable past.

Methane losses were largely reduced by increasing PUFA in the diet and under heavier soils (only per ha though). Methane increased in FYM-based systems and in young swards (<2 years old). Calving in autumn generally led to decreasing losses per L and increasing losses per ha. Only N_2O showed smaller emission in both units.

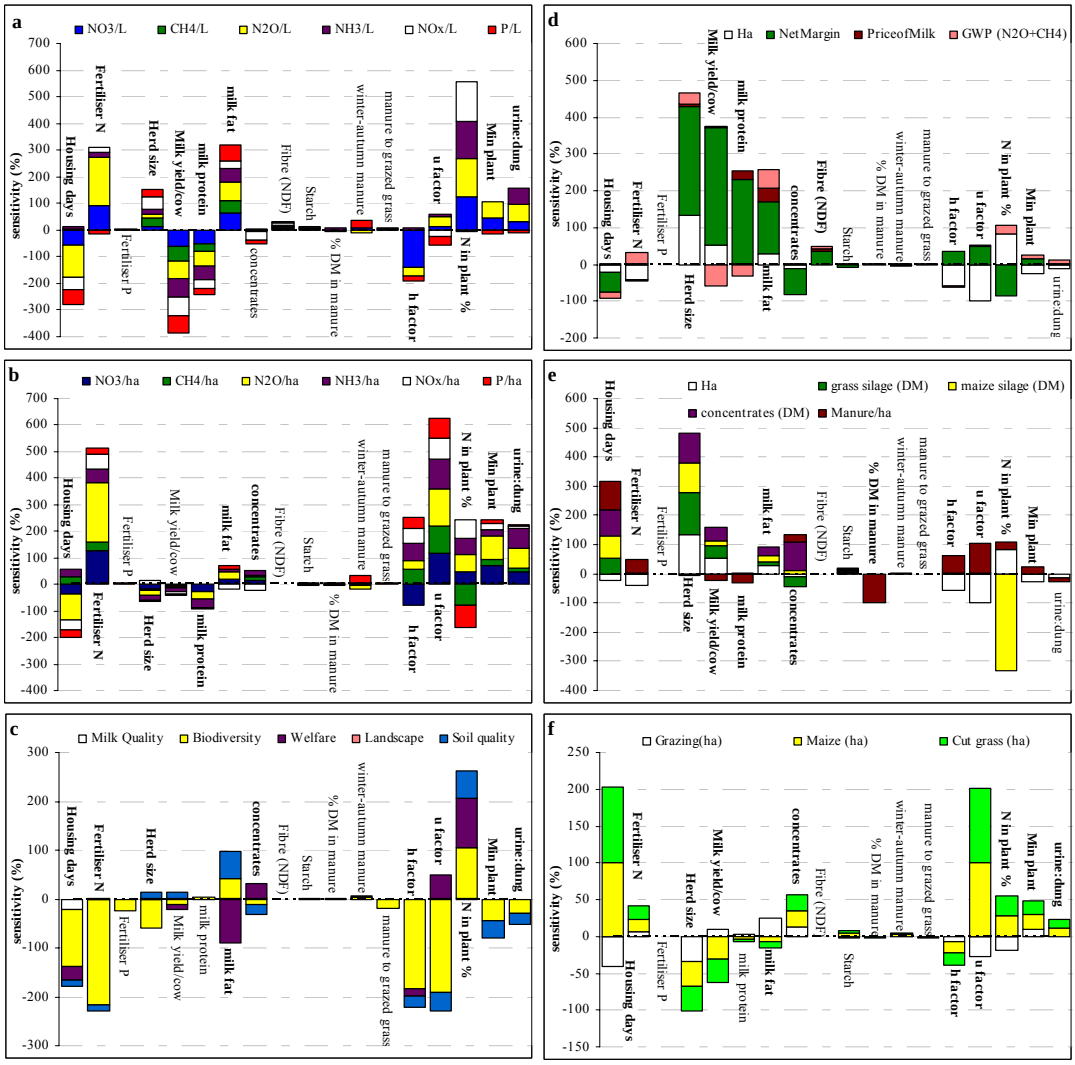


Figure 5. Cumulative sensitivity (%) effect of different E/M variables on selected state variables: **(a)** Losses per L of milk (NO_3^-, CH_4, N_2O, NH_3, NO_x, P), **(b)** Losses per hectare (NO_3^-, CH_4, N_2O, NH_3, NO_x, P), **(c)** Attributes of sustainability (milk quality, biodiversity, animal welfare, landscape and soil quality), **(d)** surface (ha), Net margin (£), price of milk and global warming potential (GWP), **(e)** surface (ha), manure (volume/ha) and amount (DM) of grazed and cut grass and maize and **(f)** surface (ha) of grazed and cut grass and maize.

Spring calving led to decreasing losses per ha and per L in terms of CH_4 and NO_x and the rest of losses hardly varied except for losses of P per L of milk that were reduced.

All of the sustainability attributes except landscape aesthetics showed sensitivity to changes in some of the studied E/M variables (Fig 6c). Global warming potential (Fig 6d) was largely increased in heavier soils and in FYM-based systems and decreased after supplementation of PUFA in the diet and in autumn-calving systems.

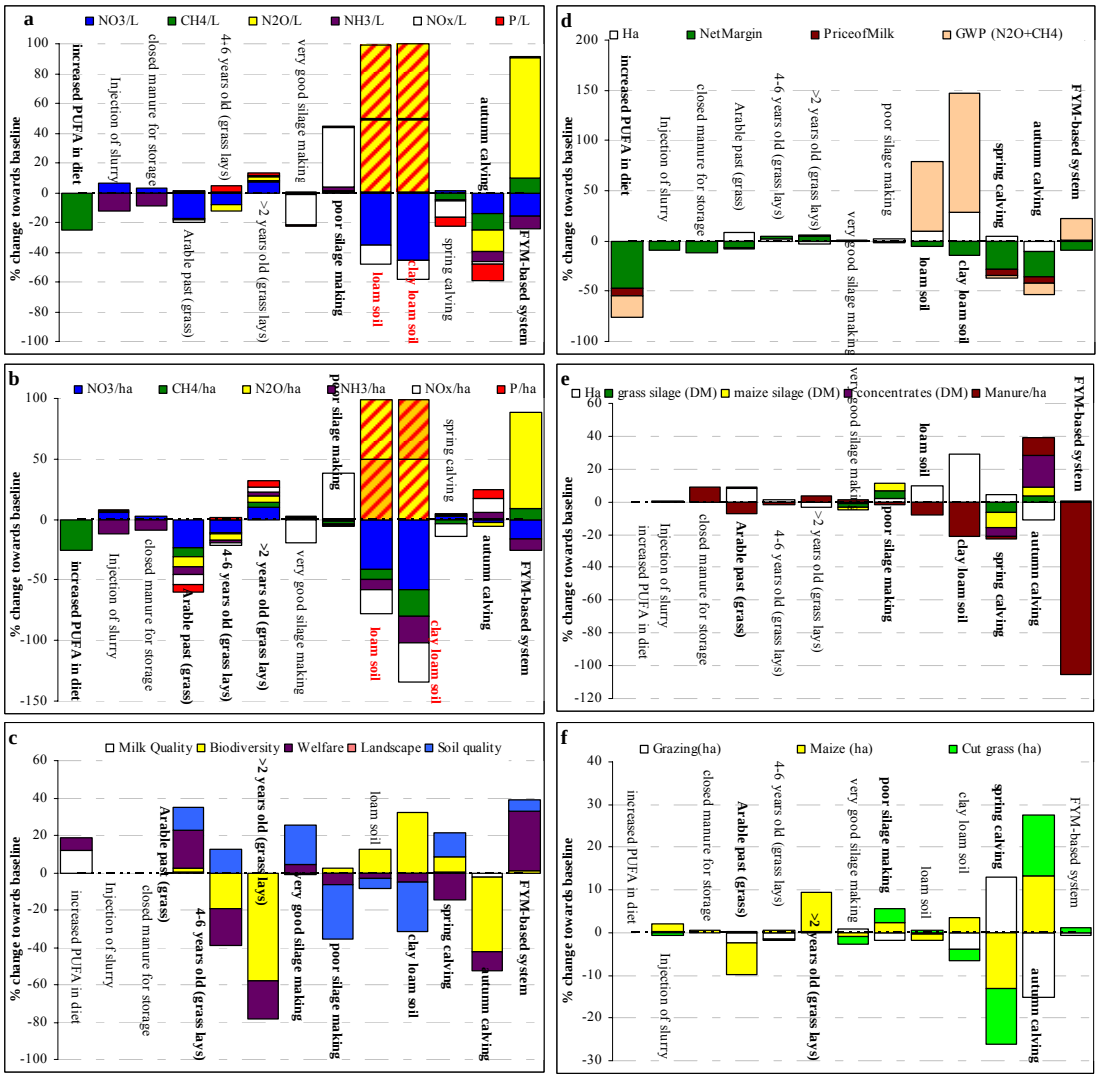


Figure 6. Cumulative change (%) towards baseline scenario of different E/M variables on selected state variables: **(a)** Losses per L of milk (NO_3^-, CH_4, $N_2O^{\lozenge}$, NH_3, NO_x, $P^{\lozenge}$), **(b)** Losses per hectare (NO_3^-, CH_4, N_2O, NH_3, NO_x, P), **(c)** Attributes of sustainability (milk quality, biodiversity, animal welfare, landscape and soil quality), **(d)** surface (ha), Net margin (£), price of milk and global warming potential (GWP), **(e)** surface (ha), manure (volume/ha) and amount (DM) of grazed and cut grass and maize and **(f)** surface (ha) of grazed and cut grass and maize. $^{\lozenge}$ The change (%) of soil type towards the baseline scenario was remarkably larger than that shown in Fig 6a and 6b (red and yellow stripped pattern). The actual % change is shown in figure 7.

Scores for biodiversity were shown to be smaller for younger swards and systems with calving pattern in autumn and larger for heavier soils and spring calving. Soil quality was positively affected by systems with grass with an arable past, good quality of silage making,

FYM-based systems and spring calving systems and negatively affected by poor silage making and heavier soils.

Animal welfare was positively affected by systems with grass with an arable past, FYM-based systems and increased PUFA in diet and negatively affected by younger sward leys, heavier soils and spring or autumn calving. Milk quality was positively affected by increased PUFA in diet.

The net margin showed large sensitivity to most factors (fig 6d). Net margin was largely decreased with supplementation of PUFA and any seasonal calving system and slightly decreased with FYM-based systems, heavier soils, when manure was injected or stored and under grass with an arable past. Young sward leys led to slightly larger net margins.

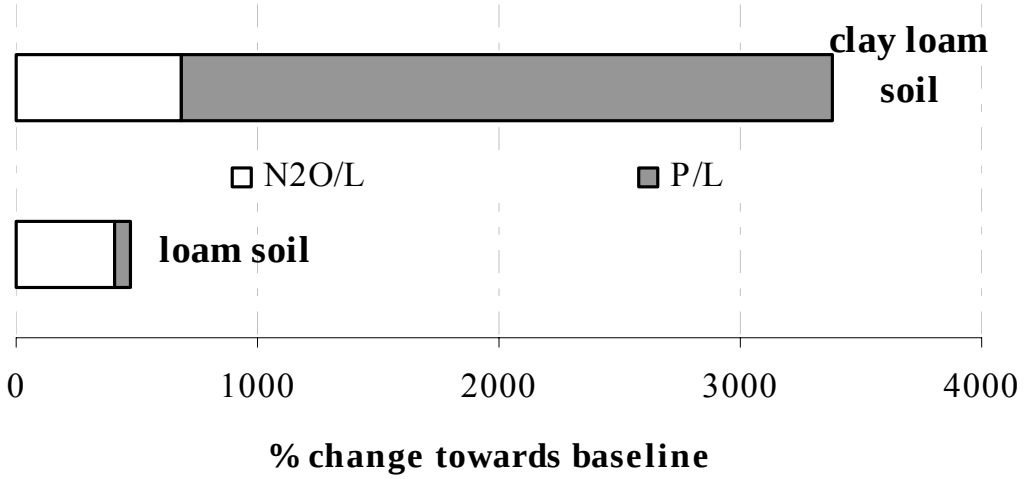


Figure 7. Cumulative change (%) towards baseline scenario of different of losses per L of milk ($N_2O^{\lozenge}$, and $P^{\lozenge}$).

Price of milk was sensitive to supplementation of PUFA in the milk and any seasonal calving (Fig 6d). They had in both cases a negative impact on the total farm net margin. The area needed in the farm for forage (Fig 6d) was positively affected by heavier soils and arable past of grass leys and negatively affected by autumn calving. The area needed for cut grass increased with autumn calving systems and poor silage making and decreased with spring calving systems and heavy soils. Maize area needs increased with autumn calving systems, heavy soils and grass young leys and decreased with spring calving systems and grass leys with arable past. Grazing area needs increased with spring calving systems and

decreased with autumn calving systems, heavy soils, poor silage making and leys with arable past (Fig 6f).

Production of manure volume per hectare (Fig 6e) was largely reduced by using FYM-based systems and to a smaller extent by heavier soils and grass leys with arable past. On the contrary, it was increased by autumn calving systems and closed system of manure storage.

10.6. Discussion

$SIMS_{DAIRY}$ modelling framework represents an advance to existing modelling approaches to study the sustainability of dairy farms. This is so because: (i) it can simulate with process-based mechanisms the N and P flows within a dairy farm, (ii) it can simulate in a soft scientific basis (scoring with indexes) the effect of the main known controls that affect the performance of those attributes that science is still trying to understand (i.e. those controls on animal welfare, soil quality, biodiversity or product quality), (iii) it integrates the interactions among attributes and controls in a transparent way and (iv) it can also optimise several objectives in dairy farms with a simple iterative procedure in order to find sustainable dairy farms, allowing the expression of impacts according to several reference units (i.e. impacts per unit of L of milk or forage ha).

$SIMS_{DAIRY}$ successfully integrates in a systems approach several models that have been recently developed and studies that have quantified or described the behaviour of isolated components of the soil-plant-animal system. Thereby, $SIMS_{DAIRY}$ is capable of investigating these components in a holistic way.

$SIMS_{DAIRY}$ sensitivity analysis showed the effect of a number of selected E/M variables on state variables, mainly those related to environment, attributes of sustainability and farm net margin. Most of the selected state variables, except for landscape aesthetics, showed substantial sensitivity to selected E/M variables. However, it must be noted that this analysis represents only a small portion of the vast solutions space and references to relationships or trends of effect for the different E/M variables may not generally be linear and hence, to study this complex surface response we would need a more complicated analysis of sensitivity. For example, when we simulate with $SIMS_{DAIRY}$ a dairy herd fed with different

diet profiles and under a combination of climatic and forage land characteristics and we plot the effect of housing period on predicted environmental impact (index comprising the effect of warming potential, eutrophication, acidification and soil erosion: according to Van Calker *et al*., (2006)), we found that this relationship fit much better to a cubic equation than into a linear one (Fig 8).

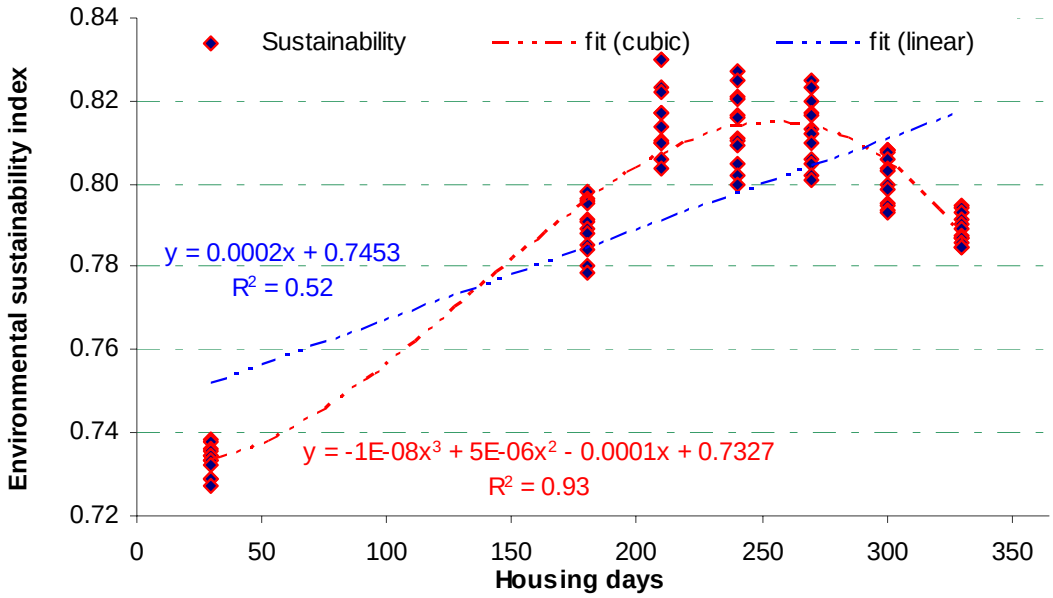


Figure 8. Relationship between housing period and environmental sustainability index (index calculated fromVan Calker *et al*., 2006).

The use of different reference units (i.e. per unit of L of milk or forage ha) by SIMS$_{DAIRY}$ in our sensitivity analysis highlighted the fact that farm E/M variables (i.e. those related to management) effect on, for instance, environmental losses can be very different if assessed per unit of product rather than per forage area. For instance, the use of plant varieties which have an enhanced ability to absorb N from the soil (increased *h* factor), reduced NO_3^- leaching both per ha and per L of milk compared with average varieties; however, for the rest of the losses, the trend is that they reduce N_2O and P losses per L of milk but increase all losses (except for NO_3^- leaching) per ha of forage land. This is so since increasing the N use efficiency of the plant leads to greater yields and smaller losses from the soil per hectare and thus, a smaller requirement for forage area. Less area and the same animal numbers results in similar losses at the animal level as total load but larger as per hectare. The controversy between what choices of reference unit to opt for sustainability assessment is not trivial.

Regional and farm approaches usually express impacts per hectare of land and other approaches, such as those of Life cycle analysis (LCA) includes the concept of the functional unit, generally expressed per kg of product (i.e. milk). However, methods like $SIMS_{DAIRY}$ which allow the expression of impacts according to several reference units are preferable (Biewinga and Van der Bijl, 1996). Farming in an EU context, where production is regulated by milk quotas, may induce us to think that it would be more logical to favour the reference of unit of milk. However, this reference unit generally gives little information about the opportunities of losses to be transported or to have an effect on other ecosystems outside the farm boundaries.

Losses were sensitive to the most studied farm variables. Some of these variables are management-related ones and thereby, they could be easily implemented by the farmer. Some other variables, such as soil type, show a large effect on losses from the soil (N_2O, NO_3^-, NO_x and P) and hence, farming on these types of soils offer little opportunities to manipulate these losses by farm management.

When analysing the predicted results of the sustainability attributes scores (those predicted by $SIMS_{SCORE}$), one must always bear in mind that $SIMS_{DAIRY}$ only aims at predicting risks and does not attempt to give absolute figures. Most of the relationships found by existing studies on these topics are still weak and need further analysis and quantification. All the sustainability attributes that are scored by $SIMS_{DAIRY}$ except for landscape aesthetics proved to be very sensitive to many of the studied farm variables. Landscape aesthetics are affected by other factors that have not been studied by the sensitivity analysis (i.e. hedging, the inclusion of traditional farm features) and that have effect on the farm net margin and on level of farm biodiversity.

Biodiversity was affected in great manner by those variables that have a large effect on the amount of inorganic N flowing in the soil-plant system, such as those directly affecting inputs of inorganic N (i.e. mineral fertiliser rate), those affecting the transformations of organic into inorganic N (i.e. reseeding) or those affecting the amount of recycling N into the soil (i.e. excretion).

The seasonal pattern affected biodiversity as systems where largest lactation requirements and grazing season coincided (calving in autumn) resulted in greater returns in urine N (inorganic N within hours) to the soil and hence affecting negatively on biodiversity. Soil

compaction by grazing activity affected in a negative way both biodiversity and soil quality strongly. Animal welfare was affected greatly by farm management factors such as those related to manure system choice, direct and indirect diet effects and the housing period. FYM-based systems and systems relying on cow grazing had positive elements for the social behaviour and free movement of animals and moreover, to reduce the risk of some health disorders. Increased PUFA in the diet affected positively animal welfare and also milk quality.

Those factors that have an effect on the amount of conserved silage grown and fed to the animals: young grass leys (<2 years), for instance, resulted in greater herbage yields, thereby more amount of conserved herbage fed to the animals and hence, increased the risk of affecting animal welfare negatively. Housing period also had an effect on milk quality and CH_4 losses from rumination. Fresh grass, compared with conserved food, had a larger content in PUFA and thereby, cows grazing have more opportunities to yield milk with high contents of PUFA, thus increasing milk qualities for human health, and decrease CH_4 outputs. Fat additions to diets can impact on CH_4 losses by hydrogenation of unsaturated fatty acids (metabolic H acceptor to reduction of CO_2), enhanced propionic acid production and protozoal inhibition. Studies, however, largely attribute this effect to decreased fermentable substrate rather than to direct effect on methanogenesis (Johnson and Johnson, 1995).

Organic farming systems have claimed their role in delivering healthier milk with increased PUFA contents. However, there is not such evidence so far. Most of this claim is likely to be more related to the fact that UK organic systems have an increased reliance on grazed grass. This would of course imply better milk quality in terms of PUFA content; however this could also be potentially attained in the same way by conventional farms if cows' reliance on fresh grass is similar to that in organic farms. It is worth mentioning that new grass varieties with enhanced PUFA contents are currently being tested (Abberton *et al*., 2006) to further improve these opportunities to enhance milk quality, animal welfare and decrease CH_4 losses. These new plants would be preferable to the current possibility of enhancing these PUFA levels in the diet by supplementation as they would be much better in cost-effective terms than the current supplementation.

$SIMS_{DAIRY}$ proved to be a very useful tool to test the effect of new plant and animal traits on the whole soil-plant-animal system. Manipulating the N absorption ability of plants (h factor), as previously mentioned, had several implications for N and P losses and their effects were not always in the same direction (i.e. they generated pollution swapping in some cases). Increasing "h factor" resulted in substantially increase plant N and DM per hectare and hence greater net farm margins through less hectare requirements or surplus of silage. This increased production per hectare, however, also increased the proportion of silage fed to animals, increasing their risks in animal welfare and milk quality. In most cases also animals were fed with excess N and thus, animals excreted more urine N and thereby, more inorganic N was recycled through the soil compartment increasing the risks towards negative impacts on plant biodiversity. Traits in plants such as those that manipulate the % N in plant and the proportion of harvestable plant showed also great sensitivity on losses, sustainability attributes and farm net margins. Manipulating animal traits such as the ability to yield milk and the ability to excrete different proportions as urine N or dung N (irrespective of diet N ingested) also showed large sensitivity on losses. Increasing milk yield per cow increased the N and P use efficiency by animals both per hectare and per cow and thus, resulting in smaller losses than the basal animal type. Higher yielding cows had an increased risk of welfare problems with fertility and mastitis. This also had implications on net farm income as income was increased as the balance resulting from gaining more money from milk, spending money for (i) extra forage surface (ii) possibly vet cares and (iii) need for larger replacement rates was still substantially positive. Future research on new animal traits should include solving these associated welfare risks on high yielding cows. Improvement of management in higher yielding cows through better health conditions (i.e. programs on detection of mastitis), although costly, is likely to tackle successfully some of these welfare risks too.

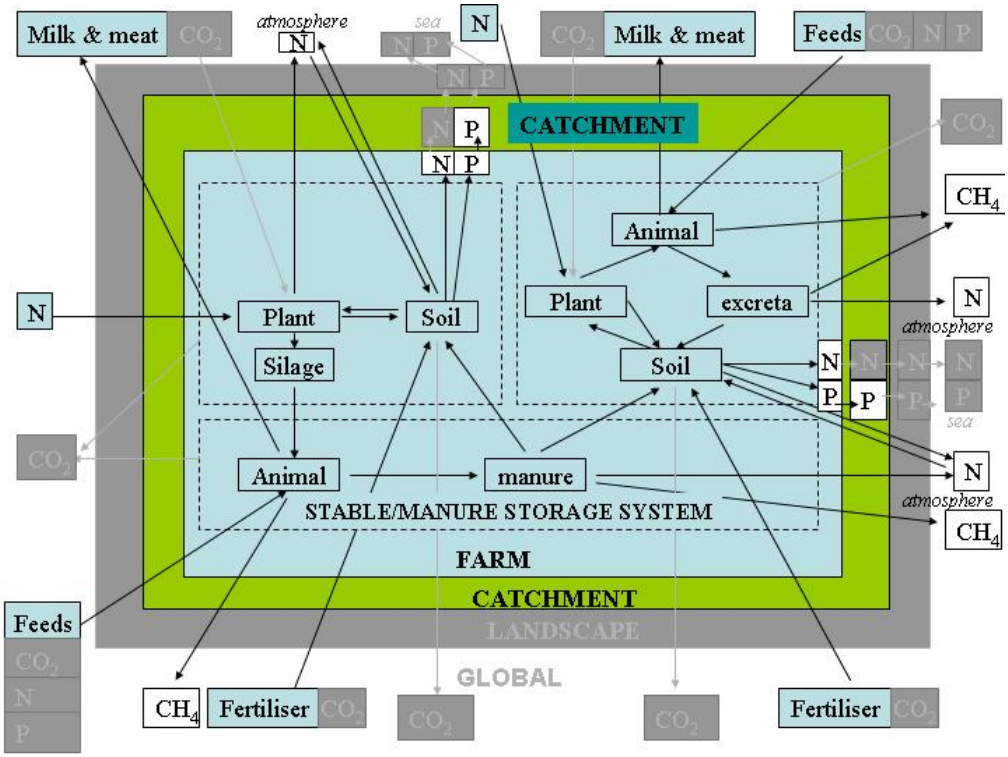
Seasonal patterns of calving largely affected the price of milk and hence net farm income. Farming systems with all-year milk attain substantially more money per L than those systems with a seasonal pattern. They also affected losses and some sustainability attributes such as animal welfare, biodiversity and soil quality.

10.7. Conclusions

Existing models and studies were used to develop an integrated mathematical simulation modelling framework to study the sustainability of dairy farms in the UK ($SIMS_{DAIRY}$ model). This study describes the details of the main submodels and the interactions among them. Different model parts are presented: (i) part of the model simulates at a farm level the flows, transformations and losses of N and P and CH_4 in the soil-plant-animal system using a monthly time step (ii) another part simulates the farm performance in terms of attributes of sustainability of animal welfare, biodiversity, landscape aesthetics, milk quality and soil quality, (iii) a third part simulates the net farm income and (iv) a fourth part is able to optimise farm management to meet several objectives and using different criteria. All simulated results are largely sensitive to nutrient management factors, edapho-climatic conditions and forage surface management. In order to see to what extent these factors influence the whole system, a sensitivity analysis was carried out where a large number of model E/M variables were tested against selected state variables. The study shows that there is not a single factor that, by isolation, can result improvements for all the aspects of sustainability studied. Moreover, in some cases, changes in some of these factors may induce the reduction of losses per L of milk but increasing the same losses per hectare. This could be explained by the fact that a lot of these factors have a large effect on yields production per hectare and hence those losses more related to animal management are likely to remain similar in total and hence greater per hectare. $SIMS_{DAIRY}$ appear to be robust and can be used to analyse the complexity and indicate the effect of management decisions and specific edapho-climatic conditions on grassland farming sustainability. However, further testing, improvements and upgrades may be necessary, specially using data from farms and future studies on those relationships that may be currently weak. The incorporation of N fixation, the full C cycle, water use efficiency and a full energy balance is needed to address the future challenges of dairy farming systems.

Chapter 11

Use of $SIMS_{DAIRY}$ modelling framework system to specify sustainable UK dairy farms



11. Use of $SIMS_{DAIRY}$ modelling framework system to specify sustainable UK dairy farms

Abstract

Sustainability in UK dairy farming is no longer secured by traditional management focused on production of commodities. Society awareness, legislations and competing markets demand farming systems which can deliver multiple attributes such as: clean environment, high biodiversity, picturesque landscapes, good animal welfare and high quality of product and soil. In order to study this complex system, a new model framework ($SIMS_{DAIRY}$) has been developed. We demonstrate the use of $SIMS_{DAIRY}$ to explore the economic viability of technical or structural system changes aimed at improving sustainability in existing UK dairy farm types. Management factors (i.e. manure, fertiliser and diet), acting singly, or in combination, are evaluated in such farms by a multi goal-seeking procedure (evolutionary trajectory towards sustainability). The following goals are sequentially achieved as this trajectory progresses, compliance with: (i) NVZ_{170} legislation, (ii) Nitrate Directive 91/414 (11.3 mg l^{-1}), (iii) Gothenburg Protocol (NH_3 reduction), (iv) Kyoto Protocol (N_2O and CH_4 reduction), (v) P eutrophication limits (100µg/l), (vi) milk with beneficial properties for human health, (vii) acceptable animal welfare and (viii) enhanced biodiversity and landscape. Although results from this exercise pinpoint the difficulty in achieving overall sustainable dairy farms under existing market/subsidies systems in the UK, they also show that some combinations of management factors may offer substantial scope for improving sustainability with no economic penalties.

11.1. Introduction

Western Europe dairy systems are facing numerous problems due to continuing intensification. It is fundamental to consider not only the productivity/economic aspect of dairy farming production but also other attributes which define farm sustainability as a

whole. Dairy farming systems must hence: (i) ensure an adequate net farm income to support an acceptable standard of living for farmers, (ii) result in acceptable environmental impacts, (iii) produce food that is safe, wholesome and nutritious, thereby promoting human health, (iv) promote a good level of animal welfare, (v) meet social expectations of picturesque landscapes (vi), enhance or maintain high biodiversity standards, (vii) improve or maintain the quality of the soil, and strike a reasonable balance among these key attributes (Bergström *et al.*, 2005). Not only may many of these attributes be unachievable under some existing systems and certain edapho-climatic circumstances but they are also so interrelated to each other that getting one of these goals may often compromise another and moreover, pose a high risk to the economic viability of the farm.

Farm level modelling is a useful tool in order to bring all this complexity into an operational and scientific *modus operandi*. Nonetheless, appropriate models to objectively determine the sustainability of dairy farming systems are still lacking. In order to fill this gap, a new model ($SIMS_{DAIRY}$) has been developed (del Prado *et al.,* 2006d). $SIMS_{DAIRY}$ integrates existing and new models, equations and 'score matrices' to optimise dairy management factors in order to find more sustainable systems (full description in chapter 10).

This paper reports the use of $SIMS_{DAIRY}$ model to explore the economic viability of technical or structural system changes aimed at improving sustainability in existing UK dairy farm types (i.e. conventional farm in the south west on sandy loam soil). Management factors (i.e. manure, fertiliser and diet), acting singly, or in combination, are evaluated on a typical UK dairy farm by a multi goal-seeking procedure.

11.2. Materials and Methods

11.2.1. Description of $SIMS_{DAIRY}$

Sustainable and Integrated Management Systems for Dairy Production ($SIMS_{DAIRY}$) is a new modelling framework which integrates existing models for nitrogen (N) cycling (NGAUGE: Brown *et al.,* 2005; NARSES: Webb and Misselbrook, 2004), phosphorus (P) cycling (PSYCHIC: Davison, *in press*), equations to simulate ammonia (NH_3) losses from

manure application (Chambers *et al.,* 1999), prediction of methane (CH_4) losses (Chadwick and Pain, 1997; Giger-Reverdin *et al.,* 2003), cows' nutrient requirements [Feed into Milk (FiM) system (Thomas, 2004)] and 'score sustainability matrices' for measuring attributes of biodiversity, landscape, milk quality, soil quality and animal welfare and an economic model (A. Butler, pers. comm). The flow diagram is shown in Fig 1.

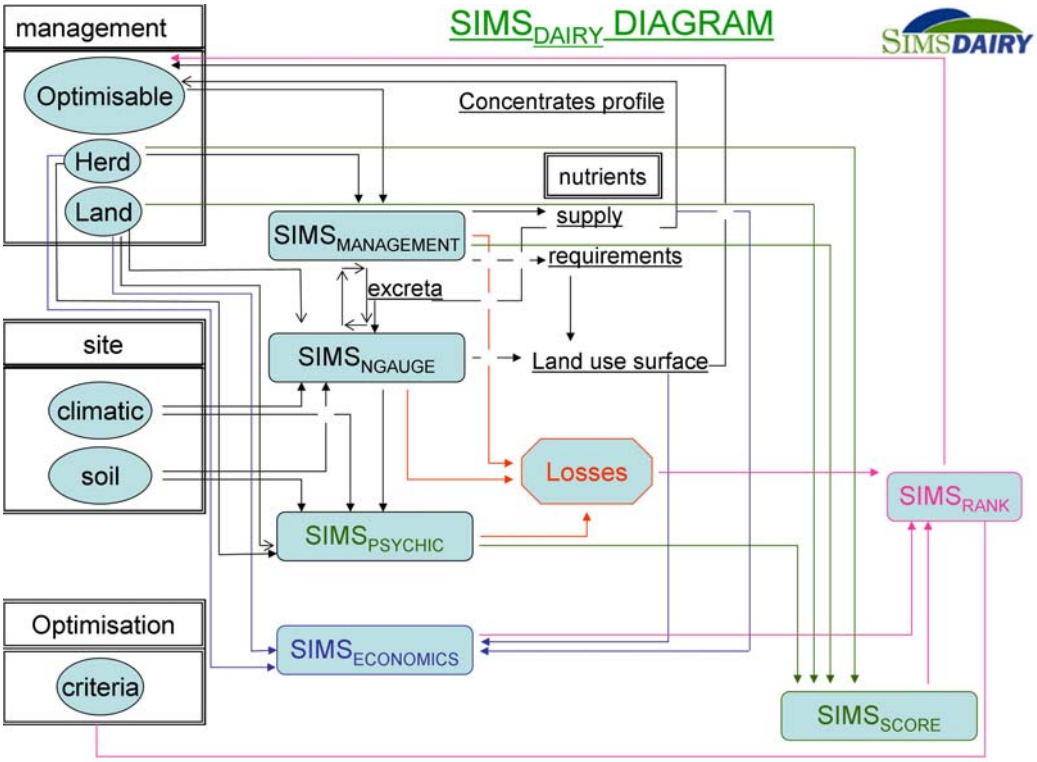


Fig. 1. General diagram of main inputs (○), flows (→) and submodels (⬭) in SIMS$_{DAIRY}$.

At the start of a model simulation the main farm herd variables (i. e. diet, manure, fertiliser, crops or animal types), land use management (i.e. fertiliser rates), site characteristics (climatic conditions and soil characteristics), management options to optimise and criteria of optimisation (i.e. environmental losses) are entered. Nitrogen and P flows are subsequently simulated throughout the different stages of the farm by the submodel SIMS$_{MANAGEMENT}$. Firstly, for a given lactating herd defined by: (i) number and type (breed, condition score, calving season, total weight, weight gain/loss, average milk yield, milk protein % and butterfat milk % target) of dairy cows, (ii) number and type of followers, (iii) grazing days and (iv) diet profile (i.e. proportion of total DM ingested during the housed period as concentrates), dry matter (DM) voluntary intake and, energy and protein requirements are

predicted for the grazing and housing period. $SIMS_{MANAGEMENT}$ then evaluates if the energy and N supplied by the existing diet profile enables all requirements to be met. Otherwise, $SIMS_{DAIRY}$ recalculates some of the initial properties of the concentrates and seeks the new concentrates characteristics. In order to simplify the complexity of a dairy system, diet profile is defined in terms of concentrates: grass grazed: maize silage ratios for both the grazing and housing period, respectively. The model, at this stage, calculates the total N and P excreted and the gaseous losses [NH_3, dinitrogen (N_2), nitrous oxide (N_2O) and CH_4] generated by the housed herd and stored manure. The resulting manure N (slurry or FYM) not lost is then applied to the arable crop/grass land according to a given area, seasonal pattern and chosen application technique (i.e. deep injection of slurry). Land on the farm is used to grow grass and arable crops in order to fulfil those animal requirements not covered by the concentrates ingestion. This land is defined in terms of use and 4 classes are allowed: (i) dairy herd grazed grass area, (ii) followers grazed grass area, (iii) area for grass conservation and (iv) arable crop area (only maize is allowed to grow as arable crop). Using the submodel $SIMS_{NGAUGE}$, N and P flows are simulated on a per hectare basis for each land use, given soil types, sward age, past management and for given rates of manure and mineral fertiliser applications. Dry matter, N and P plant yields together with losses of N [N_2, N_2O, NH_3, nitric oxide + nitrogen dioxide (NO_x) and nitrate (NO_3^-) leaching] and CH_4 are predicted and the surface required for each land use is hence calculated by simply dividing the total predicted animal requirements (previous stages) over plant yield (once silage making losses have been accounted for) of each crop source. The submodel $SIMS_{PSYCHIC}$ (Davison *et al., in press*) is automatically linked to the whole framework and predicts the risk of P diffuse pollution from a source area by estimating source, mobilisation and delivery of P and sediment: P inputs in manure and fertilisers and soil residual P, the mobilisation of P and sediment through dissolution and soil detachment and the delivery of dissolved and particulate P and associated sediment, to watercourses in surface and subsurface runoff.

Sustainability matrices are scored by the submodel $SIMS_{SCORE,}$ which simulates the effect of both nutrient management variables (i.e. effect of unsaturation of fatty acids in the diet on milk yield) and non-nutrient management variables (i.e. available surface per cow during housing) on the sustainability of the farm in terms of biodiversity, landscape, milk quality, soil quality and animal welfare. The scores assigned reflect poor (0) to very satisfactory (6)

sustainability. Subsequently, the net farm margin is calculated by subtracting the total fixed costs and overheads from the gross margin. Variables costs are calculated by the model as a function of management variables (i.e. £ per unit of applied manure volume). Some management strategies (i.e. those resulting in enhancing landscape), due to large cost variability, are user-proposed inputs and hence do not intend to reflect an accurate value.

The farm sustainability is then evaluated by the submodel $SIMS_{RANK}$, which ranks farms under different management strategies according to the user-defined criteria (i.e. minimising global environmental impacts over unit of milk).

11.2.2. Steps to find sustainable UK dairy systems

$SIMS_{DAIRY}$ was used in this study to simulate the effect of farm management on the overall sustainability of a typical dairy farm in the UK. In order to do so, an evolutionary trajectory towards sustainability was simulated by sequentially introducing management changes (i.e. in manure) on a baseline UK dairy farm (main characteristics are shown in Table 1) aiming at improving environmental sustainability as an additive process (using the optimisation menu of $SIMS_{DAIRY}$).

Table 1. Baseline Farm characteristics.

Soil type	Loam	**Animals**	
Location	Somerset	Number of milk cows	100
Annual drainage (mm)	301	Young stock	63
Management variables		Replacement rate	24%
Milk (litres/cow/ yr)	6570	Milk protein (%)	3.1
Total dairy cows/forage ha	2.5	Butterfat milk (%)	4.1
Grazing days - cows	185	**Manure management**	
Area		Type of manure used	Slurry 6 % DM
Total area (ha)	40	% manure applied to grazed grass	45
Fertiliser		cut grass	50
N to grazed grass (kg N/ha)	240	maize	5
N to cut grass (kg N/ha)	290	Storage type	slurry tank: open
N to young grazed grass (kg N/ha)	180	Application method	Broadcast
N to maize (kg N/ha)	40	Distribution (in time)	
P to grazed grass (kg P/ha)	25	Feb (%)	40
P to cut grass (kg P/ha)	35	Jun (%)	5
P to young grazed grass (kg P/ha)	40	Aug (%)	5
P to maize (kg P/ha)	40	Dec (%)	50

The non-nutrient management variables which affect the submodel $SIMS_{SCORE}$ were set in the baseline scenario at those corresponding to average conditions [i.e. no routine of

condition score (animal welfare), average maintenance of hedgerows (landscape), no buffer strips (biodiversity)]. South-west England is an important dairy region, containing 35% of the dairy holdings in England and 36% of the total dairy cows (Defra, 2005b). A typical conventional dairy farm situated in Somerset under moderately drained loam soil was chosen to represent the baseline dairy farm scenario. The main characteristics (Table 1) of such dairy farm are:

(i) The dairy cows are fed by grazed grass (half a year), on-farm feed (grass and maize silage) and bought-in concentrates.

(ii) Milk production per dairy cow is about 6500 L yr^{-1}.

(iii) The density of dairy cows per forage ha is 2.5, these dairy cows having a replacement rate of 24%.

(iv) Cows are housed in cubicles where the manure generated is stored in a slurry open tank with a volume to store slurry for about 3 months.

(v) The manure is broadcast applied to the forage land at application rates that result in spreading 50% to mown grass, 45% to grazed grass and 5% to maize.

(vi) The typical temporal patterns of distribution of the total manure applied followed the approach described by Smith *et al*. (2001b), in which, the year is divided into 4 quarters and the proportion of manure applied of the annual total is as follows: from February-April (40%), May-July (10%), August-October (25%) and November-January (25%).

(vii) The timing and percentage of annual total mineral fertiliser applied per month was designed to follow the UK fertiliser recommendations for agricultural crops (RB209), (MAFF, 2000). The amounts for N ranged from 40 to 290 kg N ha^{-1} yr^{-1} for maize and mown grass, respectively. Phosphorus rates ranged from 25 to 40 for razed grass and maize, respectively.

In order to assess environmental sustainability we used the index developed by Van Calker *et al.* (2006) as the criteria of $SIMS_{DAIRY}$ optimisation. This index comprises outputs of CH_4, N_2O, NO_x, NH_3, NO_3^- leaching and water use. We defined overall sustainability as a combination of targets:

(i) Environmental targets: compliance with NVZ_{170} rules, EU Nitrate Directive (11.3 mg l^{-1} in the leachate), P threshold for eutrophication (100µg l^{-1}) and reduction in

greenhouse gases (GHG) (comprising N_2O and CH_4) and NH_3 gases (with respect to the baseline scenario) according to Kyoto and Gothenburg Protocols, respectively.

(ii) Milk production with enhanced polyunsaturated fatty acids (PUFA) composition.

(iii) Acceptable levels of animal welfare.

(iv) Acceptable level of biodiversity and landscape.

(v) Acceptable soil quality.

(vi) Adequate net farm income for standard living.

Compliance with NVZ_{170} rules was simplified as the requirement to limit organic manure, including excreta from grazing, applications to 170 kg N ha^{-1} yr^{-1} (assuming that a 600 dairy cow will have an annual excretion of 106 kg N ha^{-1} yr^{-1}: Guidelines for farmers in NVZs: MAFF, 2001) and establishing closed periods for manure application (September-November for grasslands and August-November for maize). Kyoto and Gothenburg protocols aimed at a reduction in 12.5 % (GHG) and 12.8 % (NH_3), respectively. Threshold values for acceptable milk quality, animal welfare, biodiversity, landscape and soil quality were set at a score of 4 (see above). Due to major fluctuations on variable costs (i.e. impact of oil price rises on fertiliser price) net farm income for standard living was not set at any specific value and was used as a comparative tool.

Twelve trajectory steps were simulated (Table 2), by which management was optimised as an additive process (every step incorporates any changes being previously made). The steps imply the reduction of N mineral fertiliser rates per hectare by acquisition of more area to feed the same amount of cows at the same level of production. This extensification of the production system will bring different costs by growing a larger surface (i.e. transport by tractor). The amount of grazing time spent by the herd will bring important implications in variable costs in connection with the management of the herd. Decreasing grazing will probably lead the farmer to replace some of the land previously used for grazing into land for maize and grass for silage. By modifying the level of milk production per cow and assuming, for this study, that the number of cows remains the same, the farmer will have a different level of management complexity as the higher yielding the cow is the more care the cow generally needs. This increasing/decreasing complexity in management will be counteracted by the positive/negative impact on the economy of the farm by modification of the total milk

production. Greater levels of milk production will cause larger volumes of slurry being stored.

Table 2. Changes in the evolutionary steps of the baseline scenario towards overall sustainability.

Trajectories	1	2	3	4	5	6	7	8	9	10	11	12
Changes												
Mineral fertiliser N (%)	-5	-11	-14	-19	-24	-29	-34	-39	-44	-49	-54	-54
°Grazing days		opt	opt	opt	opt	opt	opt	opt	opt	opt	opt	opt
					Milk							
°yield			opt	opt	opt	opt	opt	opt	opt	opt	opt	opt
°proteins, butterfat				opt	opt	opt	opt	opt	opt	opt	opt	opt
°silage management					opt	opt	opt	opt	opt	opt	opt	opt
					manure							
Θ % & timing						a	b	c	c	c	c	c
°areas									opt	opt	opt	opt
application										band	band	band
°storage											opt	opt
Welfare improvements												yes
Landscape improvements												yes
Buffer strips & field margins												yes
Supplements (fat)												opt

Θ Manure % application is changed for the application months: a: [20(Mar), 20(Jun), 20(Aug), 40(Dec)], b: [30(Mar), 30(Jun), 30(Aug), 10(Dec)] and c: [20(Mar), 40(Jun), 40(Aug), 0 (Dec)] and °opt: optimised.

Changing the usual patterns (about 90% of the manure generated being applied during Autumn-Winter period) will require building larger storage systems that would let the farmer store the manure during larger periods of time to avoid winter and autumn applications. The last step will bring in improvements in animal welfare, landscape and buffer strips and field margins to enhance biodiversity. The management complexity will be then much greater.

11.3. Results

11.3.1. Optimised management results

Some of the steps involved the use of the SIMS$_{DAIRY}$ optimisation routine. These optimisations resulted in percentage changes to the following state variables: grazing days (-8%), milk yield (+49%), milk protein content (+10%), milk butterfat content (+7%), silage management (improvement in method), manure areas application (+350% to cut grass, -75 % to maize and -100 % to grazed grass), manure storage (slurry tank with crusted manure),

fat supplementation [fat (+75%), fatty acids: saturated (-42%), monosaturated (+33%), long chain PUFA (+29 %) and long chain (>=C20) PUFA (+100 %)].

11.3.2. State variables results after implementation of trajectory steps

The main effects of evolutionary steps towards sustainability are plotted in Figure 2. Environmental losses as a whole (as index of environmental sustainability increased: Fig 2g) and individually (Fig 2a-f) of N, P and CH_4 generally decreased, both per ha and per L of milk, as the steps were implemented.

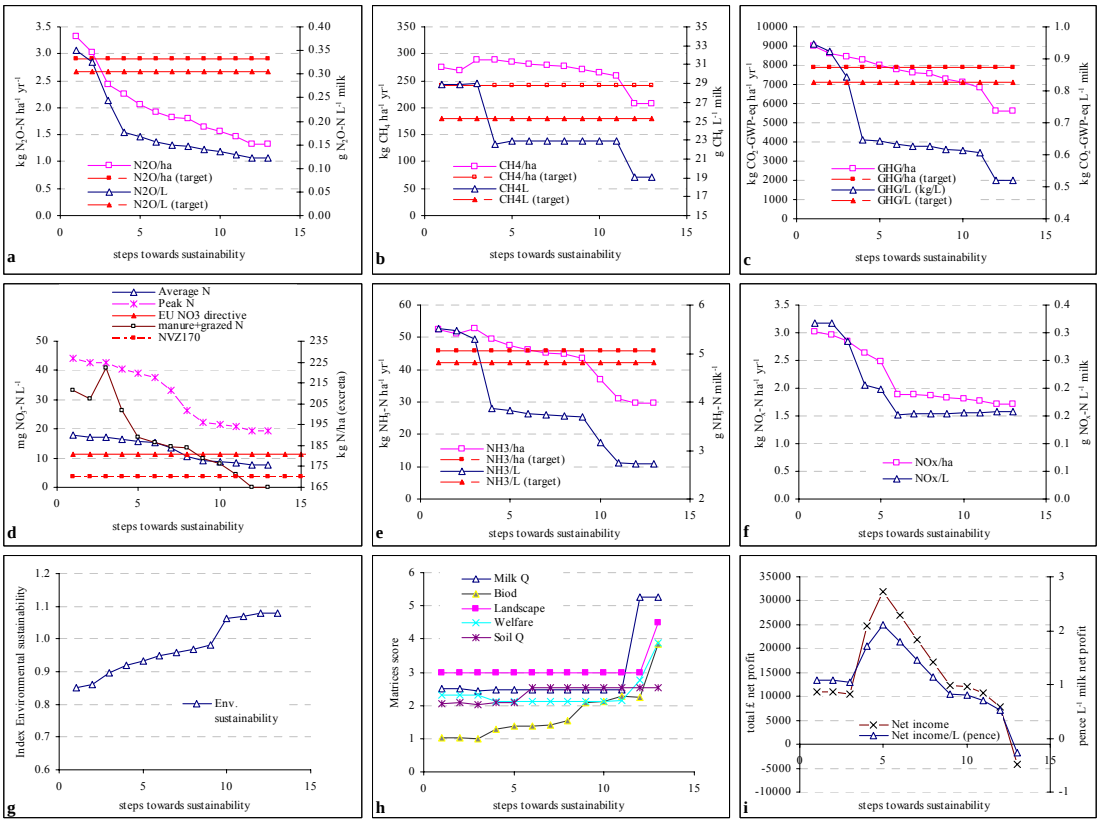


Fig. 2. The effect of evolutionary steps towards sustainability on state variables of: (a) N_2O, (b) CH_4, (c) greenhouse gases (as global warming potential CO_2 equivalents of N_2O and CH_4), (d) NO_3 leaching (as average N and peak N concentration in the leachate), (e) NH_3, (f) NO_x, (g) environmental index of sustainability (index calculated after Van Calker et al., 2006), (h) score matrices for attributes of milk quality, biodiversity (Biod), landscape, animal welfare and soil quality (Soil q) and (i) net farm income profit. Together with nutrient losses values, targets to comply with Kyoto Protocol (Fig a-c), NVZ_{170} rules and nitrate directive (Fig d) and Gothenburg protocol (Fig e) are shown. All results of nutrient losses and targets (Fig 2a-2f) are expressed per unit of surface (ha) and unit of product (L of milk). Net farm income is expressed as total and per unit of product (L of milk). The scores of the matrices (Fig 2h) are expressed in a value ranging from 0 (worst)-6 (best).

As expected, although most of the attributes of sustainability had some score improvement after steps with nutrient management changes were implemented (Fig 2h), it was not until major capital investment was carried out that these were good enough to attain the score target. Predicted net profit was large enough to maintain or even improve the baseline scenario in some of the steps. However, costs to achieve a good level of biodiversity, landscape and animal welfare resulted in largely decreasing the net farm profit in the last trajectory step.

Environmental targets were achieved at different trajectory steps. Although the target set by the Kyoto protocol was achieved as a whole at step 6 (Fig 2.c) both in CO_2 equivalent-GWP per ha and per L of milk. If we separate the N_2O and CH_4 losses, N_2O was easily reduced to this target at step 3 and CH_4, although it easily reached this target as per L of milk (step 4), it took measures of fat supplementation (step 12) to achieve the 'per ha' target. Gothenburg target was also easily achieved as a per L of milk unit (step 4) but it took more measures to decrease NH_3 ha^{-1} to this target level (step 7). Water-related targets (P threshold, EU Nitrate Directive and NVZ_{170} rules) were also achieved at different steps. Predicted P concentrations in waters complied with the eutrophication threshold (data not shown: always <75 μg l^{-1}) of 100 μg l^{-1} in all cases. Compliance with the threshold of 11.3 mg l^{-1} for the Nitrate Directive was achieved under a step (step 8) which allowed both a larger amount of farm manure and grazed N as that prescribed by the NVZ_{170} rules (step 12) but also required a more stringent closed period (no manure application between September-February). Although no target was set for NO_x losses, a large reduction was achieved both as per ha (-44 %) and per L of milk (-51 %) from the baseline scenario to the step 12.

11.4. Discussion

Although the evolutionary trajectory steps improved overall and individual sustainability, it must be noted that they only intend to show an example of trajectories and therefore, they can not be interpreted as the best possible trajectory but as an example route towards sustainability. In the future, we aim to incorporate a method by which the efficiency of multiple trajectories towards sustainability can be evaluated.

Decreasing fertiliser rate proved to be a very efficient method to improve environmental sustainability as it resulted in smaller losses either per hectare or per L of milk. As expected, it resulted in the farm requiring more land surface in order to supply the same amount of food at a smaller level of herbage production per hectare. Whereas fertiliser rate per ha was reduced up to 55 %, total forage area increased up to 30 %, thereby resulting in farm fertiliser savings. However, it is difficult to predict the profitability of this in the future as it is hard to see projections of fertiliser and land prices.

The optimum grazing period was predicted to be smaller than the average 185 days a year. $SIMS_{DAIRY}$ takes into account the combined effect of: (i) the larger risk for N_2O emission, Nitrate leaching and P losses during grazing than when the same excreta produced during housing is evenly applied to land and (ii) the greater risk of NH_3 volatilisation through managing excreta during the housing period and the production of larger volumes of manure. These volumes of manure may be difficult to manage (storage and application) and thus, pose a greater risk of N and P losses overall. Although not shown in this study, the optimum grazing period for minimising environmental losses will be highly sensitive to the type of manure-housing system chosen [i.e. FYM-based systems may pose a large risk on N_2O and CH_4 emissions (Yamulki, 2006)], type of soil and agroclimatic conditions. For example, although P concentrations in waters were always acceptable under these soil conditions, in a parallel study (data not shown), a dairy farm following the same steps and situated in the same climatic conditions but differing in soil type resulted in predicted values of P in the leachate of >450 $\mu g\ l^{-1}$ at any fertiliser rate, thus resulting in failing the P threshold for eutrophication sustainability.

Needless to say that there is no win-win situation if we look at the interactions between grazing *vs.* housing and issues such as animal welfare or soil quality. Whereas animal welfare may be positively enhanced by a greater grazing period as the risk of diseases (i.e. Listeria) or excess acidity (Wilkinson, 1999) are reduced by a smaller reliance on herbage silage and diet and social structure is improved, too much grazing may result in a negative effect on soil quality by soil poaching and compaction. Moreover, cows on silage produce milk with smaller concentrations of PUFA (Elgersma *et al.,* 2006) and hence with a lower value.

Milk optimisation resulted in higher yielding cows and raised protein and butterfat content in milk. Because this has serious implications on the welfare of the herd, especially on the fertility, diseases and metabolic disorders, $SIMS_{DAIRY}$ predicted an increase in replacement rates and veterinary costs. Environmental losses decreased per L of milk as obviously a higher yielding cow has an improved efficiency of conversion of energy, dry matter and proteins into milk. Some losses per hectare, though, increased as land surface required increased at a smaller rate than the increase in milk yield.

Landscape and biodiversity improvements would only generally be possible through investment and due to the lack of more precise economic data it is difficult to state to what extent these farms would be profitable/unprofitable.

Under the economic conditions assumed in our study $SIMS_{DAIRY}$ shows that under most circumstances UK dairy farms would not be profitable if they were environmentally compliant. Dairy farming could be profitable and environmentally sustainable through (i) substantial reduction in costs, (ii) paying farmers for environmental goods, (iii) increasing farm milk price through production of higher value product or more favourable redistribution of retail prices towards the producer.

However, achieving environmental compliance in dairy farming systems will be even more difficult with implementation of the more stringent conditions on water quality attached to the Water Framework Directive.

11.5. Conclusions

$SIMS_{DAIRY}$ proved that is a useful tool to find new sustainable dairy systems that can meet most overall targets of sustainability. In this study one trajectory towards sustainability is simulated in a step-wise order using together the $SIMS_{DAIRY}$ iterative optimisation procedure and manual modifications to the farming system. This study flagged up the fact that there is little scope to improve some sustainability attributes (i.e. landscape aesthetics and biodiversity) up to acceptable levels in intensive dairy farming systems within current socio-economics circumstances. There is also a need for dedicated studies of the impacts of variable costs to improve such sustainability attributes. These costs are currently obtained from surveys with small farm samples and thereby, subject to major errors.

Ideally, it would be most useful to study hundreds of trajectories with $SIMS_{DAIRY}$ to find new sustainable systems. However, the vast space of results and the lack of a much faster optimisation procedure prevented us from it. Currently, $SIMS_{DAIRY}$ is being considered to assess the possibilities of implementing a faster approach probably based on genetic algorithms.

Chapter 12
General discussion

12. General Discussion

12.1. Introduction

One of the major objectives of European agriculture is to have a sustainable and efficient farming sector, which uses safe and environmentally-friendly production methods and provides quality products that meet consumers demands (Van Passel *et al.*, *in press*). Sustainability is a key element to cope with the major predicted challenges linked to the food chain and thereby, to agricultural systems. The complexity of agriculture and the need to fulfil multiple objectives call for an holistic approach where the interactions of the components can be integrated and analysed as a whole. "*Systems modelling*" is a useful tool to put this into practice.

Agricultural systems can be studied at different scales and for different purposes. Although all scales are useful to study varied aspects that influence sustainability, the choice of scale determines the scope of your study. Field scale is the first level for a detailed process analysis, because traditional flux measurement techniques can be used (Leunin *et al.*, 1999). These measurements allow for the development, calibration and validation of the models. This is also the scale at which farmers influence nutrient flows from cropping systems through decisions on, e.g. the choice of variety, sowing date, irrigation and fertilisation schedules. Farm scale is regarded as the scale more specific to agriculture (Seguin *et al.*, 2007). It is widely held that farm nutrient management accounts for most of the variability of the environmental losses in a dairy farm. The landscape scale spatially integrates the effects previously described at smaller scales, and also takes into account the most significant contribution of land use (for the biogeochemical aspects) and land cover (for the biophysical aspects). It is mainly governed by regional and national policies.

Although, to date, there are large uncertainties in our understanding of most mechanisms (e.g. accounting for all the variability of factors that affect N_2O fluxes from soils) at all levels, there are also a large number of isolated studies and data that need integrating within system studies (i.e. through modelling).

The empirical mass-balance modelling of the late 80s (in the UK by Scholefield *et al.*, 1991 and in the Netherlands by Van de Ven, 1992), originally developed to simulate N flows

in grasslands systems, was chosen to be used as the basis to carry out more complex and sophisticated systems approaches. These modelling approaches have been widely used and have proved to be adequate for a large number of systems (see chapter 3, section 3.2).

This thesis focused on the role of systems analysis/modelling to examine the effect of nutrient management on dairy farm sustainability. Two chapters also showed examples at 2 scales of measuring the effect of nutrient management on an environmental issue that is still poorly quantified /understood (i.e. effect of management on N_2O and NO_x emissions from grassland soils).

I started by asking myself what existing environmental and production problems are associated with dairy farms management. For every simulation model, I defined time, space and which, is generally more difficult, subsystems to be incorporated in the different models. I used a systems way of thinking to grasp the big picture. The sets of relations that attempted to formally describe the behaviour of grassland and a dairy system in these models were obtained by analysing and reviewing: existing models, data from existing single-issues modelling approaches and multi-site trials and finally, developing my own modelling approaches. I tested and analysed the sensitivity of the most important parameters on the behaviour of the main state variables. Simulation models were developed in such way that a model would result in improving the understanding of the relationships defining the behaviour of the system in an increasing holistic way and thereby, increasing levels of complexity (more subsystems and more integration) were attained as the models were developed in time.

The N and P use efficiency at the field and farm scale can be studied through simple mass-balance empirical annual modelling. Simple models are capable of simulating the effect of general management factors, soil and climatic factors on the main internal and external flows of N. However, they have several limitations to simulate N and P losses. Models with a shorter time-step structure can overcome this constraint and be used as effective tools to analyse the interaction between nutrient use efficiency and single pollutant issues or, moreover, the combination of them. Modelling also offers the possibility to optimise factors (e.g. management) for single or multiple objectives to study sustainable farms at present or in the future.

Some of the findings in this thesis provide new insights, while other findings may be seen as a confirmation of what other studies have found already. Some of the research findings are important for policy makers, land managers and for farmers as well.

12.2. Discussion

Modelling nutrient use efficiency

Achieving a balance between production and environmental losses is one of the goals for sustainable farming systems (Jarvis and Aarts, 2000). One way of decreasing N and P losses to the wider environment and increasing production in dairy farming systems is through improving the efficiency of nutrient use (especially N and P) (Schröder, 2005). Nitrogen and P can be lost from dairy systems via numerous pathways. These pathways are regulated by different processes (leaching, run-off, volatilisation, denitrification or nitrification) which interact at different levels (i.e. herd, yard, field or farm). Both N and P pools are subject to competing processes that eventually result in either losses to the wider environment, or production (milk, meat or herbage) or sequestration in the soil (i.e. N and P immobilisation). It must be emphasised that soil have a finite capacity to immobilise nutrients and that sooner or later immobilisation and mineralisation will reach an equilibrium (Jarvis *et al.*, 1996b).

a. Improving the nutrient use efficiency by manipulating the internal cycling.

Different mass-balance mathematical models are proposed in this thesis as valuable tools to examine the effect of manipulating management at different levels (field or farm) and under different edapho-climatic conditions on the efficiency of nutrient transfers through all the stages of the N and P cycles of dairy farming systems.

Nutrient use efficiency, especially at farm scale has been also studied elsewhere using nutrient budgets (Van der Meer, 1982; Watson and Atkinson, 1999; Domburg *et al*., 2000). Nutrient budgets, through the calculation of the N and P surpluses, although they may be useful to give a broad indication of losses (i.e. Salo and Turtola, 2006) or to show changes in soil mineral N (i.e. Nyborg *et al*., 1995), do not give an estimate of the different forms of emission to the wider environment and neither do they indicate risks of N losses from a

particular component (e.g. soil) (Schroder *et al.*, 2004). Nitrogen surpluses, for example, can identify areas of high livestock densities, which would be associated with increased risk of pollution. However their use in isolation as indicators of N leaching, or of progress towards mitigation, could be misleading especially if comparing areas differing in land use, climate and soil type (Lord *et al*., 2002). Models such as NUTGRANJA 2.0 and NCYCLE_IRL can predict losses as they incorporate the soil and climate conditions and the processes by which N is transformed and cycled in the soil-plant-animal system. They, thereby, can be used to study the effect of not only management, but also edapho-climatic conditions on the nutrient use efficiency and internal and external nutrient flows.

The efficiencies of N conversion from the different components in the system can be manipulated through different management options. These efficiencies are generally less than 100% and their ranges widely differ between the different system components. For instance, NCYCLE_IRL can simulate a large number of scenarios to provide an indication of the range of conversion coefficient values (dimensionless) through the different mass flows of the N cycle in cut-only (Fig 1a) and grazed-only fields (Fig 1b). Those coefficients that are related to the processes of leaching and denitrification are those with wider ranges of efficiencies and those related to volatilisation of $_{NH3}$ (competition between NH_3 volatilisation *vs.* infiltration of NH_3 or nitrification), animal product (competition between digestion and partition into milk & meat production *vs.* excreta production) and plant uptake (competition between plant absorption vs. denitrification, leaching, volatilisation or immobilisation) have the smallest ranges.

The degree to which these ranges affect the N use efficiency of the system, obviously, is intimately related to the amount of N that flows through these competing processes. Thereby, assessing which components of the system have a larger scope to influence outputs, both useful (e.g. herbage) and undesirable (losses) ones, is critical. In general, reducing overall N inputs to the farm has the scope for increasing N farm efficiency. Otherwise, when inputs are large, a decreasing flux in one part of the system may be compensated elsewhere (Dou *et al.*, 1998). This, however, may reduce total production in the farm and thereby, it poses a risk for production. Finding a balance between N use efficiency and production is hence generally needed.

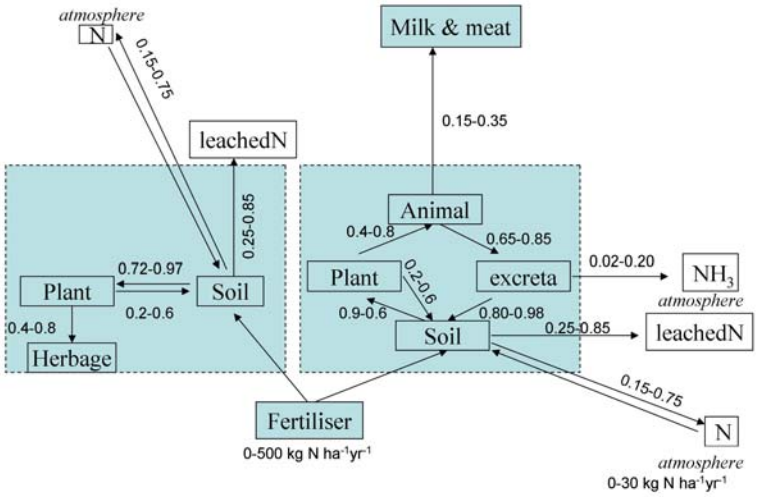


Figure 1. Indicative range of conversion coefficient values for cut (a) and grazed (b) grassland fields simulated with NCYCLE_IRL (after calculations using NCYCLE_IRL: del Prado *et al*., 2006a).

Using a modified version of NCYCLE_IRL (del Prado *et al.* 2006c), the coefficient of N absorption ability by plants (*h* factor), after changing +1% different efficiency coefficients, was the coefficient with a greater positive effect on milk N increase and total leached N reduction (and also on total N use efficiency). Other coefficients that showed a remarkable but smaller increase in milk N and leached N reduction were the efficiency of harvesting (*u* factor) and the efficiency of N use by the animal to convert diet N into milk (*milk* factor) (Fig 2).

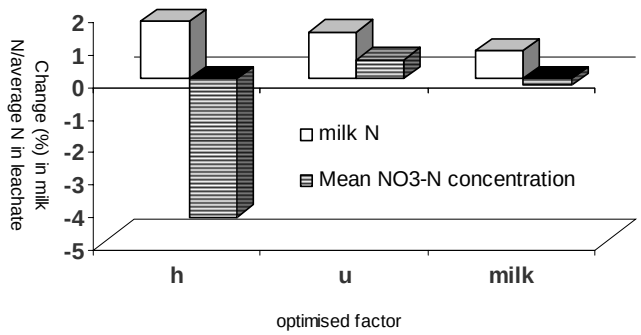


Figure 2. Percentage change in milk N and leached N (mean NO_3^--N concentration in the leachate) after increasing 1% N efficiency in plant uptake (h), harvest (u) and animal conversion of ingested N into milk N (milk) in a grazed grassland (after del Prado *et al*., 2006c).

These findings give us a clear indication of what components of the system may offer a larger scope for improving the N use efficiency of the system: improving N use efficiency in the plant by either improving the match between N supply from the soil and the N plant demand or by breeding grass varieties with an enhanced N use efficiency.

So, in order to develop management options that efficiently reduce N losses by improving the N use efficiency of the system at little production cost, a strong focus must be directed to improve the N use efficiency in the plant. Increasing the predictability of the N use efficiency by the plant will also be critical as the plant controls a large proportion of the internal flows of the N cycle.

b. Limitations of the simple modelling approaches.

One assumption to consider is that these models apply to steady-state systems. Thereby, these models can only be used to compare different systems which, unless stated (i.e. specifying arable past history), would be supposed to employ similar management throughout a large period of time. Perturbations to these systems in terms of discontinuous management can hence not be generally investigated by these modelling approaches.

Models at the farm or field scale can only predict changes in P status but not losses of P due to the slow mobility of P. That P which is not taken up by the plant nor resulting in milk or meat is not necessarily lost, but can accumulate in the soil and be used by the plant or animal in subsequent years. As nutrient surpluses approaches, modelling P at this level will only be useful to provide broad indications. A landscape/catchment level will be more appropriate to relate P use efficiency and losses.

Another limitation of these simple models like NUTGRANJA 2.0 or NCYCLE_IRL is that the effect of factors which affect processes and hence the conversion coefficient values (i.e. mineral fertiliser input, edapho-climatic conditions, cutting regime) can only be simulated on average for an annual context, as the relationships used to construct the models are empirical and resulted from annual averages data-sets. Most of the processes represented in Fig 1, especially those related to the plant itself (uptake), microbial activity (denitrification, mineralisation, immobilisation, and volatilisation) or with a physico-chemical basis (leaching) are very sensitive to edapho-climatic conditions and hence, a shorter calculation

time-step would be more adequate to account for the interaction between edapho-climatic conditions and management. In a farm scale this could be extended to the farm animal management (grazing *vs.* climatic conditions).

Some of these limitations were exposed for NCYCLE_IRL using a data-set from recent Irish leaching experiments on grazed grasslands (del Prado *et al., 2005*), in which the discrepancy between predicted and measured data was large. This particular example demonstrates that simple models like NCYCLE_IRL can give reasonable predictions on average and especially on grass fields under cutting (chapter 3) but are likely to fail with those systems where the uncertainties are large (i.e. grazed systems).

c. Ways to overcome the limitations of the simple modelling approaches.

In more complex modelling approaches like NGAUGE and $SIMS_{DAIRY}$ the mass-balance basis to study N use efficiency is similar to those used in simple models. However, the main differences are that the more complex models can produce a larger solution spaces for each process competing for the N, since these models describe in more detail (temporal and biogeochemical) these processes and transfers of mass and energy between components. This implies that these models can simulate grassland and dairy farm systems with a stronger dynamic basis and thereby, the interaction between management (animal or fertiliser management) and edapho-climatic conditions can be investigated in a more precise way. It is, however, important that the models do not become too complex. More complex models (more subsystems) do not necessarily imply more accurate accountancy of the reactions of a real system as they generally require more parameters and each parameter has its associated uncertainty (error) and this uncertainty is carried through in the model (Addiscott and Whitmore, 1991).

Part of the uncertainties associated to the processes that are not accounted for in NCYCLE_IRL/ NUTGRANJA 2.0 could be quantified by incorporating stocasticity into both models. For instance, the use of a Monte Carlo (MC) simulation is a means of transforming a deterministic model into a stochastic one (Husson, 2001). This is an analytical method that is commonly used to analyse the propagation of uncertainty in evaluations of environmental impact (Stevick *et al.*, 2005). The MC approach has successfully been applied to analyse the uncertainty associated with the estimation of N

losses from farming systems (Gibbons *et al*., 2006; Payraudeau *et al*., *in press*) when the uncertainty is high and/or the probability density function (PDF) is not normally distributed (e.g. N_2O emissions: log-normal distribution).

NGAUGE and $SIMS_{DAIRY}$ (chapters 7 and 10), although capable of simulating N and P flows at a finer time-resolution (monthly time-steps), still lack of this stochasticity. In both models, uncertainties driven by climatic conditions can be at least accounted for by the incorporation of monthly climate statistical data where climatic factors are represented by different percentiles (10, 30, 50, 70 and 90). However, future approaches should address implicitly stochasticity in a stronger way (e.g. Monte Carlo).

Modelling the interaction between nutrient use efficiency and pollution and their influence on global/local environmental issues

The finer resolution that modelling approaches like NGAUGE and $SIMS_{DAIRY}$ have in terms of processes allows linking the inefficiencies of the systems to specific environmental issues since the different losses can be specified for individual compounds. This is very useful as different N, P and C compounds can be quantified for different farming systems and they can be associated to a particular environmental issue (eutrophication: NO_3^- and P, acidification: NH_3 and NO_x or global warming potential: N_2O, CO_2 and CH4). The $SIMS_{DAIRY}$ modelling framework can be used to investigate direct GHG of CH_4 and N_2O from dairy farms.

a. Modelling the interaction between nutrient use efficiency and N_2O.

Management (e.g. fertilisation, grazing, tillage), climatic and soil conditions have been found to strongly affect N_2O emissions from soils (Granli and Bockman, 1994). This fact is confirmed in this thesis (chapter 5 and 6) for factors such as mineral fertiliser; manure fertiliser and weather conditions (e.g. soil temperature, soil water content, seasons). Thereby, understanding to what extent some of these management factors may influence N_2O fluxes at different weather conditions and under different soils is critical in order to decrease N_2O emissions from soils. Experimental studies, although feasible for a limited number of combinations of management and edapho-climatic conditions, can not cover all of the combinations. Thereby, tools that are able to simulate many combinations of management x

soil x climate in a relatively small period of time are desirable for estimating the total contribution of grasslands to N_2O emissions. Models offer this possibility.

The models used to simulate N_2O fluxes at the field level are generally based on experimental data. So far, although field experimental studies have allowed improved confidence in the estimates of rates of N_2O emission from a range of sources, they have also demonstrated wide-ranging temporal and spatial variability (Jarvis *et al.*, 2001). This fact may actually hinder the statistical confidence of both our study estimates and model predictions. Different managements may also bring a different level of variability in the N_2O measurements. The variability of the N_2O fluxes from the maize plot of the commercial farm studied in chapter 6, for example, was remarkably smaller than that from the grazed grasslands. Thereby, the effect of factors such as soil %WFPS, soil temperature, soil NO_3^- content and soil NH_4^+ content on N_2O emissions from maize lands could be fitted to equations with a large R^2 and hence with large potential to be used for predictions. The variability was remarkably large in grazed grassland systems (>200% in a lot of cases) as found by other authors (Velthof *et al*., 1996a; Williams *et al.*, 1999; Merino *et al*., 2001b). This large variability supports the idea that there is a need to improve techniques to accommodate the large spatial and temporal variability of emissions from grazed grass soils before any relationship can be used with confidence as predictors.

As in other studies (Velthof *et al*., 1996) results of the measurements can be used to derive simple empirical equations to be included in existing models. These equations may attempt to include, as in chapter 5 or chapter 6, soil NO_3^-, soil NH_4^+, soil temperature or soil water content (as %WFPS). Soil water content was fitted to quadratic equations , similar to those derived by other authors (e.g. Schmidt *et al.*, 2000) in grassland (chapter 5) and maize land (chapter 6), with R^2>0.60, and thereby, with large potential to be used for predictions not only for N_2O but also for NO emissions. Other relationships were tested such as multiple regressions, but they were not as successful for predictions as those derived in other studies (i.e. Flechard *et al., in press*). This example highlights the difficulty to generalise one or another statistical method as the most appropriate one to predict N_2O emissions. A site-specific assessment may be more adequate instead.

Those relationships with statistical significance (for cut grasslands and maize) can be incorporated into models such as NUTGRANJA 2.0 and NGAUGE for general predictions

of N_2O emissions. NGAUGE and $SIMS_{DAIRY}$ predictions of N_2O losses from soils are based on the hole-in-the-pipe conceptual model (Firestone and Davidson, 1989), by which pools of denitrifiable (NO_3^-) and nitrifiable N (NH_4^+) are simulated to flow through the *pipe* for every monthly step and where the size of the *holes* where N is lost as N_2O, N_2 and NO is determined by the effect of soil water content, mineralisation and amount of mineral N.

The sensitivity analysis of both NGAUGE (chapter 7) and $SIMS_{DAIRY}$ (chapter 10) showed that models that are capable of including processes affecting the N cycle with a sufficient time resolution and sophistication may have the potential to explore the effect of the interactions between climate x soil x management on N_2O losses. As previously discussed, shorter time-scales will improve the accountancy of weather variability (e.g. storms). Models like DNDC (Li *et al.*, 1992ab), CENTURY/ DAYCENT (Del Grosso *et al.*, 2000; Parton *et al.*, 1987, 1996, 2001) or PaSim (Riedo *et al.*, 1998 and Schmid *et al.*, 2001) have at least daily time-steps. Both types of time-scales modelling approaches will have their shortcomings and strengths. These will be discussed in the following subsection for prediction of total GHG.

b. Modelling the interaction between nutrient use efficiency and GHG.

Estimations of GHG emissions in every country are generally carried out by using the IPCC methodology. The IPCC Guidelines aim at a comprehensive inventory of emissions of GHG. Although useful as a common guidance, the IPCC methodology may over-simplify some aspects that can actually lead to large errors in the GHG inventories. The IPCC methodology uses for estimations of N_2O emissions from soils a default Ef for mineral fertilisation applied (1.25 %) and it does not consider the effect of the interactions between soil, climate and management. Numerous studies have found that these Efs may actually vary substantially, for example, with weather conditions (Hyde *et al.*, 2006: 3.5-7.2% for warmer and drier conditions in Ireland), crop choice (Yan *et al.*, 2003: 0.15% for maize) or soil type (Dobbie and Smith, 2003: 6.5% for clay soils and Merino *et al.*, 2004: 0.5 % for silt-loam soil). Taking into account the variability found by several studies on this Ef, one and only default Ef does not seem to be adequate for this level of variability (more than 100%).

The IPCC methodology also provides a method to quantify emissions from animal excreta (grazing and manure management). However, IPCC only provides a rough estimate of the

amount of N excreted by the animals and the N loss before the spreading of slurry or manure (Dämmgen and Webb, 20006).

In dairy farming systems, diet and milk production per cow are factors that can influence the amount of excreted N per cow and indirectly, the risk of N_2O emissions (as shown in chapter 10 in sensitivity analysis of $SIMS_{DAIRY}$); thereby models which can simulate the flows of N through the different stages of the N cycle at the farm level could be used as the basis to improve the predictions of the IPCC by incorporating such factors into the Efs. $SIMS_{DAIRY}$ sensitivity analysis also highlighted the importance of including the interactions between soil type and climate. In fact, these interactions were by far the most sensitive factors to not only N_2O losses but also the global warming potential of N_2O and CH_4 together. This fact also indicates that until a large effort is taken in studying the effect of soil type on N_2O emissions for different crops, managements and climatic regions, a large uncertainty should be expected in the contribution of agriculture to the global anthropological GHG production. Experimental data are needed for all countries, not only countries with developed economies, and experiments for over a sufficient continuous period of time.

Methane emissions at the farm level, per animal in particular, have been found to show relatively smaller variability compared with N_2O (as shown in chapter 10). Among the factors affecting CH_4 output per cow, diet plays the most important role. Through using a default Ef per animal type (e.g. dairy cow) for enteric fermentation, the IPCC methodology may over-simplify the effect that diet management has on CH_4 losses. There is a need, therefore, to incorporate factors such as fibre/starch (e.g. models by Mills *et al*., 2001 and Kebreab *et al.*, 2004) and fat diet profile (e.g. models by Kebreab *et al.*, 2004 and $SIMS_{DAIRY}$ as seen in chapter 10) to improve such prediction of CH_4. This will, however, require more detailed quality data on farm practices specific to each country. Hence, until it becomes readily available in most countries such data will have an insignificant effect on global estimates of GHG.

Mechanistic models such as DNDC (Li *et al*., 1992ab), CENTURY/ DAYCENT (Del Grosso *et al.*, 2000; Parton *et al*., 1987, 1996, 2001) or PaSim (Riedo *et al.*, 1998, Riedo *et al.*, 2000 and Schmid *et al*., 2001) have been successfully used in studies to simulate GHG from different agricultural systems (e.g. DNDC: Levy *et al*., *in press;* Miehle *et al.*, 2006;

Saggar *et al*., 2004, Brown *et al*., 2002; CENTURY: Desjardins *et al*., 2005; Pasim: Calanca *et al*., *in press*, Lawton *et al*., 2006). Although they are generally regarded as good predictive tools for GHG, because of their mechanistic nature and large requirements of calibration they have the practical limitation of generally requiring a large number of specific parameters (each with its associated variability) that are not easily found in the existing measured data. Therefore, the use of such models to estimate GHG from different countries will become even more relevant once the data-sets are improved for all the countries, including those less developed.

Simpler models (or modelling frameworks) at the farm scale with an empirical (Dairywise: Schils *et al*., 2006b; FarmGHG: Olesen *et al*., 2006) or semi-empirical ($SIMS_{DAIRY:}$ chapter 10) nature have been recently proposed (Schils *et al*., *in press*) as functional tools to complement the IPCC methodology. Moreover, such tools are practical for development of cost-effective GHG mitigation options as they reveal relevant interactions between all farm components. They are also very applicable as they use easily available data-inputs and can account for other impacts that affect the environment (i.e. losses to waters or NH_3 emissions). Empirical approaches, however, have the drawback that they may require a large number of modifications if used for other sites.

c. Modelling the interaction between nutrient use efficiency and leaching/run-off losses.

Nutrient use efficiency is also related to leaching/run-off losses from farms. Such losses affect the eutrophication of water bodies outside the field or farm boundaries and can be studied by NGAUGE (NO_3^- leaching) and $SIMS_{DAIRY}$ (NO_3^- leaching and P leaching/ run-off) on a monthly time-step. A shorter time-step together with a stochastic approach may improve the simulation of the effect of storm events on N and P leaching/run-off by accounting for the variability of such events.

Modelling with monthly-time steps, through NGAUGE or $SIMS_{DAIRY}$, may still be valid for policy purposes as it enables us to average the effect of management, climate and soil on NO_3^- leaching losses. It may be used to explore the efficacy of policies such as those from the Nitrate Directive (chapter 8). In chapter 8, outputs from NGAUGE showed that there was scope for improving the NVZ rules (through better use of fertiliser and modest export of manure to adjacent farms as long as receiving farming systems are low-input farms). There

is however a need for integration between different policies, the science base and their implementation (Macleod *et al.*, 2007). For example, to establish predictions of water quality in watercourses a hydrologically-based approach at a catchment scale and incorporating as many environmental processes affecting pollution as possible would improve the study of more complex legislations (i.e. WFD) or the combination of a number of them.

d. Modelling the interaction between nutrient use efficiency and NH_3 losses.

Ammonia emissions are simulated in NGAUGE and $SIMS_{DAIRY}$ following similar approaches as those described by Chambers *et al*. (1999) and Webb and Misselbrook (2004). By simulating the internal and external flows of TAN at the different components of the farm and having Efs per mass of TAN and being moderated (these Efs) by, for instance, seasonal factors, this type of modelling goes beyond the simple calculation which uses Ef per animal as they enable the exploration of mitigation measures (e.g. diet, manure application methods & timing, storage types) to decrease NH_3 emissions considering the effect on other pollutants and also on the profitability of the farm (Webb *et al.*, 2006). It is hence critical that comprehensive emission inventory are obtained by combining existing methods with adequate modelling approaches (e.g. $SIMS_{DAIRY}$), where the methods describing a given source are complementary and cross-referenced throughout (Dammgen and Webb, 2006).

e. Modelling the interactions between nutrient use efficiency, production and losses.

Farm economics and farm N use efficiency are intimately correlated. Increasing the N use efficiency generally will lead to increasing production and decreasing losses. Plant growth and nutrient use efficiency is generally limited by a combination of genotype and environmental factors. New genotypic varieties with increased nutrient use efficiency have been recently developed (e.g. Aber varieties at IGER) and may indirectly result in decreasing pollution to the wider environment.

Modelling and experimental data can actually be effectively combined to quantify the effect of these new varieties on losses under different scenarios. The results from these exercises may then be used to decide what varieties, where and under what circumstances one may use one or another variety.

For instance, a scoping study was carried out to evaluate the global environmental benefits of some existing and future varieties of grasses developed by IGER. In order to do so, the results obtained from a study (Wilkins *et al.,* 2000) on N use efficiency of grazed perennial ryegrass varieties was used. The N use efficiency at the plant level was used to calibrate the N plant use efficiency parameter of NGAUGE for the 7 varieties of ryegrass. NGAUGE simulated the N flows of a grazed grassland and losses of N and milk N per hectare were predicted for the baseline and different ryegrass varieties. The percentage change (N pollutants and N losses) of the different ryegrass varieties compared with the baseline ryegrass was plotted (Fig 3). Using the basis to compare total efficiency performance of the different varieties as decreased lost N: N in Milk (Fig 3a) varieties 3 and 6 showed great reductions in lost N: N in Milk of up to 72 %. This efficiency enhancement was mostly due to a large decrease in N losses (Fig 3b) and to a smaller extent due to a modest increase in milk N (Fig 3c). Less scope was hence found to increase N in milk than to decrease N losses by using these new varieties of ryegrass.

On the other hand, NH_3 losses increased in most cases (Fig 3d). Excreted N was greater as more N was also ingested by the cows, resulting in larger amounts of urine deposited in the soil and hence, more N subject to NH_3 volatilisation. The fact that the absorption ability of the ryegrass varieties is enhanced, allows this N to be more efficiently recycled within the system and more N is accumulated as recalcitrant organic pools from the recycling of plant residues. To a smaller extent, the varieties with greater N content in their leaves than in the baseline ryegrass resulted in an increase in urine: dung ratio and hence yet more N to be lost as NH_3.

This kind of approach, where one can focus at the system level, utilising iterative cycling between experimentation and modelling, and the use of genomic tools, facilitates precision breeding. Thereby, it may assist to fully realise the potential of crop improvement to multifunctional agriculture, where both productivity and ecosystems services are major goals (Abberton *et al*., 2006).

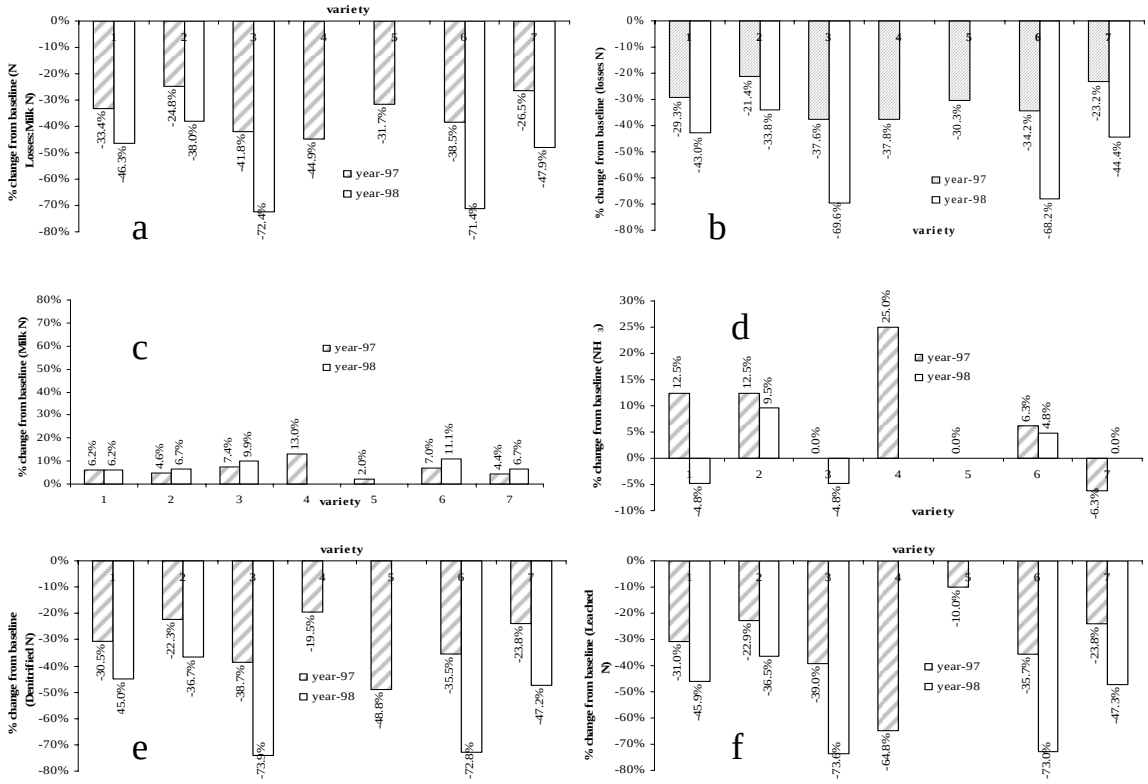


Figure 3. Predicted percentage change of the different ryegrass varieties and in different years compared with the baseline ryegrass in terms of: (a) N losses: N in milk, (b) Losses N, (c) Milk N, (d) NH_3 losses, (e) Denitrified N and (f) Leached N.

f. Modelling the interactions between the different losses (pollution swapping).

As seen by the previous example, sometimes reducing N losses of one N compound may have potentially negative effects on other N compounds 'pollution swapping'. Models like NGAUGE and $SIMS_{DAIRY}$ allows the potential effects of 'pollution swapping' to be studied.

In chapter 8, this is shown to be especially relevant when assessing the success of implementing a certain measure to decrease a particular type of loss (NO_3^- leaching), for instance by mineral fertiliser optimisation. NGAUGE outputs showed that optimising fertiliser through and improved N efficiency (maximising plant N: N losses), NO_3^- leaching decreased but the risk of undesirable losses in other N forms such as N_2O and NH_3 increased. This degree of *pollution swapping*, however, may or may not be acceptable. In the

absence of legislation specifically related to the concentration of these gases this issues become a choice of policy makers.

Because of the different spatial level at which different pollutants can effect ecosystems and travel within the environment, up-scaling field or farm approaches to landscape or regional scale may help to further understand or quantify the extent of this pollution swapping. In chapter 9, the modelling framework LANAS was developed to simulate N fluxes at the landscape-scale. LANAS only simulated the dispersion of NH_3 emissions in the atmosphere, however, in the future other frameworks that can study the transport of N_2O and NO_3^- should be developed as the effects of such pollutants will have impacts over greater distances than NH_3. $SIMS_{DAIRY}$ modelling framework, in the future, would be improved if it could be used at larger spatial scales such as regional and global, as these would offer the possibility of identifying the shifts from one type of impact to another. Modelling approaches at larger spatial scales by averaging results from existing approaches developed at smaller scales will however have to overcome the potential problems of non-linearity with respect to their parameters

Optimisation of field and farm management for multiple objectives towards sustainability

a. Optimisation of a single-issue management factor (i.e. mineral fertiliser)

Improving N use efficiency in the plant is not only achieved by breeding more efficient varieties, as previously discussed, but it can also be achieved by improving the synchronisation between supply of inorganic N in the soil and the plant N demand at each stage of the plant development. This can be done by means of optimisation of fertiliser timing and amount. The optimisation of resource use is a key issue to achieve the different goals with respect to food supply, income and protection of the environment (Kropff *et al.* 2001).

To make a decision about N fertilisation, one must project into the future (Sebillote and Soler, 1990) using a predictive tool and this tool must be flexible enough to be initiated at any moment of the crop cycle (Meynard *et al*., 1997). Although theoretically this should apply to both mineral and organic fertiliser, in practice, tactical timing and amount

management of organic fertiliser (manure) is generally more constraining (limitation of manure storage available and by legislation).

NGAUGE only optimises N mineral fertiliser (chapter 7). However, it also takes into account the effect that manure N can have on such optimisation. This manure simulation within NGAUGE proved to be very helpful when assessing the scope for manure timing and type choice to decrease NO_3^- leaching (chapter 8, section 8.4). The model outcomes evidenced: (i) the poor synchrony between the N demand by the crop and release of inorganic N from manures (Stockdale *et al*., 2002), (ii) the limitations to replace inorganic fertiliser with organic fertiliser (i.e. manure) and (iii) the fact that when manures are spring-applied, grass demand is generally better matched with supply by liquid manures (slurry) than by solid manures (FYM), even if the long-term residual effect of the solid manure is taken into account (Berry *et al*., 2002; Schröder, 2002).

The criteria to be satisfied in NGAUGE optimisation procedure aims at maximising the efficiency ratio defined as kg in herbage: kg loss, which is an indication of N use efficiency in the system and a way to achieve a balance between 2 conflicting goals (production *vs* loss). Obviously, targets must be established in terms of total amount of fertiliser applied, herbage needed per hectare or N lost, as otherwise the optimisation would generally result in predicting very small or no fertiliser N as a way to achieve the most efficient system in term of N use efficiency. This allows N to be used more efficiently while still retaining the focus of the system on production targets.

The scope for improvement in efficiency through optimisation is limited by site factors, but more importantly by the level of N input to the system. The latter is obvious from the shape of the N response curve in plants: there is greatest scope for improvement with steepest gradient of the curve. At low N inputs, N response is dominated by mineralisation (largely unmanageable) while at high N inputs, response to incremental N input is very low.

One of the main criticisms to this optimisation approach is that while the model is capable of optimising the efficiency of N use for a particular grassland system, the optimised pattern of herbage production (high yields in early summer) may not be compatible with the farmer’s preferred stock management (chapter 8, Fig 3). Maximising herbage N production during grazing must be matched by for instance the lactation stage of the dairy cows when protein and energy requirements are large. The criteria of optimisation in NGAUGE consider

all kinds of N losses. However, N_2 emissions are not environmentally pollutant. Some changes to the operation of NGAUGE may be required, *viz* making all taking N_2 losses out of the criteria of optimisation or moreover, using a compound index that provide a weighted assessment of the potential of the predicted N losses to contribute to water eutrophication, acidification, soil erosion and climate change (i.e.Van Calker *et al*. 2006).

In NGAUGE, in contrast to the existing UK fertiliser recommendation system (MAFF, 2000), the potential losses of N are taken into account in the production of this recommendation, both by ensuring that the target is achieved with the greatest ratio of herbage N to N lost, and by providing the facility for N losses to be entered as a target. Thereby, NGAUGE could be very practical to improve such recommendation systems.

There have been several other approaches for farm focus on strategic levels (De Haan, 2001) and on operational management level (Carberry *et al*., 2002; Flinn *et al*., 2003) and decision support for N fertiliser management, originating in the Netherlands (Dairy Farming Model; Van de Ven, 1996; STONE: Wolf *et al*., 2003), France (AzoPât; Decau *et al*., 1997 and Delaby *et al*., 1997) and New Zealand (NLE: Di and Cameron, 2000, and Overseer: Wheeler *et al.*, 2003), however, policy makers generally have restricted their use for scientific or policy purposes only.

b. Optimisation of several factors for multiple objectives towards sustainability

Sustainability as a broader sense than that studied at NGAUGE requires that the optimisation can target more multiple management factors and introduce multiple goals that go farther than those proposed by the NGAUGE efficiency ratio. $SIMS_{DAIRY}$ optimisation objectives include those that aim at maximising farm net margin, biodiversity, milk quality, landscape aesthetics, animal welfare and soil quality and minimising the risks of environmental losses. The targets are the acceptable levels of achievement for any of the attributes (i.e. Nitrate directive threshold or an acceptable net income for the farmer) and the goals (or constraint) are the combination between a target and an attribute (Romero and Rehman, 2003).

Finding optimal solutions for a large amount of combinations of management factors and goals sought produce a vast and complex solution space. If the objectives and the constraint are linear functions the optimisation may employ linear programming (simplex algorithms) [Berentsen and Giesen, 1995; Zander and Kächele, 1999; Hengsdijk and Van Ittersum, 2003]

or the theory of games (Becu *et al*., 2004) as the methods. However, the relationships found in $SIMS_{DAIRY}$ are not generally linear and hence, for non-linear optimisation problems there are other methods. As a first approximation and due to the mathematical complexity of non-linear methods $SIMS_{DAIRY}$ optimisation was carried out through a simple iterative approach. This kind of approach has been already used by many studies (i.e. Friedrich and Reis, 2000) and its main limitation is the computational speed. $SIMS_{DAIRY}$ needs faster optimisation procedures that could actually be built using the basis of existing non-linear methods.

Although selection and application of these mathematical methods is beyond the scope of this thesis, it should be acknowledged, however, that evolutionary (as well known as 'genetic') algorithms (EA), for instance, could be an ideal basis for a new optimisation procedure in the future. This type of approach is likely to be useful as they allow you to test a large number of possible solutions in parallel (computationally faster), to select the best solutions based on fitness criteria, and to introduce novelty through mimicking stochastic mutation. Although they have not been widely applied in the field of farm modelling yet (Reis *et al*., 2005), they have already been successfully used for instance, to explore sustainability trade-offs in cropping systems (DeVoil *et al*., 2006) or for bioeconomic optimisation of fisheries (Mardle and Pascoe, 2000). They are recommended when the search space is large, complex and poorly understood and traditional search methods fail (i.e. linear programming). These specifications would fully apply to $SIMS_{DAIRY}$.

At the moment the slow optimisation speed limits $SIMS_{DAIRY}$ to explore a small part of the optimal solution space (solutions of sustainable dairy systems). The extent to which the goals to become sustainable are more or less constraining will affect this solution space. They may be too constraining like in the example in chapter 11, where the level of desired biodiversity can by no means be achieved with an adequate farm income for the farmer (unless subsidised or relaxing the biodiversity target). Obviously, the more relaxed the goals for sustainability are, the greater likelihood of finding sustainable systems may be. Ranking, however, such systems will differ among different sets of stakeholders and will require whole socio-economical studies.

c. Existing approaches to study farm sustainability and their applicability

Soussana (2006), in a review analysing the scope of consumption of energy and GHG from farming systems indicated that there is a need to develop refined analysis systems of flows (energy, nitrogen, carbon, greenhouse-effect gases flows) at the scale of the whole farm for useful diagnoses and projects of improvements (reduced energy consumption or greenhouse-effect gas production, creation of bio-energy, storage of C…). Apart from those farm models described in previous sections, a number of other models have been developed and applied to the evaluation of livestock production in grassland farming systems. Although these models function at the farm level, most do not include all major farm components, or these components are not modelled with enough detail to provide a robust research and teaching tool.

Most farm models may be classified as either linear programming or simulation models. Linear programming is often used for farm economic evaluation and optimisation. This approach has been used to evaluate dairy production in New Zealand (McCall and Clark, 1999), the USA (Schmit and Knoblauch, 1995), and the Netherlands (Berentsen and Giesen, 1995; Van de Ven and Van Keulen, 1996, *in press*; Pacini *et al.*, 2004). Although these models are primarily used for economic evaluation, environmental issues have also been addressed by tracking N, P, and K balances at the soil, animal, and farm levels (Berentsen and Giesen, 1995; Van de Ven and Van Keulen, *in press*). The limitation of linear programming has already been discussed previously in this section. Process-level models have been used to evaluate the bio-economic efficiency of pasture dairy production in France (Cros *et al*., 2003). A simulation-based decision support system has also been developed to provide crop and livestock management support at the whole-farm level, with emphasis on water, nutrient, and pesticide management (Ascough *et al.*, 2001). Comprehensive models provided tools for evaluating and comparing the performance and economics of various technologies and management strategies for dairy farms (McGechan and Cooper, 1995; Rotz *et al.*, 1999; Rotz *et al.*, 2002; Rotz *et al.*, 2005a) or in agricultural systems in general (Vatn *et al.*, 2006).

Some more integrated approaches at other levels have been developed as decision support that considers both biophysical and socio-economic approaches (i.e. Rossing *et al*., 1997; Vereijken, 1997; Van Calker *et al.*, 2006). However, they generally lack process-based

mechanisms and thereby, lack sensitivity to major factors that affect sustainability and show a partial reflection of the complex chain of causes and effects (Van Cauwenbergh *et al*., 2007).

Other models, based on the life cycle analysis (LCA), have also been developed to asses the environmental impacts of farming systems (i.e. Sandars *et al*., 2003). Although in concept is a very sound method as it systematically follow mass and energy from '*cradle to grave*' of a particular product (i.e. milk), in practise employing the whole LCA towards the study of a dairy farm, for instance, is limited to the quality of the data and assumptions made. It is also limited as it only includes the concept of one functional unit, generally expressed per kg of product (i.e. milk). The assessment of a multifunctional activity like agriculture poses the question of the reference unit for the impacts. Regional and farm approaches, as opposed to LCA, usually express impacts per hectare of land. However, methods which allow the expression of impacts according to several reference units are obviously preferable (Biewinga and Van der Bijl, 1996).

Its use in combination with the more-process based approaches may however be very useful. For instance, when I analysed the efficacy of exporting manure as a measure to reduce NO_3 leaching from dairy farms in chapter 8, I concluded that one of the successes of this measure would lie on how much distance were between the dairy farm exporting manure and the low-input farming system receiving this manure (due to transport trade-offs: energy used and CO_2 emitted). Although, not mentioned in this chapter, exporting manure could also be directed to biogas plants, provided they were close enough or they could be connected by a waste pipeline system. In order to analyse both options a whole LCA could be developed were energy, CO_2 or increased CH_4 generation from biogas plants would be estimated together with our original NGAUGE predictions. Incorporation of some LCA approaches focusing milk product once it goes beyond the boundaries of the farm would also enable us to widen the boundaries of the study.

Modelling the overall sustainability of a dairy farming system involves knowledge of a varied number of attributes and generally requires the inputs from varied disciplines. $SIMS_{DAIRY}$ modelling framework, for instance, deals with attributes that define socio-economic and ecological-environmental sustainability. However, this definition may still be too narrow. Other studies, for example those from Van Calker *et al.* (2005, 2006) although

insufficiently sophisticated on the ecological-environmental modelling side, can improve the definition of overall sustainability of $SIMS_{DAIRY}$ by providing more relevant attributes. Farm sustainability in these studies was subdivided into the following aspects: (a) economic, (b) internal social, (c) external social and (d) ecological sustainability. Within these aspects, Van Calker *et al*. (2006) indicated a selection of attributes that can be used (Fig 4, except those with a $^{\Phi}$symbol).

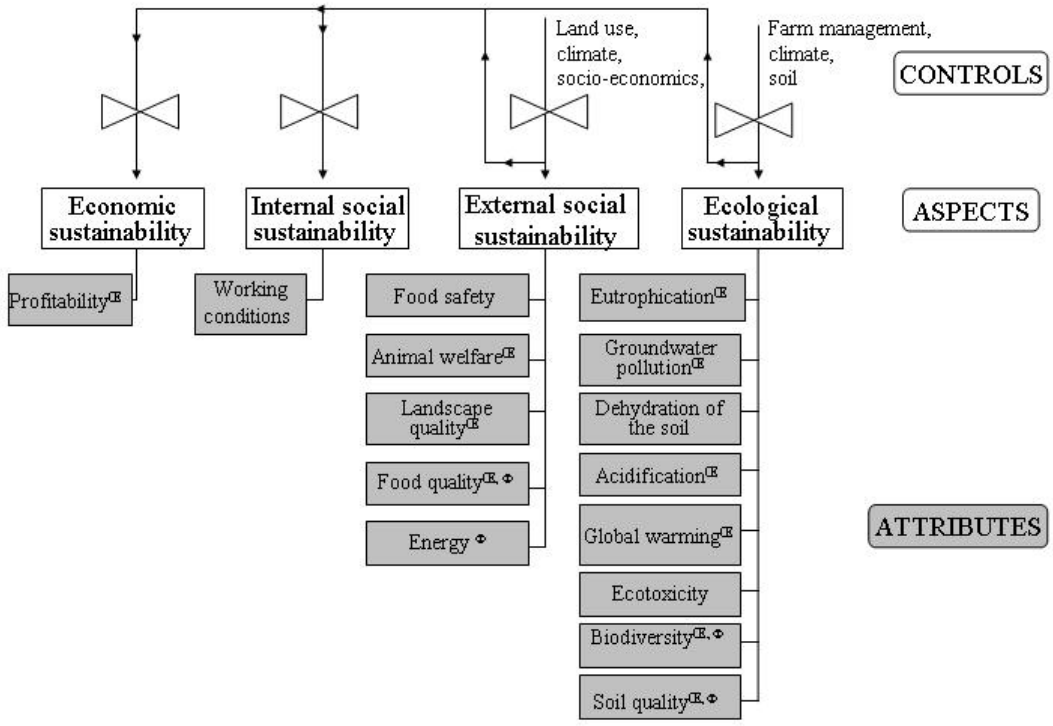


Figure 4. Decomposition of overall sustainability of dairy farms into aspects, attributes and controls that affect the dynamics of the attributes (adaptation of Van Valker *et al*., 2005; Van Calker *et al*., 2006).

Some of the proposed attributes are already simulated and optimised within the $SIMS_{DAIRY}$ model (marked with a $^{\Phi}$ symbol) and some key attributes that are included or easily includable within $SIMS_{DAIRY}$ are not mentioned by this study (marked with a $^{\Phi}$symbol). This example shows that this type of research is rapidly growing and there are ample opportunities to extract useful information from the different existing approaches (i.e. Van Calker *et al*., 2006) in order to improve other approaches (i.e. $SIMS_{DAIRY}$). In this particular example, $SIMS_{DAIRY}$ could be easily modified to include energy flows and water flows

provided that data are gathered, analysed and synthesised into simple indicators (Piorr, 2003; Belcher *et al*., 2004; Van Calker *et al*., 2006) or more process-based approaches.

Modelling frameworks ($SIMS_{DAIRY:}$ chapter 10 or LANAS: chapter 9) integrate different existing models which are coded with a different calculation time-step, different input data and different programming language. Their intended spatial scales may be different from each other but they can be modified and aggregated to a common and different scale such as the LANAS model framework (chapter 9). These models may have a focus on different systems and scales. Thereby, their integration may enable us to study systems in a broader sense and whereby the interaction from different disciplines (e.g. hydrology and animal science) is required. Although in principle frameworks may sound a sensible and rational exercise to bring together existing modelling tools in a cohesive way, in practise they are still a very challenging task since, to date, models have been generally developed with no standardised structure. Each model may be coded with a different calculation time-step, different input data or different programming language. This may in the end result not only in large conceptual but also technical problems.

Investigating future scenarios in dairy farming systems

The implications and trade-offs for farms following one or another trend can be studied by modelling, thus enabling policy makers to take decisions about what trends to actually favour/encourage. For instance, there is an increasing trend in some countries in Europe (i.e. Spain) to have dairy systems almost fully housed during the whole year, basing hence their reliance on concentrates produced from cereals, legumes or other feedstock. In countries like England, farmers are still uncertain about what system to chose. The impact of both types of systems on farm sustainability can be studied by modelling.

For instance, $SIMS_{DAIRY}$ outputs suggest that a certain movement towards increasing the housing period could be beneficial towards reducing certain environmental losses. It was shown that increasing the number of housing days decreased the risk of global warming potential (GWP) of CH_4 and N_2O both per ha and per L of milk (Fig 5b in chapter 10). This is a result of a balance between the decrease (up to a certain level of housing time) in N_2O emissions from soils through less grazing and decreasing the proportion of urine N in excreta

through a rich starch-based (maize) diet (Kebreab *et al*., 2001), and the small increase in CH_4 emissions due to an increase in impact of CH_4 emissions from rumination through an increased animal intake and larger volumes of manure generated. The relationship between GWP and housing days (Fig 5, adapted from Fig 8 in chapter 10), however, did not always follow a linear trend.

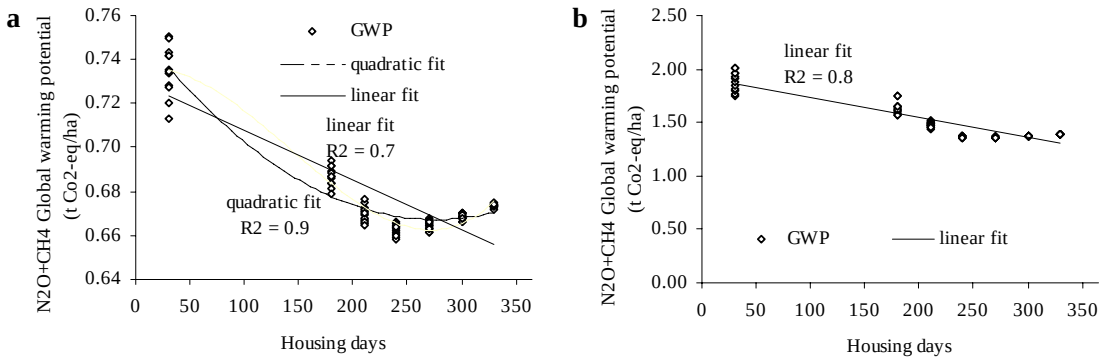


Fig 5. Effect of housing time (in days) on predicted losses per hectare of: global warming potential caused by N_2O+CH_4 emissions on UK dairy farms under sandy loam (a) and clay loam (b) soils. The % of maize area was proportional to the number of housing days ranging from 3 to 14% and 4 to 17% in sandy loam and clay loam soils, respectively.

The fact that GWP decreased with increasing housing days up to an inflection point at about 240 days (in sandy soils) and increased after these number of days, suggests that for dairy systems (especially intensive ones) there may be a housing time per soil type and probably per management choice where the positive effect on N_2O emissions of replacing grazing with increasing manure production (and subsequently apply it to land) and increasing, for instance, maize area is counteracted by excessive manure per ha to be applied. Increasing housing time led to a decrease in NO_3^- leaching losses (for a sandy loam soil) but an increase in P, NH_3 and NO_x losses, this increase (NH_3 and NO_x) mainly caused by silage losses. Losses from silage must be considered in any integrated farm approach. Increasing housing time and reliance on maize could have an increased risk of negative effects on issues such as animal welfare (housing may have a negative effect on animal social relationships), plant biodiversity (through more even distribution of excreta in the land) and the % PUFA in the milk content (through the reduction of ingested PUFA through reduced fresh grass feeding).

These results obviously highlights the fact that for this particular issue there is no win-win choice and policy makers must establish their priorities for attributes that are not economically based.

Extensification, for example, is an option to decrease the environmental impact per unit of hectare. Such farming systems may be attractive as they provide the opportunity to combine production with other functions such as supplying habitats for wild flora and fauna and improving landscape qualities (Schröder *et al*., 2005a). However, impacts per unit of product (i.e. milk) are likely to increase as product per hectare decreases and thereby, to maintain the same level of production more land is required. Society, in contrast, may desire that land for other purposes (i.e. recreational, pristine areas…). At a higher scale, society may be better served by intensive systems, which in total loads, may also be as pollutant as extensive systems. Too strong a focus on the environmental impact per unit of product may also stimulate farmers to fully specialise into either arable or livestock production. Such a development can have a negative effect on the nutrient use efficiency of the society as a whole (Schröder *et al*., 2003) or may cause a high consumption of fossil energy due to the high energy demands per unit of output, transport of manures, feedstuffs, bedding materials and farm products including animals (Corré *et al.*, 2003). At the same time, policies such as those originating from the CAP reform, where subsidies are decoupled from production, may well polarise farmers towards largely subsidised extensive systems and unsubsidised very intensive systems.

The role of organic farming in feeding a growing population may also pose similar questions as those already discussed for extensive systems. Organic dairy farming is also generally a legume-based system and thereby, it will be partly advantageous as legumes can replace manufactured fertiliser with fixation of atmospheric N. Therefore, these systems indirectly require less fossil-fuel energy and emit less CO_2 emissions. Modelling approaches to forecast the impact of such systems on the sustainability should incorporate plant fixation and predict the effect of climate change (temperatures, rainfall and CO_2 atmospheric concentrations) on the fluxes of N, P and C at different levels.

Animal and plant breeding may well have an even larger implication on food security and sustainability of farming systems. For example, grass varieties with high sugar content may reduce the impact of N losses (i.e. simulated with NGAUGE in Fig 6).

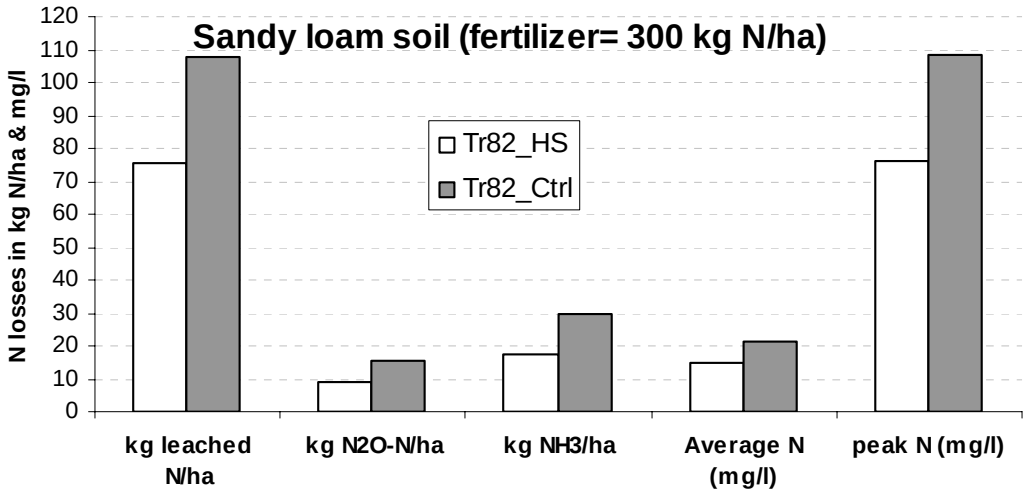


Figure 6. Predicted N losses reductions of a new variety of grass with a higher content in sugars (Tr82_HS) compared with non-improved ryegrass (Tr82_Ctrl) growing in a sandy loam soil fertilised with a high rate of mineral N (300 kg N $ha^{-1}yr^{-1}$).

Manipulating the scope for future animal traits such as the ability to yield milk and the ability to excrete different proportions as urine N or dung N (irrespective of diet N ingested) although useful at the moment in reducing losses per unit of product, they have important trade-offs in animal welfare (fertility and mastitis), animal replacements and milk quality. Enhanced focus on traits that balance milk yield, milk quality and animal health will help to improve the sustainability of dairy farming systems.

Although there is no doubt that some of the technological changes offer scope for some sustainability aspects. It is still quite uncertain to forecast to what extent changes will impact on the human population and the environment. The level of adaptations required may be too high as the world changes in land uses, increased urbanisation, climate and under a much larger population pressure (demanding more food and energy).

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