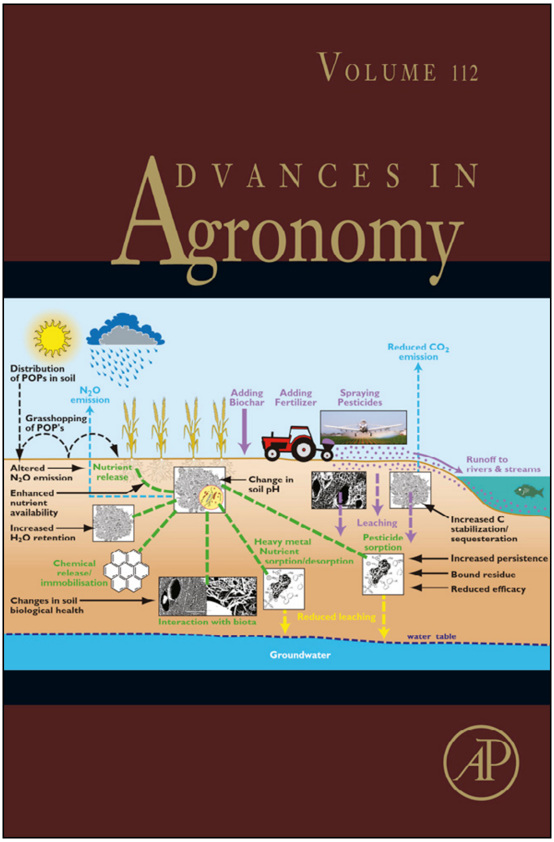

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CHAPTER ONE

A Review of Quantitative Tools for Assessing the Diffuse Pollution Response to Farmer Adaptations and Mitigation Methods Under Climate Change

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Contents

Abstract

In an era of global climate change, the agricultural sector faces the challenge of increasing the production of safe and nutritious food supplies to meet a growing world population while safeguarding the environment. Farmers will adapt their agricultural practices to a changing climate to safeguard against loss of production and to take advantage of any positive climatic conditions. Certain management practices have been found to reduce the effects of agricultural practices on the environment and a key question is how efficient these are under the current climate, and will these management practices still be relevant under a changing

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climate? Mathematical modeling is the only tool available to assess the potential efficacy of proposed agricultural management practices to help evaluate their impacts on the environment in a future climate. This chapter attempts to evaluate a range of published models for their capability to simulate agricultural production systems and associated environmental system losses under a changing climate, and their ability to introduce farmer adaptation and mitigation methods. The chapter focuses on the applicability of the models given a set of essential criteria related to scale, biophysical processes, and land management. Thirty models are initially examined, based on details found in published papers, against specific criteria, viz: (1) spatial scale and temporal scale, ease of use, and ability to consider a change in climate; (2) ability to simulate nutrient cycling processes, specifically carbon and nitrogen dynamics with microbial turnover, mineralization–immobilization, nitrification and denitrification, plant nutrient uptake, and phosphorus cycling; (3) ability to consider a water balance and water movement through soil; and (4) ability to introduce and modify agricultural practices relating to crop and livestock management. The chapter does not compare any actual model simulations. It was concluded that albeit no single model incorporates all above stated requirements, there were three models, DAYCENT, PASIM, and SPACSYS which will accommodate most features. These models may therefore be considered in the context of this chapter to be the most suitable for a general assessment of the effects of farm mitigation and adaptation on environmental losses under a changing climate.

1. Introduction

1.1. Safeguarding the environment

There is a need to increase agricultural production while safeguarding the environment (Defra, 2009; Horrigan *et al.*, 2002; Morris and Winter, 1999), and this challenge is set in the era of a changing climate. It is clear that previous and current agricultural practices impact adversely on a number of ecosystem services (Beman *et al.*, 2005; Pilgrim *et al.*, 2010; Van Wesemael *et al.*, 2010) including water and air quality. For example, agriculture is a major source of phosphorus (P) to the aquatic environment (Granger *et al.*, 2007; Hawkins and Scholefield, 1996; Lewis and McGechan, 2002), hence future research directions will need to better link P losses with soil nutrient and moisture conditions, ecological effects, and climate change (Blackwell *et al.*, 2010; Kronvang *et al.*, 2009; Turner and Haygarth, 2001). Diffuse nitrogen (N) loss from agriculture is also a major contributor to the aquatic environment, in the form of nitrate (NO_3^-) in surface and groundwater (Bust and Haycock, 1993; Froschl *et al.*, 2008; Lerner and Harris, 2009; Ryden *et al.*, 1984). In addition, the processes of nitrification and denitrification are responsible for gaseous emissions of nitrous oxide (N_2O; Cardenas *et al.*, 2010; DeBusk *et al.*, 2001), while methanogenesis in ruminant livestock and livestock manures is responsible for methane (CH_4)

emissions (DeRamus *et al*., 2003; Matthews *et al*., 2006; Pinares-Patino *et al*., 2007). These are two key greenhouse gases (GHGs) whose production is enhanced under intensive agricultural production (Beauchemin *et al*., 2010; Millar *et al*., 2010). Both management and environmental factors influence the rates of N_2O and CH_4 emissions from the range of agricultural sources (Del Prado *et al*., 2010; Meijide *et al*., 2010; Pereira *et al*., 2010). Current studies are investigating the potential influence of nutrient amendments to agricultural soils such as compost from food waste and agricultural residuals such as straw (Suntararak, 2010).

Agriculture is also a major emitter of ammonia (NH_3; Cooter *et al*., 2010; Misselbrook *et al*., 2001; Nunez *et al*., 2010), which represents an agronomic loss of N; is associated with N deposition, soil acidification and loss of general biological biodiversity (Fraser and Stevens, 2008); and is also a precursor of fine particulate matter, considered a public health threat (Shih *et al*., 2006).

Current legislation and advice tries to mitigate diffuse water pollution from agriculture by promotion and adoption of good management practice (Monteny *et al*., 2006; Van Der Meer, 2008). Agricultural diffuse pollution and soil degradation have led to a reconsideration of agricultural policies in Europe (Collins and McGonigle, 2008). For example, farm income support payments are now linked to compliance with standards (cross compliance rules) to protect the environment and animal health. In addition, the Water Framework Directive (WFD) represents a major effort toward the conservation and management of aquatic ecosystems (Basset, 2010). The Directive runs concurrently with a European Nitrates Directive, to reduce or prevent water pollution caused by NO_3^- from agricultural sources (WFD-UKTAG, 2001). Nitrate vulnerable zones are designated areas of land draining into waters polluted by NO_3^- from agriculture, and farmers with land in NVZs have to follow a mandatory action plan to tackle NO_3^- loss from agriculture.

Major emitters (such as China and the United States) of GHGs have agreed under the Copenhagen Accord that global average temperature increase should be kept below 2 °C (Ramanathan and Xu, 2010). Temperature increases have been linked to an increase in global soil respiration, indicating an acceleration of the carbon cycle (Bond-Lamberty and Thomson, 2010). Actions to stabilize carbon dioxide (CO_2) concentration below 441 ppm during this century, targeting applicable air pollution laws and reducing greenhouse emissions of short-lived CH_4 and hydrofluorocarbons, can reduce the probability of exceeding the 2 °C barrier before 2050 to less than 10%. Specific targets to reduce GHGs and NH_3 emissions have also resulted in a range of agricultural practices to limit emissions, for example, shallow injection of slurry and slurry store covers to reduce NH_3 emissions; supporting biogas production on farms (Regina *et al*., 2009); techniques to improve carbon sequestration (Lal, 2010); improving the performance of ruminants; regulating the ruminal fermentation; and reducing the emission of GHGs from feces (Li *et al*., 2010).

1.2. Tools to support agroenvironmental legislation

Nutrient cycling in agricultural systems is complex, and it is important that any potential secondary effects of introducing a mitigation method to reduce pollution are understood. There is a risk that the mitigation method used may stimulate a different form of pollution from another component of the nutrient cycle. There is the potential to either reduce another form of pollution at the same time (a "win–win" situation) or possibly to increase another form of pollution (i.e., "pollution swapping"; Stevens and Quinton, 2009b). However, it is increasingly evident that no single mitigation option will reduce all pollutants (Stevens and Quinton, 2009a).

Stressors of changing climate, land use, and demands on water resources, and their resulting effects on nutrient cycles are predicted to increase over the coming decades (Heathwaite, 2010). Future climate scenarios for the UK predict wetter winters and hotter, drier summers than the historical baseline UK climate (Malby *et al.*, 2007; Mills, 2005; Palmer and Ralsanen, 2002; Vidal and Wade, 2008). It is important to predict the impact of our current thinking of climate change mitigation, in a whole-system context, on gaseous emissions and water loss. For example, what are the physical effects of wetter winters and more intense rainfall events on diffuse water pollutants (Granger *et al.*, 2010b), and will current mitigation advice be adequate, that is, use of buffer strips, cover crops, etc.? (Stevens and Quinton, 2009a) What will be the impacts of hotter, drier summers on preferential flow and losses of diffuse water pollutants or on NH_3 volatilization and N_2O emissions, and will current mitigation advice still be effective? The effects of changed temperature and rainfall patterns and increased atmospheric CO_2 concentrations on nutrient cycling (e.g., nitrification, denitrification, mineralization) and effects on gaseous emissions, diffuse water pollution and, importantly, crop nutrient uptake and yields will be complex.

Agriculture involves a high degree of management but is still susceptible to failure under extremes in weather. As such, there is a need to continuously evaluate farming practices and implement those that minimize adverse effects of weather and take advantage of conditions that promote production and food quality, that is, adaptation. With the likelihood of climate change, agricultural practices will require adaptation to meet the new climate constraints on food production (McGinn and Shepherd, 2003). In addition to mandatory regulations, farmers will naturally adapt their land management to mitigate the effects of a change in climate (Gifford *et al.*, 1996). To determine what current legislation and advice to reduce diffuse pollution to air and water is sufficient to cope with the potential effects of climate change, simulation modeling is required because it has the potential to integrate the complexity of the system, provide a quantitative insight of the direction of change in a flux that occurs as a result of the perturbation of the system, and help to determine the potential outcomes of climate change on agricultural productivity and effects on the environment (Giltrap *et al.*, 2010; Janzen *et al.*, 2006; Pattey *et al.*, 2007).

1.3. Reviewing the tools to fit the purpose

Although there have been a number of nutrient model reviews for agroecosystem applications and climate (Bryant and Snow, 2008; Challinor *et al.*, 2009; Kersebaum *et al.*, 2007; Lewis and McGechan, 2002; Parton, 1996; Smith *et al.*, 1997), only a limited number or those dealing with single matter cycling models were involved in the reviews. The purpose of this chapter is to determine the strengths and weaknesses of a range of international models (Table 2a and b), based on characteristics essential and desirable in a model (Table 1) to evaluate the adaptation of farming practices to mitigate diffuse pollution under climate change, specifically, the models' ability to simulate the direct effects of climate change on agricultural productivity at the field or farmscale for a range of crop types, environmental losses to water and air, as well as their ability to introduce farmer adaptation and specific mitigation methods. However, we do not undertake any actual performance test or compare accuracy of the model outputs in this chapter. The chapter focuses solely on the applicability of models to meet a given set of essential criteria:

- **(i)** to be able to operate at appropriate spatial and temporal scales;
- **(ii)** to be capable of simulating the processes, transformations, and losses relevant to climate change impacts on agriculture;
- **(iii)** to have capability to simulate and evaluate mitigation methods (e.g., a tool kit for diffuse pollution), and enable examination of potential secondary effects (e.g., win–win and pollution swapping);
- **(iv)** to be able to simulate the effects on outputs resulting from farmer adaptations; and
- **(v)** to have ease of use for the operator.

Ideally, these models should be at farm or field scale to reflect management decisions on farms and for policy; a minimum of a monthly timestep is necessary to reflect management decisions and the cropping calendar.

2. Rationale for Selection of Model Criteria

2.1. General selection

Before any model was chosen for the chapter, we have limited our scope of model selection: first, this chapter is not trying to be exhaustive, only those that have been commonly cited or proven and validated in the literature will be included. And second, our particular focus is on a farming application as well as nutrient cycling and environmental losses. There are an infinite

Table 1 Selection criteria of processes

Criteria	Climate change	Nutrient cycling	Water	Agricultural management
Essential	• Temperature • Precipitation	• Mineralization • Immobilization • Nitrification • Denitrification • C and N dynamics with microbes • Root and shoot partitioning and uptake	• Water balance • Movement through soil layers (i.e., leaching)	• Crop type and timing of agronomic factors • Land-use change • Livestock grazing/housing periods • Fertilizer and manure application, timing, and rates
Desirable	• Fixed/actual weather file input • Atmospheric CO_2 concentrations	• Phosphorus nutrient concentration in streamflow	• Runoff • Sedimentation	• Tillage and physical modification • Modification of animal diet

number of environmental applications that models are written for. The models that fall outside our focus will be excluded in the chapter.

Availability of model details is a recurring problem previously commented on in papers (Tiktak and Vangrinsven, 1995). The documentation of models is the last phase in model building, and sometimes a detailed description of a model in an institute report is a difficult thing to find, even though the model itself may be well known. Lack of details can render models unusable to wider research groups other than their creators (Landsberg *et al.*, 1991), and a model could be overlooked that has a greater capability than is documented, and prevent the model from being more widely used.

In order to select models, we have built on previous reviews (Lewis and McGechan, 2002; Smith *et al.*, 1997), added more recently published papers on appropriate models and added relevant new models not included in these reviews. This chapter is to be used to enable readers to select the most applicable computer model for projects concerning an evaluation of the effectiveness of agricultural practices resulting from farmer adaptation. It is also to be used to enable readers to select the most applicable model for examination of the necessary mitigation methods for various crops as a response to a change in climate, with relevance to productivity and environmental losses.

A list of models used and sources are summarized in Tables 2a and b.

We have separated model *characteristics* into two main levels for this chapter, that is, desirable and essential (Tables 1 and 2a, b; Sections 2.2–2.5). We also consider three other aspects of models which influence their use and application, that is, ease of usage (Section 2.6), spatial scale, and temporal time step (Section 2.7). Processes, transformations, and losses simulated are dealt with in Sections 2.2–2.4. Usefulness of models for diffuse pollution, pollution swapping, and farmer adaptation is dealt with in Section 2.5. Appendix contains brief descriptions of each model included in this chapter along with key descriptive publications, hence these same references after each model are not generally given unless the information was taken from a separate source.

Which model is eventually most applicable will depend largely on what results are expected as output, and therefore processes needed, and for this we need to define some rules to place relative importance on processes. If our focus is on the sustainability of agriculture with adaptation and mitigation under climate change, it may be seen in terms of its resulting pollution, hence the need for a model including processes relating to nutrient loss and pollution. In case models do not include all processes, we must decide which processes take most priority to include in a model. One important source of agricultural pollution is nitrogen. Its output from the soil is in the detrimental forms of NO_3^- and ammonium (NH_4^+) into a watercourse (Granger *et al.*, 2010a; Lu *et al.*, 2009), and N_2O and NH_3 emitted into the

Table 2 Characteristics of reviewed models

(a)

					Processes, transformations, losses relevant to climate change									
			Resolution		Losses to waters					Atmospheric losses				
ID	Models	Characteristics, focus of model	Spatial	Temporal	Leached N	Runoff N	P	Sediments	Fecal/ pesticides	NH_3	N_2O	NO	CH_4	Transformations in soil
1	ANIMO	A nutrient model strong on manure and slurry components	Field scale, 50 soil layers	Daily–weekly	y	Y	Leaching, surface dissolved runoff			y	Gases treated as one sink			Decomposition, nitrification, denitrification, min/immobiliz (P, N), P soil sorption/ desorption, C dynamics
2	APSIM	Crop production, N and C cycling, water	Field scale	Daily	y			Soil erosion			Gases treated as one sink			Decomposition, min/immobiliz, nitrification, denitrification
3	BASINS	Water quality and erosion model; open GIS tool with web dataset	Catchment	Daily	y	Y		Soil erosion						
4	CNSP Pasture	A pasture uptake model	Field	Monthly	y	Y								
5	PASIM	Mechanistic pasture simulation model	Field scale, one-dimensional	Daily	y	Y		Soil erosion	Pesticides	y	y	y		Net mineralization, nitrification, denitrification, and NH_4 sorption
6	DAISY	Crop, C and N and water flows with heat balance and land management	Field scale, over 20 layers, one-dimensional	Daily	y	Y			Pesticides		Gases treated as one sink			Min/immobiliz, nitrification, and denitrification

7	DAYCENT (daily version of CENTURY)	Rainfall, temperature, NH_4 simulated within 15 cm on the top soil	Field scale, 10 soil layers, one-dimensional	Daily	Leaching (P)		Leaching, surface dissolved runoff	P erosion			y	y	y	Decomposition, nitrification, denitrification (N) min/immobiliz (P, N), P soil sorption/desorption, C dynamics
8	ECOSYS	Complex integrated terrestrial system	Various scales (field to km)	Hourly to centuries						y	y	y	y	Decomposition, nitrification, denitrification, Min/immobiliz (P, N), C dynamics
9	EUROSEM	Erosion model of sediment transport, potential to be coupled with an agricultural P cycling model	Catchment	Short-term			Soil erosion	Sediment transport						
10	EVENFLOW	Complex stream N model	Catchment	Daily	y									No separate processes, empirical from experimental nitrate data
11	GLEAMS	Nonpoint source stream loading, P, uptake of NO_3	Field scale 10 soil layers	Daily	y	Y	Leaching, surface dissolved	P bound to particulate, detachment + transport	Pesticides	y	Gases treated as one sink			Decomposition, nitrification, denitrification, min/immobiliz (P, N), P soil sorption/desorption

(*Continued*)

Table 2 (*Continued*)

(a)

			Resolution		Processes, transformations, losses relevant to climate change									
					Losses to waters					Atmospheric losses				
ID	Models	Characteristics, focus of model	Spatial	Temporal	Leached N	Runoff N	P	Sediments	Fecal/ pesticides	NH_3	N_2O	NO	CH_4	Transformations in soil
12	HURLEY	Pasture growth and soil nutrient cycling	Field	Hour										C cycling, plant N uptake, nitrification and denitrification, min/immobiliz (N)
13	INCA	Process-based N cycle in plant–soil-stream loading, macro- and micropore drainage	Catchment	Daily	NO_3^-, NH_4^+, separate for soil water and groundwater					Since nitrification and denitrification included, no gaseous output, a wasted opportunity				Plant uptake, nitrification and denitrification, min/immobiliz (N), matrix and macropore soil drainage
14	MACRO	Water pollution, 2-domain with macro- and soil matrix micropores	Field scale, 15 soil layers	Daily–hourly or less			Colloid + soluble, bound to particulate		Pesticides					Not a C/N cycling model
15	MONERIS	Point and diffuse streamflow loading	Catchment	Annual	y	Y								Conceptual approach, no detailed processes
16	MOTOR	A unique, flexible SOM framework for interchangeable processes based on reaction kinetics	Expressed as mass, flexible units	Daily										Based on pools and fluxes, does not explicitly name processes

17	NGAUGE	Detailed N cycling	Field scale	Monthly	y					y	y	y		Decomposition, min/immobiliz, nitrification, denitrification
18	NOPOLU	Nutrient loss to surface water	Catchment	Annual		Y								No soil processes
19	OVERSEER	Livestock management model	Farm	Annual										
20	PSYCHIC	Phosphorus flow, not stream routing	Field/Catchment	Monthly										
21	REALTA	Nutrient loss to surface water	Catchment	Annual	y	Y	y							No soil processes
22	RZWQM	Tillage, macropore transport	Field scale, up to 10 soil layers	Daily	y	Y		Soil erosion	Pesticide, fecal	y	y	y		Decomposition, min/immobiliz, nitrification, denitrification, C dynamics
23	SIMSDAIRY	Detailed farm N cycling	Farm (dairy)	Monthly	y		y	y		y	y	y	y	
24	SOIL + SOILN	An integrated C/N dynamics model	Field scale, number of soil layers depends on soil simulation, can have over 20	Daily	y	Y					Gases treated as one sink			Decomposition, min/immobiliz, nitrification, denitrification (all N gases included)
25	SOMM	Specialized SOM mineralization and humification	Plot to global	Long-term										Decomposition, nitrification, denitrification, N release

(*Continued*)

Table 2 (*Continued*)

(a)

			Resolution		Processes, transformations, losses relevant to climate change									
					Losses to waters					Atmospheric losses				
ID	Models	Characteristics, focus of model	Spatial	Temporal	Leached N	Runoff N	P	Sediments	Fecal/ pesticides	NH_3	N_2O	NO	CH_4	Transformations in soil
26	SOURCE AP			Annual										Simplistic, no soil processes
27	SPACSYS	Flexible, integrated plug-and-play nutrient model for plant, roots, agricultural management	Field scale, layers flexible	Daily	y	Y			Fecal		y	y		Decomposition, min/immobiliz, nitrification, denitrification
28	MODCOU	Hybrid spatial scales	Modcou regional scale (and plot-scale version-STICS)	Daily	y	Y					Gases treated as one sink			Decomposition, net mineralization, nitrification, denitrification
29	SUNDIAL/ MAGEC	Crop and Nutrient flow	Four fixed layers, field output	Monthly/ daily	y					y	Gases treated as one sink			Decomposition, min/immobiliz, nitrification, denitrification
30	UK-DNDC/ DNDC	Integrated C/N dynamics with crop growth	Plot, regional	Daily	Attempted but not well-developed water module					y	y	y	y	Decomposition, nitrification, denitrification, plant growth, ammonia volatilization

(b)

ID	Models	Processes, transformations, losses relevant to climate change: Plant: Climate	Plant: Shoot:root	Hydrology	Other	Pollution Swapping (C, N, P)	Mitigation	Farmer adaptations	Limitations	Source of info (see references in full)
1	ANIMO	Soil temperature, saturated and unsaturated systems, ground and surface water		Field drains, lateral, vertical, saturated/ unsaturated, groundwater and surface water	Natural areas, forest, wetland plant types	C dynamics	Manure, fertilizer	Different crops, grazing	No N_2O, focuses on leached nutrients	Groenendijk and Kroes (1999), Schoumans and Silgram (2003)
2	APSIM	Plant water uptake, soil temperature, water	Active uptake, mass flow, diffusion to roots	Vertical drainage		C dynamics module			Originally developed for sugarcane, other crops need to be developed	Huth *et al.* (2010), Shaffer and Ma (2001)
3	BASINS	Takes in hydrological data from GIS including future climate projections		Strong in catchment flows					Not agricultural management, limited US web-based geo-related dataset	Mohamoud *et al.* (2009)
4	CNSP Pasture	Soil temperature, water	Root length and uptake; alter ratio if deficient; mycorrhizal effects	Soil water dynamics affecting C/N dynamics		C dynamics	Fertilizer		No N_2O; no separate SOM decomposition pools	McCaskill and Blair, 1990
5	PASIM	Plant uptake, soil water dependent, temperature, microclimate submodel	Partitioning between shoot:root; root uptake and exudation	Vertical percolation	Physiological effects of CO_2 increase			Animal manures, fertilizer	Detailed plant growth and simple soil SOM models introduce uncertainty (Riedo *et al.*, 2000)	Riedo *et al.* (2000)
6	DAISY	Plant water uptake, temperature, soil water dependent		Vertical percolation				Animal manures, fertilizer	No N_2O	Grant (1995), Shaffer and Ma (2001)

(*Continued*)

Table 2 (*Continued*)

(b)

ID	Models	Processes, transformations, losses relevant to climate change: Plant: Climate	Plant: Shoot:root	Hydrology	Other	Pollution Swapping (C, N, P)	Mitigation	Farmer adaptations	Limitations	Source of info (see references in full)
7	DAYCENT (daily CENTURY)	Soil temperature, plant temperature, plant water	Allocation to roots increases as precipitation decreases, and a function of time since planting for crops	Vertical percolation		C dynamics		Limited organic waste	Only vertical drainage	Parton *et al.* (1987, 1998, 2001), Shaffer and Ma (2001)
8	ECOSYS	Plant uptake, temperature						Animal manures	Can be too detailed for application with greater calibration requirement	Shaffer and Ma (2001)
9	EUROSEM								Erosion model, vegetation related to obstruction of flow	Morgan *et al.* (1998)
10	EVENFLOW	No climate link with growth or N cycling			Frequency of exceedance of N concentration				Crop processes limited, isolated N cycle	Schoumans and Silgram (2003)
11	GLEAMS	Soil temperature, plant temperature		Vertical percolation				Animal manures	No N_2O	Leonard *et al.* (1987)
12	HURLEY	Yes, very specific, soil moisture, soil temp	Yes, very specific	Some representation	Energy, physiological effects of CO_2 increase				No N_2O	Thornley and Verberne (1989), Arah *et al.* (1997)
13	INCA	Soil moisture, air and soil temperature, plant water		Matrix (slow) and macro- (fast) drainage	Land-use change		Various crops	Manure, fertilizer application	No C cycling or microbes	Whitehead *et al.* (1998), Wade *et al.* (2002)

14	MACRO	Soil temperature, plant water, rainfall, temperature		Multilayer, macro/micro				Limited organic waste	Pesticide model rather than nutrients	Jarvis (1994)
15	MONERIS								Very coarse scale, simplistic	Venohr *et al.* (2005), Schoumans and Silgram (2003)
16	MOTOR (review based on Verberne version, although modifiable)	Indirect reduction factors to rates for drying of soil or temperature effects; fixed weather files	Plant processes not explicitly modeled	Verberne version: water flow not explicitly modeled	Emphasis on microbial effects, isotropic tracers modeled	C and microbial dynamics with N	Different crop types	Manure application	Steep learning curve, no GHG's, no productivity (yield) versus pollution information	Whitmore, 2007, Verberne *et al.* (1990)
17	NGAUGE	Temperature not from observed weather data		Precipitation, not observed weather data			Manure, fertilizer	Animal manures	Isolated N cycling, no carbon or microbes, fixed weather	Brown *et al.* (2005)
18	NOPOLU								Coarse scale	Schoumans and Silgram (2003)
19	OVERSEER	Limited climate variation		Topographic slope and flow with land management					Coarse temporal scale	Ledgard *et al.* (1999), Wheeler *et al.* (2008)
20	PSYCHIC	Monthly long-term statistical means of rain, temperature, sun hours		Drainage, runoff						Davison *et al.* (2008), Stromqvist *et al.* (2008)
21	REALTA								Coarse a scale	Magette, 1998, Schoumans and Silgram (2003)

(*Continued*)

Table 2 (*Continued*)

(b)

ID	Models	Processes, transformations, losses relevant to climate change: Plant: Climate	Shoot:root	Hydrology	Other	Pollution Swapping (C, N, P)	Mitigation	Farmer adaptations	Limitations	Source of info (see references in full)
22	RZWQM	Plant uptake, soil temperature, plant nutrients	Not considered	Infiltration, drainage			Fertilizer recommendation	Manure applications, growing seasons, animal weight, grazing/cutting, dairy cow intake	Simple soil hydrological flow	Ma *et al.* (2001), Shibu *et al.* (2006)
23	SIMSDAIRY	Temperature not from observed weather data	Not considered	Precipitation, not observed weather data			Fertilizer recommendation	Animal manures	Isolated N cycling, no carbon or microbes	Del Prado *et al.* (2006)
24	SOIL + SOILN	Plant uptake, temperatures, soil water (derived)	N uptake function of root distribution	Vertical and lateral		C and microbial dynamics with N	Fertilizer recommendation	Manure applications, growing seasons	A good model but SPACSYS has further developed on this model, for example, root component	Eckersten *et al.* (1996), Janssen (1998), Shaffer and Ma (2001)
25	SOMM	Soil temperature, soil moisture			Earthworm decomposition of humic substance		Natural/grazed system/forest biomass		Specialized SOM mineralization and humification derived from microorganisms/microfauna experiments	Chertov *et al.* (1995)

26	SOURCE AP								Too simple, no soil processes	National Environmental Research Institute (2000), Schoumans and Silgram (2003)
27	SPACSYS	Plant uptake, soil temperature, plant nutrients	1D and 3D comprehensive root system implemented	Infiltration, drainage and lateral	Changes in root architecture, salt dynamics	C and microbial dynamics with N	Fertilizer recommendation	Manure applications, growing seasons, tillage, fertilizer	P component not added yet	Wu *et al.* (2007)
28	MODCOU	Soil water, and temperature		Vertical and lateral			Fertilizer recommendation	Manure applications, growing seasons	No N_2O	Ledoux *et al.* (2002)
29	MAGEC/ SUNDIAL	Plant uptake maximum and minimum temperature, rainfall and ET required	Root:shoot ratio to maximize uptake	Vertical only			Fertilizer recommendation	Manure applications	No N_2O	Bradbury *et al.* (1993), Smith *et al.* (2006)
30	UK-DNDC/ DNDC	Soil temperature, hydrology			Forest and wetland versions	Weakness in hydrology limits leaching versus GHG's	Fertilizer and manure	Different crops, woodland biomass, tillage	Not well developed water module, not detailed partitioning for crop	Brown *et al.* (2002), Li *et al.* (1997, 2010), Shaffer and Ma (2001)

Note: For brevity in table, min/immobiliz, mineralization and immobilization processes.

atmosphere (Cardenas *et al.*, 2010; Cooter *et al.*, 2010). Good management systems will try to avoid N application immediately preceding heavy precipitation to minimize NH_4^+ loss, so simulating runoff and associated NH_4^+ loss may not rank so high in importance to us as simulating soil water drainage and associated NO_3^- loss. Since N_2O emitted into the atmosphere is 310 times more potent than CO_2 (Cuellar and Webber, 2008), it is logical to also include it as an essential output for soil flux model simulation. Neither NO_3^- loss nor N_2O losses can be completely eliminated from a farming system, but we can determine which land management strategy gives the overall optimal balance between farming and associated N losses and this is why a useful model should include both outputs.

The dynamics of carbon (C) and N is core to the processes affecting leaching and N_2O emission in the majority of published soil N cycle models/modules. New ideas about organic decomposition and nutrient cycling can be implied from results of isotope studies (Amelung *et al.*, 2008; Bol *et al.*, 2009). For example, it has been shown that some fungi feed only on fresh plant material, little evidence has been found of inert soil C and there is nutrient flow information from the dissipation of bacterially derived C and N through soil food webs (Murray *et al.*, 2009). However, many recent ideas have not been formed into a coherent system which has been used in many computer models; simulations are based firmly on the traditional understanding of organic matter dynamics. Carbon and N occur together in all types of organic matter in varying ratios. Organic matter plus applied nutrients are cycled in the soil through various decomposition stages, partially acting as assimilate for the microbial biomass which transforms it (DeBusk *et al.*, 2001). Ratios of C:N vary through these stages, and an excess organic matter with lower C:N ratios can result in an excess of N which the microbes will release resulting in N mineralization. High C:N ratios will cause the microbes to immobilize soil mineral N to convert into an organic complex with C. Both immobilization and mineralization can occur, and if the result is net mineralization, excess mineral N in the soil could be at risk to produce leachate through excess water percolation. After mineralization, several things could happen. Under aerobic conditions (dry soil), the nitrifying microbes convert NH_4^+ to NO_3^-, rendering it susceptible to leaching when the soil rewets. NO_3^- diffusing into anaerobic soil layers (wet soil) can also be reduced by denitrifying microbes to N_2O, a potent GHGs. Hence a change in climate, or in land management adapting to the changing climate, will stimulate a change in microbial activity and organic matter turnover (Bond-Lamberty and Thomson, 2010; Lal, 2004), and hence affect leaching and gaseous emission, the two processes being systematically related. Thus, it would be preferable to use a model which includes a sophisticated organic matter turnover simulation.

The detrimental environmental impacts of agriculture can only be minimized if there is more efficient use and recycling of nitrogen and phosphorus (Tilman, 1999).

Manures represent a substantial resource of N and P but have smaller N:P ratios (2–6:1) than most crop requirements (7–11:1), leading to soil P enrichment over time. It is necessary from an economic yield aspect to maintain a high plant P-use efficiency over time, and to do so, it is necessary to build up the soil P to a critical level, at which there is a high percentage recovery of phosphorus from fertilizer in crop harvest offtake. In developed countries, where soil P is in excess, farmers attempt to strike an economically viable balance between maintaining a soil at a critical level while preventing excessive phosphorus levels. European agriculture is currently operating on an annual P surplus, which can have a major impact on water quality (Dils *et al*., 2001). It will therefore be important to include P cycling in an integrated multinutrient model, but this could limit the choice of a more advanced model of C and N dynamics, in which case it would be better if either P were simulated by a separate model or, in the longer term, a new holistic N, C, and P model were developed.

We have included in our chapter, models that simulate a particular nutrient cycle in isolation such as the N cycle in NGAUGE, or focus on a particular process, for example, erosion in EUROSEM. These were useful to review because there is the possibility of using them in a framework with other models, for example, an N model related to soil moisture via a water flow model being added, or a stream-routing model with an agricultural management model added. Sometimes certain models are particularly strong in one feature, shown by that process being simulated in more detail than others. We try to show the diverse methods by which models simulate processes in the following sections and focus on what is included or missing from a model for our study. The next section breaks modeling details down into criteria, discussing merits and limitations of the listed models.

2.2. Model issues with regards to climate change impact

2.2.1. General background

The rates of most biological processes are sensitive to the factors of temperature and water availability being related to enzyme activity. Considering future climate effects (essential now in most studies of environmental processes), we need to know by how much climate changes from a historical baseline. Climate scenarios from general circulation models (GCMs) provide us with this information. In order to assess the impacts of climate change on diffuse pollution, and the effects of mitigation management practices and adaptation on diffuse water pollution, models need to be able to directly or indirectly use climate data, and preferably use climate scenarios. This would mean a direct use of observed climate parameters and future climate scenarios on a daily basis. Alternately, an indirect use of climate data, such as a modification of a fixed climate, could also be considered.

Climate parameters are driving variables for energy transformation, water balance, plant growth, and nutrient cycles in agricultural production systems. Therefore, the parameters of temperature and precipitation as a minimum requirement should be included in a model. Daily maximum and minimum air temperature should be integral to a model for determining climate information and crop processes. Knowing the minimum temperature allows an approximate assessment of whether precipitation will be in the form of snow which can increase soil surface water retention time and can delay flow. Minimum temperature also influences vernalization for annual over-winter plants and determines the date of flag leaf appearance for cereal crops (Slafer and Rawson, 1995). Most soil–crop–weather models require a time function for crop development which may be a calendar time or heat unit accumulation. Robertson (1968) introduced the concept of biometeorological time, involving photoperiod, maximum and minimum temperature, for calculating the rate of development of different crop stages. Photoperiod is a preferred climate parameter relating to crop development but it can be calculated using Julian day and latitude. Likewise, wind and humidity would be preferred parameters to allow a calculation of evapotranspiration which will affect crop growth and development rate and the soil water balance.

Results have shown from two decades of free-air CO_2 enrichment (FACE) experiments that elevated CO_2 stimulates photosynthetic carbon gain but increase in crop yield is smaller than expected (Leakey *et al.*, 2009). Plant responses to CO_2 vary and underlying mechanisms are not clearly understood, hence it is not considered an essential simulation to include in a model. However, the PASIM and HURLEY models and SPACSYS have the option to include a range of atmospheric CO_2 concentrations.

2.2.2. Observed or simulated climate files

ANIMO does not use direct weather data, instead it uses output from earlier run weather-driven simulations with a separate soil water model, operating at the same timestep as the soil water simulations, daily or weekly. NGAUGE and $\mathrm{SIMS}_{\mathrm{DAIRY}}$ have a static climate file derived from historical climate statistics instead of observed climate. GLEAMS can take climate data from observed or simulated sources and it operates on a daily timestep, using observed weather data to drive the hydrology, erosion, and temperature submodels. An optional climate generator can be used within GLEAMS for daily rainfall, temperature, and radiation data. Otherwise, most complex models with a shorter timestep use observed climate data, such as APSIM, RZWQM, DAYCENT, MAGEC, and SPACSYS, requiring daily timestep weather data to drive the hydrology, energy, and nutrient submodels. MACRO operates with observed weather data on a daily, hourly, or shorter timestep.

2.2.3. Precipitation

The fixed climate files of NGAUGE and its farmscale extension $\mathrm{SIMS}_{\mathrm{DAIRY}}$ take the 30-year mean monthly precipitation for locations around the UK, and there is a choice of one of six rainfall values. Precipitation indirectly impacts on the submodels of denitrification, mineralization, and plant uptake. Each precipitation file can be modified by a fixed amount to give five classes representing a very wet to very dry month. It is recognized that the period since precipitation is a major factor in determining denitrification rate (Jarvis *et al.*, 1991), so the temporal and spatial scales are a limiting factor. It is the monthly and longer timestep models which sometimes use a derivation from climate archives like NGAUGE and $\mathrm{SIMS}_{\mathrm{DAIRY}}$, most use weekly rainfall. ANIMO takes daily precipitation information from its separate hydrological model. MAGEC, RZWQM, DAYCENT, SPACSYS, APSIM use daily precipitation. As regards climate change, any annually scaled models for precipitation are immediately limited in terms of adaptation, as they cannot use climate data seasonally, that is, drier summers or wetter winters.

2.2.4. Temperature

Soil nutrient–microbe dynamics are temperature dependent, and demonstrating a typical modeled C and N cycle response with respect to air temperature change, a sensitivity test was conducted on MAGEC (Smith *et al.*, 2006). When temperature was increased, amounts of decomposable and resistant organic pools were reduced. Mineralization and denitrification were significantly increased reflecting increased microbial activity. Nitrate and ammonium in the soil, along with leaching, were reduced, possibly with increased microbial N requirement (Smith *et al.*, 2006). Many of the models reviewed such as MACRO, GLEAMS, DAYCENT, and ANIMO require daily air temperature to calculate daily soil temperature and thermal conductivity, which affect the chemical and biological processes (Lewis and McGechan, 2002). The dependence of N processes is based on air rather than soil temperature in the SUNDIAL model (Smith *et al.*, 2004), the model inputs average weekly air temperature. SPACSYS requiring daily maximum and minimum air temperature has a specific soil thermodynamics portion of the model, with optional extra components such as ice water infiltration and snow dynamics. In some models, for example, SOIL and SOILN, heat modules link soil water and heat with freezing and thawing of soil water (Bergstrom *et al.*, 1991; Lewis and McGechan, 1999). In other models, the temperature comes from a derivation of archived climate data. The fixed climate files of NGAUGE and $\mathrm{SIMS}_{\mathrm{DAIRY}}$ take the 30-year mean monthly temperature for locations around Britain, and there is a choice of one of six temperature zones. Weather impacts on the submodels of denitrification, mineralization, and plant uptake. Each temperature file can be modified by a fixed amount to give five classes representing a very warm to very cold month (Brown *et al.*, 2005; Del Prado *et al.*, 2010).

2.3. Consideration of the water cycle

2.3.1. General background

Soil water modules are often used to link climate into other soil processes via evapotranspiration and precipitation. Chemical and physical processes in nutrient cycling such as a portion of N mineralization and immobilization are modified by soil moisture and also by water flow. Water is also important as a carrier for the mobility of nutrients into and out of soil layers. Most models have some form of water balance, shown in Table 2b. Since we are reviewing models to determine the effect of climate change on diffuse pollution, a simulation of water balance and availability would be useful. Results have shown NH_4^+ to be lost predominantly by runoff, while NO_3^- is lost into streams by percolation of water through soil (Eunice Lord, ADAS, personal communication, 2010; Fey *et al.*, 2010; Lu *et al.*, 2009). Hence, runoff and leaching are both important processes depending on the expectation of simulation output.

2.3.2. Water balance

Soil water models generally require hydraulic conductivity and water response functions for various soil layers (DeJong and Bootsma, 1996) to determine throughflow or a deficit. Whereas ANIMO uses a separate soil water module, NGAUGE and $\text{SIMS}_{\text{DAIRY}}$ have no soil water processes simulated within the models, but soil moisture deficit is read as an input with the weather files. The percentage water-filled pore space in these two models (related to soil moisture deficit) modifies N processes and is related to monthly denitrification using a relationship based on experiments (Scholefield *et al.*, 1997).

GLEAMS, an update of the CREAMS model for nutrient and pesticide flow and RZWQM (Shibu *et al.*, 2006), determines surface runoff by employing the surface runoff curve number technique with evapotranspiration and soil-routing simulations. The Soil Conservation Service Curve Number (SCS-CN; Tramblay *et al.*, 2010; US Department of Agriculture Soil Conservation Service, 1972) is a method to determine soil water runoff, or overland flow, depending on antecedent moisture conditions. The method is based on two hypotheses: that the ratio of direct runoff to potential maximum runoff is equal to the ratio of direct soil infiltration to maximum potential soil retention and that initial abstraction, or temporary surface storage, for example, puddles, is a fraction, commonly 20%, of the potential maximum soil retention. SCS-CN has been widely used for flooding because it uses a minimal number of parameters compared to other methods. GLEAMS also uses two optional calculations of evapotranspiration depending on climate parameters available, which is a very practical step, considering data sources vary or have missing data. GLEAMS can also account for irrigation.

Models deal with soil moisture throughout the soil layers differently depending on their soil water complexity: GLEAMS uses five soil layers; RZWQM and DAYCENT (the daily scaled CENTURY model) use 10 layers. GLEAMS can relate the water balance to wetland, subsurface drainage, and tillage systems. SPACSYS can have unlimited soil layers, it stores water in surface, matrix pool, or canopy pools, extra water from a groundwater source can occur, and the water in the soil matrix can be redistributed since it uses SOIL's numerical solution to the Richards equation (Janssen, 1998). This a common feature in other models such as DAISY which also employs Richard's equation requiring water release characteristics and hydraulic conductivity. PASIM can also have an unlimited amount of soil layers and, like SPACSYS, employs Darcy law so that water fluxes between soil layers relating to percolation, capillary rise, and drainage depend on soil water content, matric potential, and hydraulic conductivity. UK-DNDC and the 2002 version of DNDC employ a "tipping bucket" method of vertical soil drainage through layers, that is, when field capacity is reached, 50% of the water over this threshold moves into the soil layer below. In addition, gravitational redistribution and matric redistribution of soil water (Ritchie, 1998) are then employed.

2.3.3. Runoff, water movement, and drainage

The hydrological component of GLEAMS, EVENFLOW, and RZWQM simulate runoff using an adaptation of the SCS curve number method (Tramblay *et al.*, 2010; US Department of Agriculture Soil Conservation Service, 1972). The downward movement of water is simply based on the excess of field capacity for many models such as GLEAMS, RZWQM, SUNDIAL, and MAGEC. Other models such as DAISY and SPACSYS base their soil water on the Richards equation (Richards, 1931), relating water flow to hydraulic conductivity and water tension. DAYCENT has multiple soil layers for water flow. MACRO, a model particularly strong in water flow through soil, has its own module for multiple soil layers and water movement in macro- and soil matrix pores.

GLEAMS and DAYCENT only consider vertical flow, not lateral flow under the soil surface. MACRO and SPACSYS consider flow to groundwater and subsurface lateral flow to field drains. GLEAMS therefore simulates the vertical transport of nutrients and pesticides down through root layers, and its surface flow detaches and deposits sediments providing transport for the full description of C, N, and P cycles contained within GLEAMS. Contrasting with detailed nutrient transport processes, NGAUGE and $SIMS_{DAIRY}$ simply relate water-filled pore space to a leaching component, but their emphasis is the N cycle.

SPACSYS is a complex, process-based, integrated agroecosystem model. It has a daily timestep and operates at the field scale. Driven by weather, it has a thorough water flow module for field drainage and vertical flow plus groundwater flow. Water flow interacts with plant growth, separated into consideration of roots and above ground processes. Ammonium and NO_3^- are included in vertical drainage and in groundwater flow; surface runoff loss of organic matter is also an output in water flows.

MACRO has been recommended for use as a tool to study leaching (Mantovi *et al.*, 2006). Nitrate accumulation in surface soil during warm periods was shown to be susceptible to fast drainage related to shrinking/swelling properties of clay minerals. The model results confirmed the observed role of macroporosity in accelerating the throughflow of soluble compounds. MACRO has separate simulations of contaminant flow in soil matrix pores (micropores) and macropores, as well as contaminant movements between the two domains. MACRO simulates water movements vertically through the profile including deep groundwater and horizontally to field (tile) drains. The hydrological routines in MACRO are similar to many other soil water models, with the soil water tension and hydraulic conductivity relationships enabling the Richards' equation to be solved (Richards, 1931). MACRO differs from other models in its treatment of larger soil macropores when capillary forces are very low, so water movements can be assumed to be driven by gravitational forces alone (McGechan *et al.*, 2008).

APSIM has been used to explore components of the water balance for a range of farming systems. APSIM was used to explore the impact of climate on water balance, with all other factors held constant, including the soil type. The impact of climate on water balance was said to identify the relative magnitude of transpiration, soil evaporation, runoff, and drainage and to explore temporal variability in these terms for selected locations over the 1957–1998 climate record (Keating *et al.*, 2001). Evidently, then APSIM appears suitable to investigate the effect of climate change scenarios on soil hydrology.

We can group models into their resultant output by referring to Table 2b. ANIMO, APSIM, PASIM, DAISY, DAYCENT, INCA, MACRO, RZWQM, SOILN, SPACSYS, MODCOU, and MAGEC produce vertical drainage. ANIMO, SPACSYS, and SOILN produce lateral flow to field drains. The documents that we have reviewed for ECOSYS, EUROSEM, MACRO, MOTOR, NOPOLU, SOMM, and SOURCE AP do not specify that they output leached nitrate.

2.3.4. Catchment flow

A few models such as EVENFLOW, MONERIS, NOPOLU, SOURCEAP, REALTA, and PSYCHIC are strong catchment models, considering stream pollution (Table 2a). The HSPF model is packaged in open GIS form as BASINS. Using web-based data for a geographic location is a strong tool for multiple nonpoint source data considering surface flow drainage over catchments to one or multiple rivers, but it is not an agricultural tool. BASINS would however have potential if linked with a model simulating agricultural land management effects on nutrient cycling. It can consider fecal indicator organisms, P and sediment transport, and can link with inputs of biota in watersheds, for example, indices such as biodiversity of invertebrates representing the fitness of aquatic communities. BASINS can utilize online climate scenarios. However, without agricultural management, it is limited for our application, and further since it is an American model, having a full complement of data for other countries in its GIS database is doubtful. When a model is using online data, this can be useful to access data availability, but there is no control over the quality of the data, and questions arise of flexibility and specifically of the ability to use one's own observed data.

EUROSEM is an erosion impact model, useful therefore for determining sediment transport and relating to nutrient loss. Like HSPF/BASINS, it focuses on strong water flow modeling to catchment scale, but instead of stream loading, it focuses on erosion of the gulleys and channels. It is not an agricultural model and lacks land management, its consideration of vegetation is related to interception and infiltration, but as with BASINS, such a model would be useful linked to a land and nutrient management model.

INCA also accounts for water flow to a catchment. Inputs required are climate, initial water flow and N loading, land management, fertilizer timing and application, crop type, and sewage flow rate. Key processes are mineralization, immobilization, denitrification, nitrification, plant uptake of nitrate, and ammonium; the concentration of these is dependent on the water cycle. The process equations are solved in a manner ensuring that no one process takes precedence over the others. Parameter sets are derived through calibration, that is, model parameters being adjusted a little at a time until the difference in observed and simulated data is acceptable. Hydrological calibration is key to this because it controls N stored and transferred. Soil, air temperature, and hydrological processes incorporate features suitable for climate change applications. INCA has really been designed for studying river system functioning, nevertheless, it does include all agricultural soil N processes and land use and land management.

2.4. Capability for nutrients and carbon cycling

2.4.1. C and N coupling

Soil C and N dynamics affect crop and soil quality, as well as the resulting pollution from agriculture. Through their greenhouse effects, they have an influence on the stability of the climate. In recent years, it is this global environmental importance that has resulted in a focus on this subject, while at the same time, new biogeochemical tools have been developed which can improve understanding of these cycles, for example, isotope tracing and remote measurement techniques (Amelung *et al.*, 2008; Boegh *et al.*, 2004; Bol *et al.*, 2009; Gilmanov *et al.*, 2010; Rubino *et al.*, 2010). Meanwhile faster computing has enabled improvements in modeling, especially at field or microscale, to include more mathematical complexity in the simulation of processes, which has enabled the improvement of models of C and N dynamics (Lu *et al.*, 2006; Ptashnyk *et al.*, 2010).

There are knowledge gaps in the fine details of C and N cycle processes, so they are commonly modeled using pools of common components within a cycle and, from experimental results, transformation rates are determined between the pools. Some models simulated the N cycle without linkage to the dynamics of the C cycle, for example, NGAUGE. However, C and N dynamics are intricately linked via microbial growth and turnover. Modeling trends have moved away from isolated nutrient cycles (Bergstrom *et al.*, 1991; Brown *et al.*, 2005; Chertov *et al.*, 1995) toward integrated simulations of multinutrient cycles, also incorporating crop, atmosphere, microbial biomass, soil water, and other components (Grant, 1997; Groenendijk and Kroes, 1999; Wu *et al.*, 2007). Some models have developed separately from the original model. For example, UK-DNDC and DNDC (Li *et al.*, 1997) have similar functions, but UK-DNDC (Brown *et al.*, 2005) was modified for use in the UK and both have been updated separately since.

2.4.2. Mineralization/immobilization

Heterotrophic soil microorganisms, primarily fungi and bacteria, use C from decomposition in a specific proportion with N (C:N ratio of ca. 6) which they obtain from mineralization of organic N, soil NO_3^-, or NH_4^+. If microbial organisms are supplied with C rich and N poor residues (generally anything with C:N ratio over 30) such as wheat straw, this will result in immobilization of N in the biomass, leaving little N available to a growing crop. N is released with microbial turnover, or when microbes are consumed by higher trophic levels which excrete excess N, resulting in N mineralization. Conversely, decomposing organic materials with lower C:N ratios can result in an excess of N and net soil mineralization (Chadwick *et al.*, 2000; Shaffer and Ma, 2001). Simulations adopt a mixture of methods to represent mineralization and immobilization.

Models which integrate simulation of the C and N cycles commonly capitalize on the C:N ratio as the key link between the two nutrient cycles and a way of determining net N immobilization and mineralization (DNDC, SPACSYS, SOILN, DAYCENT), a C:N value above a threshold value signifies immobilization (high organic C residues after harvest and ploughing), and a value under the threshold signifies net N mineralization. Meanwhile, the rates of the processes plus microbial growth and decay are influenced by temperature and soil moisture (Melillo *et al.*, 1989).

In RZWQM, mineralization and immobilization are determined by the decay of organic pools and growth of microbes. Organic pools decay according to a first-order equation and the rate coefficients are modified for temperature and moisture effects. It is assumed that a fraction of organic C decayed becomes part of the microbial biomass, and the N assimilated into microbes is calculated via the C:N ratio. RZWQM separates soil functions by different microbial groups, for example, it is the aerobic heterotrophs which obtain their energy and growth via organic pool decay. In GLEAMS, organic pools also decay according to first-order reactions.

NGAUGE and $SIMS_{DAIRY}$ calculate N mineralization empirically. These models do not account for organic C, so do not link C:N ratios to organic matter cycling. Annual preexisting mineralization is calculated from previous land use, herbage production, dung, and applied manures, based on experimental results and modified by sward age, soil texture, and drainage. The values are partitioned between 12 months. Mineralization is modified by 30-year means of temperature and soil moisture from specific locations in the UK. Mineralization is added from the current year's residues empirically derived and based on monthly plant N content. A key feature of this process is that for each monthly timestep the model iterates through the N cycle, until the resulting value returned from the previous step in the cycle for mineralization is within a threshold difference.

Not all models have to have a detailed description of N processes. MONERIS considers soil N simplistically, mineralization and immobilization are ignored, and the net N surplus (input minus harvest offtake) is assumed to be released as dissolved inorganic nitrogen. In EVENFLOW, there is no explicit representation of the N cycle, being based on empirical relationships between cropping and grazing regimes and nutrient output instead.

Among the catchment models, SOURCE AP, REALTA, and NOPOLU do not consider soil processes but can nonetheless serve as "broad brush" tools to assess pollutant loads at catchment level (Schoumans and Silgram, 2003). For all these models, soil processes are lumped and implicitly derived from measured monitoring data.

2.4.3. Denitrification/nitrification and nitrous oxide emission

Representations for nitrification/denitrification vary among models, often in accordance with the complexity of the whole model. In SOILN, ANIMO, and DAISY, nitrification is determined by a nitrification rate, NH_4^+ content, and environmental modifiers of the rate (Hansen *et al.*, 1991; Ma and Shaffer, 2001; McGechan and Wu, 2001).

NGAUGE and $SIMS_{DAIRY}$ use this approach, too. Their source of ammonium is pools of ammonium mineralized from organic matter, including excreta, NH_4^+ from fertilizer, and urine from slurry application.

Nitrification in NGAUGE and $SIMS_{DAIRY}$ is a zero-order reaction, hence independent of substrate concentration but with temperature and moisture modifying the rate. Processes producing NO and N_2O have a representative value to produce a maximum amount, a modifier accounting for moisture and the amount of ammonium nitrified (Brown *et al.*, 2005). Denitrification is simulated as a function of the amount of inorganic N modified by temperature and moisture. Considerable temporal and spatial variations in denitrification rate occur in the field, and during a dry month, a sudden downpour increases the denitrification rate, so a limiting factor of a monthly model is that it obscures temporal variation. Production of N_2O and N_2 is determined by the denitrification rate modified by the minimum of three factors; water-filled pore space in soil (related to moisture), mineralization rate, and the amount of mineralized N.

In APSIM, nitrified N_2O is proportional to the nitrification rate. The simulation of the N_2:N_2O ratio from denitrification is related to the amount of nitrate to heterotrophic CO_2 respiration (Thorburn *et al.*, 2010).

The complex ECOSYS model links the net mineralization to the nitrification process. Each microbe functional type in each substrate–microbe complex seeks a consistency of its C:N ratio during growth by mineralizing or by immobilizing ammonium. These reactions control soil mineral N concentrations which in turn drive nitrification and denitrification reactions in the model (Grant *et al.*, 2006). ECOSYS is a model based on physiochemical transformations, such as oxidizing reducing equations and energy transformations, and considers eight types of microbe separately.

RZWQM considers functional groups of microbes separately, autotrophs obtain their energy from nitrification, and a fraction of NH_4^+ is assimilated, whereas facultative heterotrophs grow via denitrification and take a fraction of denitrified NO_3^-. RZWQM calculates nitrification as a zero-order rate modified by temperature, pH, autotroph biomass, and oxygen content. Unlike most models, RZWQM can account for nitrification inhibitor application. Denitrification is determined by a first-order rate coefficient modified by soil C, lack of oxygen, temperature, pH, and denitrifier biomass.

DAYCENT calculates nitrification to be proportional to mineral N turnover, and its N_2O production to be related to turnover rate and excess ammonium in the soil. N gas fluxes from nitrification and denitrification are driven by soil NH_4^+ and NO_3^- concentrations, water content, temperature, soil texture, and labile C availability. DAYCENT's simulation of combined N_2O plus N_2 gas flux from denitrification is limited by the minimum value of three factors: (1) maximum N gas flux for a given soil respiration rate, (2) for NO_3^- content, and (3) the soil moisture effect on denitrification.

DNDC's denitrification module tracks microbial dynamics and availability of substrate (NO_3^-) and modifies the rate reaction on the substrate by moisture and temperature (Zhang *et al.*, 2002). ANIMO links denitrification to the amount of decomposable organic matter; SOILN connects denitrification to the amount of NO_3^-; and DAISY relates denitrification to the amount of NO_3^-, organic decomposition, and emission of CO_2 (Hansen *et al.*, 1991; McGechan and Wu, 2001).

Denitrification in the OVERSEER model is based on IPCC methodology where the amount of each type of N input into the system (excreta, fertilizer, effluent) is multiplied by the emissions factor for that type of N source. Excreta from livestock is partitioned into urine and dung, and further partitioned into paddocks, lanes, dairy, or housing. Dairy and housing contribute to the effluent system.

The variety of different empirical methods reflects the unknown nature of the processes of nitrification and denitrification, which are so complex and vary in time and space with different species of microbes affected by varying environmental factors in the soil.

Referring to Table 2a, the models which specifically output N_2O are PASIM, DAYCENT, ECOSYS, NGAUGE, $SIMS_{DAIRY}$, RZWQM, SPACSYS, and UK-DNDC.

2.4.4. Organic matter decomposition, carbon and nitrogen dynamics

Most models (e.g., MOTOR, UK-DNDC, DAYCENT, RZWQM) link the C and N cycles by the ratio in which they are found in their organic matter component, thus knowing how much C gives the amount of N and vice versa. Simulated C and N dynamics commonly comprise algorithms for the decomposition of organic matter combined with plant uptake; mineralization/immobilization; and, if included denitrification and nitrification, input of plant litter, manure, and root exudates.

The core algorithms of C and N dynamics are the C decomposition of organic matter pools. These vary across models but are generally split into fast decomposition pools with a higher C:N ratio such as fresh litter, and slow more stable decomposition such as humus with a lower C:N ratio. This concept can be seen in GLEAMS, MAGEC, RZWQM, and SPACSYS. The nutrient model of GLEAMS has an organic matter and microbial pool dynamically linked to the N and P cycles. GLEAMS incorporates crop residue and active and stable organic matter pools. MAGEC links decomposition and C:N ratio to soil type. RZWQM has a specific microbial biomass pool and separates the microbes into aerobic heterotrophs, autotrophs, and facultative heterotrophs. In SPACSYS, organic matter pools have specific decomposition rates further modified by soil water and temperature and the C:N ratio. The C:N ratio in the microbial biomass has a feedback effect on mineralization and immobilization.

SPACSYS has four organic matter pools: (1) fresh organic material, (2) humus, (3) dissolved organic matter, and (4) microbial biomass. Part of the organic matter dynamics also includes dissolved organic carbon (DOC) from residues lost from the surface of the soil in runoff, and DOC lost from within soil by leaching.

PASIM has C fluxes moving between an animal submodel, a plant submodel, and a soil submodel. Considering this represents grazing from grass to animal, urine/feces from animal to soil, and root exudation from plant to soil, this is a framework common to other models.

CENTURY/DAYCENT separates plant residues into structural lignin and structural cellulose pools and a metabolic pool based on the lignin:N ratio. Metabolic and cellulose pools are more active, and lignin the stable pool. DAYCENT decomposition of litter and soil organic matter and nutrient mineralization are functions of substrate availability, substrate quality (lignin %, C:N ratio), and water/temperature stress (Parton *et al.*, 2001). The final residual organic fraction which cannot be further broken down (condensed tannins, phenolics, waxy alkyl compounds, and lignins) is referred to as the acid unhydrolyzable residue (AUR). The CENTURY model, when applied to leaf litter only, has 5C pools: structural, metabolic, microbial (or active), slow, and passive. The undecomposed litter is divided into the structural and metabolic pools, as determined by the AUR/nitrogen ratio, the higher this ratio, the more of the organic matter in the litter is considered to be structural. Carbon from the structural and metabolic pools is partitioned into CO_2 losses and transfers to the active and slow pools, and further CO_2 losses with transfers to the passive pool. Pool-centered decomposition rates are calculated empirically by reducing a maximum decomposition rate by a multiplicative function that depends on mean July temperatures and annual precipitation rates. The N pools and processes are considered to have same structure as the C pools and processes, with prescribed C:N ratios by pool type. N rates entering or leaving the pools are adjusted such that the C:N ratio of each pool remains fixed, except for the C:N ratio of the metabolic pool which is allowed to vary. External N inputs are via atmospheric deposition and fertilizer applications or N_2 fixation (Del Grosso *et al.*, 2009).

In ECOSYS, microbial biomass is an active agent of organic matter transformation in the model. Soil organic matter is divided into four substrate–microbe complexes: plant residue, animal manure, particulate (active), and nonparticulate (passive) organic matter in five different states: solid, solubilized, adsorbed, microbial, and microbial residue. Each organic state in each complex is further divided into carbohydrate, cellulose, and lignin with varying rates of relative decomposition. Microbial communities are further grouped into obligate aerobic and anaerobic, facultative anaerobic, and methanogens (Grant, 1997). Rates of decomposition of each substrate–microbe complex depend on the substrate–microbe density relationships, temperature, and water content. Residue decomposition products depend on soil clay content.

SOMM considers organic decomposition and the N cycle separately (Zhang *et al.*, 2008) and includes mineralization and humification by microbes and soil fauna with separate soil microfauna and mesofauna pools. Limited in its view, SOMM could be useful seen as an addition to models which lack this aspect such as NGAUGE and $\mathrm{SIMS_{DAIRY}}$. However, in comparison with other models such as CENTURY, it was found to require far more temperature and moisture sensitivity coefficients (Zhang *et al.*, 2008), since each coefficient empirically derives from independent process studies, for each of the mass and N turnover processes. Despite its greater parameter requirement, SOMM simulations tested against experimental measurements were not found to give as high a quality of fit between calculated and observed values for mass remaining and N concentrations over time as CENTURY.

MOTOR is primarily concerned with the flow of C linked to N via the C:N ratio's of different matter. The model deduces the fraction of each source pool that within a daily timestep becomes a particular product in another pool. The fractions are multiplied by the rate term and the amount of C in the source pool can be modified by the efficiency of the process (Verberne *et al.*, 1990). MOTOR is based on a body of work including the Verberne organic matter turnover model (Verberne *et al.*, 1990). The system tries to accommodate the change in C:N ratio during nutrient flows. Gross mineralization of N determines its supply and immobilization its demand. The supply and demand are compared, and if out of balance, there are several strategies used to rebalance the N flow. Decomposition kinetics is modified repeatedly until the supply matches demand. One strategy is to include a partitioning factor, putting emphasis on a greater transformation of a pool to a specific product for which there is a high demand, out of a number of potential products. Another strategy is to reduce the decomposition rate of fresh residue pools (manure and litter). The values of C:N are variable in a pool, although it is stated that how much these latter two strategies reflect real life is unclear. These strategies increase N supply, conversely C retention time in soil can be reduced to reduce excess N. Production of microbial biomass from the residue pool and its decomposition will create a need and an excess of N, respectively. Hence, the microbial turnover is modeled integrally with the nutrient flows. The reaction rates are modified by temperature and soil moisture decreasing from an optimum value as soil dries, although the model has no explicit water simulation.

DNDC's decomposition module quantifies the organic C gain from crop litter (roots and aboveground residue) and/or manure incorporation, as well as the C loss through decomposition. DNDC partitions litter into three soil litter pools, very labile litter, labile litter, and resistant litter, based on the C:N ratio of the bulk litter. There is a specific decomposition rate for each litter pool, modified by temperature, moisture, and N availability in the soil profile. During the decomposition of litter, part of the litter C is consumed as the energy source by the soil microbes and becomes CO_2, and part of the litter C is turned into microbial biomass. After death, microbial remains will become humus to undergo further decomposition.

2.4.5. Root/shoot partitioning and uptake

Plant N uptake relates to plant growth, root distribution, and integral with this is partitioning to different parts of the plant. DAYCENT and PASIM deal with biomass growth separately for roots and shoots modified by temperature and moisture, and SPACSYS includes root growth in detail apart from the rest of the plant, roots getting priority for assimilate. A component of SPACSYS develops the root architecture, which will have further effects on nutrient uptake. Under substrate shortage, root growth is restricted which modifies the proportion of assimilate translocated to different parts of the plant. SPACSYS also contains a mycorrhizal pool since fungi often attaches to the root system. DAYCENT plant production is a function of genetic potential, phenology, nutrient availability, water/temperature stress, and solar radiation. Net primary production is allocated to plant components (e.g., roots vs. shoots) based on vegetation type, phenology, and water/nutrient stress. Nutrient concentrations of plant components vary within specified limits, depending on vegetation type, and nutrient availability relative to plant demand (Del Grosso *et al.*, 2009).

DNDC root growth is also determined by partitioning of assimilate from crop growth processes, and then rooting processes include the increase of root front depth, distribution of root length density, and biomass. Root depth is limited to a maximum. Daily variation of root density depends on new growth and senescence. Root depth, density, and biomass distributions will affect the capacity to uptake N. SPACSYS has a detailed option to investigate the three-dimensional architecture of roots. This root simulation is related to soil temperature and strength, and water nutrient concentration for growth, and assimilate to determine root elongation and volume expansion. The previous root direction, geotropism and mechanical resistance affect the orientation of a root and root branching is simulated. A simpler option for root growth simulation in SPACSYS considers root growth based, like DNDC, on rooting depth, vertical distribution of root length density, and root biomass.

N uptake in models is usually simulated from plant demand from a crop growth module or from studies using an empirical curve. Some models, for example, DAYCENT, SPACSYS, and RZWQM, have plant growth modules to estimate demand of the inorganic N at different phenological stages. ANIMO bases crop uptake of nutrients on a balance between crop demand and soil supply, and adjusts crop growth rate if the soil supply is limiting. The GLEAMS model assumes uptake of total N. Plant nitrogen is returned to the soil via crop residues and roots. Allocation of assimilate to roots increases as precipitation decreases; this potentially could be of use in simulating adaptations to climate change.

2.4.6. Phosphorus

ANIMO, GLEAMS, DAYCENT, and MACRO incorporate the P cycle. The models contain the transport of soluble and particulate P, the application of manure and fertilizer and the mineralization/immobilization of organic/inorganic matter. MACRO considers micro- and macroflow containing P and has the capability to simulate the movement through the soil of P bound to particulate material. ANIMO also considers preferential macropore flow. It considers P sorption onto and diffusion within soil particles, described by a combination of instantaneous and time-dependent sorption and chemical precipitation of phosphates, and overland flow of dissolved organic phosphorous, inorganic phosphate, and particulate phosphate with water flow to adjacent fields (runoff and erosion). Erosion and sediment yield from fields is estimated in GLEAMS via soil particle detachment and the subsequent transportation of this sediment. Particle detachment is assumed to be a function of soil properties, management, and rainfall and runoff characteristics.

When runoff occurs, the sediment load is assumed to be limited by the transport capacity; deposition takes place with usually the coarse and dense particles deposited first. DAYCENT considers surface losses from the labile inorganic and active organic P pools. The model also considers soil erosion effects in addition to surface runoff losses.

With respect to P, MONERIS has no sorption and desorption mechanisms, just an overall equation used to describe the relationship between P content of the soil and the P concentration in soil solution (Schoumans and Silgram, 2003). The catchment models focusing on streamloading, REALTA, MONERIS, NOPOLU, and SOURCE AP all consider total P load from land to water, but no detailed soil processes concerning P cycling.

A complete consideration of P in soil should consider transport of both soluble and particulate P, and of both inorganic and organic P, by surface runoff, through the soil to field drains, and vertically through the soil down to deep groundwater. In addition, it should consider the transformations from one form of P to another following applications of both mineral fertilizer and manure (Lewis and McGechan, 2002). Most models considered here seem to be missing one or more of these processes. GLEAMS considers everything except transport to field drains. DAYCENT also only considers vertical transport. ANIMO has the most comprehensive inclusion of manure and slurry, and includes a rigorous description of soluble forms of phosphorus, but lacks consideration of particulate transport. MACRO has the most comprehensive inclusion of through soil transport processes and particulate transport but not surface runoff and currently has only simplistic representation of P transformations. A comprehensive nutrient model focused on P would be a combination of these four with a full representation of the C:N:P cycle as described by GLEAMS, with manure and slurry components as described by ANIMO, and plant residue decay equations taken from the DAYCENT model. Finally, the overland flow and erosion losses could be represented by components from the GLEAMS model (Lewis and McGechan, 2002).

PSYCHIC accounts for the mobilization and delivery of P and suspended sediment (SS) using empirical data. It includes transport of soluble and particulate P, and inorganic and organic P, by surface runoff, through the soil to field drains and vertically through the soil down to deep groundwater. The model determines the fraction of mobilized phosphorus and sediment delivered down rivers based on the connectivity of drains and watercourses, with preferred particle size for each pathway of diffuse pollution. Over predictions have been reported (Stromqvist *et al.*, 2008) although this seems the most comprehensive P model in our chapter.

2.5. Land management

2.5.1. General modeling issues with respect to land management

This section reviews which models have the ability to simulate agricultural management. It may be the capability to simulate different types of crops and their period of ground cover, or breeds of livestock and timing of grazing, or the timing and application of fertilizer, or a physical alteration of the soil such as tillage. Viewed in light of climate change, these are parameters a farmer can choose to adapt. The most likely mitigation measures we feel would be recommended are listed by (Cuttle *et al.*, 2007).

Any change in either the natural conditions or the farming management can simultaneously alter several soil environmental factors including temperature, moisture, pH, and substrate concentration gradients. This can affect a series of biogeochemical reactions such as physical movement, oxidation and reduction, dissolution, adsorption, assimilation which finally determine CO_2 and N_2O emissions from the modeled ecosystems (Zhang *et al.*, 2002).

For example in SPACSYS, if ploughing is opted for as part of the simulation, all remaining living leaves and stems, roots down to ploughing depth, and all above ground residues are evenly included in the litter pool for that depth. The roots below the ploughing depth are incorporated in the corresponding litter pools (Wu *et al.*, 2007). This has a huge impact on the organic matter cycling via different C:N ratios, soil aeration, and altering active biomass functional types, that is, nitrifiers or denitrifiers.

Considering how farmers may adapt to climate change or what mitigation policies may be made, the most likely seem to be connected to field management strategy, crop types, and the length of time that the ground is covered. Cover crops can reduce NO_3^- loss if well established, using the cover with crop rotations and accurate timing to reduce leaching (Shepherd *et al.*, 1993). The ability to schedule land management events daily is one the most important benefits of a model with a shorter timestep (Del Grosso *et al.*, 2009).

As will be seen in Section 2.5, no one model accounts for every agricultural management. Model applications can be divided into those biased toward livestock farming and those biased toward arable. Choice of model for management effects depends on the application required; a mix of use for land-use change may require use of more than one model. Models with shorter temporal timesteps, daily, weekly, or monthly, are better suited than models with annual timesteps to simulate land management effects. A shorter timestep will allow, for example, specific dates of sowing and cropping, and to allow for a specific grazing period. A shorter timestep can also take into account the interaction of the management with climate events and crop stages, for example, an application of slurry a day before a heavy rainfall at an early crop developmental stage with less than full ground cover, which would be expected to promote fast sediment carrying runoff.

2.5.2. Crop type and timing

Crop type and timing are necessary parameters to account for land-use change. SPACSYS accounts for different crop types, seeding date, cultivation/planting schedules, amount, and timing of nutrient amendments. UK-DNDC accounts for crop type, sowing date and density, harvest date, straw management, and irrigation amount. DAYCENT and INCA allow for vegetation type, cultivation/planting schedules, and amount and timing of nutrient amendments. DAISY incorporates a crop planting date and harvest date. RZWQM accounts for crop type, seeding date, and irrigation. APSIM allows for crop rotations. ECOSYS accounts for crop type, seeding and harvest date, type of harvest, and fraction of plant removed.

2.5.3. Livestock grazing/housing periods (including feed input and excreta output)

PASIM, NGAUGE, and $\text{SIMS}_{\text{DAIRY}}$ are biased to livestock systems. PASIM, HURLEY, OVERSEER, NGAUGE, $\text{SIMS}_{\text{DAIRY}}$, and SPACSYS consider separate systems of grazing or cut grass. PASIM and $\text{SIMS}_{\text{DAIRY}}$ consider live weight gain and lactating cow feed intake. $\text{SIMS}_{\text{DAIRY}}$ also takes into consideration different types of feed supplements, housing date and calculates the associated gaseous emissions from housing and manure storage. NGAUGE considers feed supplements. Diet can modify CH_4 output. CH_4 output is only considered by DAYCENT, ECOSYS, $\text{SIMS}_{\text{DAIRY}}$, and UK-DNDC/DNDC. PASIM, OVERSEER, NGAUGE, $\text{SIMS}_{\text{DAIRY}}$, SPACSYS, and MACRO all consider dairy and sheep farming. The HURLEY and OVERSEER pasture models for livestock consider stocking rates.

2.5.4. Nutrient application: Fertilizer and manure

ANIMO, GLEAMS, and DAYCENT include a livestock manure pool for input to nutrient dynamics. MACRO can simulate slurry via an addition to its irrigation component. NGAUGE, INCA, $\mathrm{SIMS_{DAIRY}}$, and RZWQM simulate manure additions. SPACSYS simulates nutrient addition via fertilizer and manure applications. It distinguishes between six different types of manure based on their C:N ratios. SPACSYS, NGAUGE, and $\mathrm{SIMS_{DAIRY}}$ consider slurry application and distinguish between application by splash plate or injection. NGAUGE and $\mathrm{SIMS_{DAIRY}}$ also have an optimization routine for fertilizer rate and timing. ANIMO allows for slurry application, but also additions of fertilizer, manure, and crop residues. A few models like ANIMO, DNDC, NGAUGE, and SIMSDAIRY also consider soil N input by atmospheric deposition of N. DNDC simulates application date and amount of NO_3^-, NH_4^+, NH_3 and urea, and manure. DAYCENT, ECOSYS, HURLEY, INCA, RZWQM, and DAISY allow for fertilizer application, amount, and date. As mentioned previously, NGAUGE and $\mathrm{SIMS_{DAIRY}}$ have monthly timesteps, ANIMO can have a daily or weekly timestep, MACRO can have a daily or hourly timestep, HURLEY has an hourly timestep, and the rest of the models have a daily timestep, which renders them all applicable for simulating fertilizer and manure management.

2.5.5. Tillage and other physical modification of land

ANIMO, ECOSYS, RZWQM, and SPACSYS simulate tillage. DNDC simulates tilling date and depth. As with SPACSYS, the GLEAMS tillage module incorporates crop residue, animal waste, and fertilizer, and mixes the respective pools in the ploughed layers. DAISY requires tillage date and method. All of these models have a daily timestep.

2.6. Ease of use for the operator

Logically, the more simplistic models with larger temporal and spatial scale, that is, NOPOLU, MONERIS, REALTA, have lower data requirements than finer scale and more complex process-based models like ANIMO. The lower the data requirements the smaller the workload and the quicker an operator would be able to learn to simulate nutrient output, as a large part of model run would simply consist of data collection. If detail and accuracy are not paramount and general trends are required with a limited budget and timeframe, this type of model may be the one most suitable. The most detailed model included in this chapter is ECOSYS. If a detailed spatial scale or timestep is needed, this terrestrial ecosystem model will usually suffice. The model can also be applied regionally and over long time periods, up to centuries. It has a longer list of parameter requirements of any models considered in this chapter. To speed data access, several models are now linked into a GIS, accessing a national database. PSYCHIC uses this approach to predict P and sediment transport, accessing a database common to Agriculture Development and Advisory Service (ADAS) users where it was developed. The next step is a web-based public access database, which BASINS uses. BASINS makes it possible to quickly assess large amounts of point source and nonpoint source data in a format that is easy to use and understand. Installed on a personal computer, BASINS allows the user to assess water quality at selected stream sites or throughout an entire watershed. It integrates environmental data, analytical tools, and modeling programs for a cost-effective approach to watershed management. BASINS integrates national databases (elevation, hydrography, meteorological, land use, and soil), assessment tools, data management and graphing programs with models (HSPF, SWAT, PLOAD, and AQUATOX), and analysis tools. HSPF is a watershed hydrology and pollutant transport model (Whittemore and Beebe, 2000) and is the core watershed model in BASINS. A custom GIS interface for BASINS is available in ArcGIS through a toolbar. The program invokes web data download for US databases of hydrologic units across the US available online. This, however, somewhat limits the applicability to other countries. HSPF uses BASINS to extract soil, land cover, and geomorphological data and parameter values from geographic information databases, using the BASINS GIS analysis tools (US Environmental Protection Agency, 2001).

2.7. Spatial scale and temporal timestep

2.7.1. Spatial scale

Spatially most models we reviewed are field scale, for example, SPACSYS, PASIM, DAISY, ANIMO, which meet the requirements for this study (Table 2a). Some models have more than one scale: ECOSYS simulates from field up to regional scale; PSYCHIC is at field and catchment scales; SOMM from plot to global scale; MODCOU from plot to regional scale; and UK-DNDC/DNDC which operate at field or regional scales. The models which work on a catchment scale are generally those whose main focus is stream loading of nutrients, for example, BASINS, EVENFLOW, INCA, MONERIS, NOPOLU, SOURCE AP. In the models looked at, only $\mathrm{SIMS_{DAIRY}}$ and OVERSEER were farm scale, incorporating livestock housing and associated emissions and nutrient loss.

2.7.2. Temporal timestep

Most models reviewed worked with a daily temporal scale. Models based on a monthly scale are CNSP, NGAUGE, $\mathrm{SIMS_{DAIRY}}$ and PSYCHIC. Daily and monthly timesteps mean a model has the potential to simulate farm management decisions and can reflect monthly variability in weather (precipitation, temperature). Large timescale models considering over a hundred years are the annual MONERIS, REALTA, NOPOLU, SOURCE AP, and organic matter turnovers in SOMM and HURLEY Pasture are also on a large timescale. On the issue of temporal scale, OVERSEER would be potentially a good agricultural management tool if it had a finer temporal scale. It has been developed for livestock systems, incorporating stocking, fertilizer and manure management operations, but it operates with annual quantities, so the climate does not have a separate wet or dry season, and with an annual scale individual weather events, no matter how extreme, are missed. Models that give results on an annual basis are not really applicable for diffuse water pollution, unless annual pollutant load is the target output. If linked to a streamflow model, a smaller scale could help produce frequencies of exceedance of pollutant concentration and loads. MOTOR is a specialized model based on reaction kinetics, with output expressed in terms of reaction rates of pool components converted in milligram per kilogram of soil, its timestep is not specified explicitly in documentation (Whitmore, 2007) but is inferred that it is daily.

Models which have variable scales are: ECOSYS with a timescale which runs from hourly to centuries; ANIMO with daily to weekly scales; MAGEC which is daily and its SUNDIAL monthly counterpart; and MACRO which runs hourly to daily. NGAUGE and $\mathrm{SIMS_{DAIRY}}$ are monthly and annual models.

3. Conclusions

While no model will incorporate all our requirements, there are some that will accommodate more than most. In practice, we have to make some assumptions and accept the limitations of whatever model we use. Thus, we look for a reasonably detailed, flexible, and integrated model with a robust, validated approach and yet one where the processes are explicit.

If we compare which of these models outputs both N_2O emission and NO_3^- leaching, both processes are common to PASIM, DAYCENT, NGAUGE, $\mathrm{SIMS_{DAIRY}}$, RZWQM, and SPACSYS. This would make these six models good candidates for assessing secondary effects of mitigation and adaptation, and all output on shorter daily/monthly timescales for field or farm. It is our opinion that when diffuse pollution and its mitigation is considered, taking into account the balance between gaseous emissions of N and leached or overland flow of N, creates an integrated and holistic assessment of the problem. Additionally, DAYCENT and $\mathrm{SIMS_{DAIRY}}$ include P cycling.

Of the six models, DAYCENT, PASIM, RZWQM, and SPACSYS incorporate organic turnover which is integral with nitrogen cycling and makes for a more accurate process simulation attuned to biomass dynamics than empirical studies based on experimental results. All four of these models take in daily climate data and include water movement through the soil.

PASIM, DAYCENT, and SPACSYS consider root dynamics and root: shoot ratio which affects nutrient uptake capacity with decreased precipitation. For land management, PASIM, biased toward dairy farming, considers grazing or cut grass, animal weight, and intake by the lactating cow; however, it is a pasture model so cannot account for a change of land use, such as a different crop or a rotation. Whereas DAYCENT is biased toward cropping and considers vegetation type, cultivation/planting schedules, amount and timing of nutrient amendments, such as fertilizer application. SPACSYS applicable to both livestock and cropping considers tillage, vegetation type, cultivation/planting schedules, amount and timing of nutrient amendments, fertilizer application, cut grass or grazed grass.

In summary, it can be concluded that no single model incorporates all our stated requirements, there were, however, three models, DAYCENT, PASIM, and SPACSYS which would accommodate most features, and would be candidates for further development in the light of our current and future modeling requirements.

Appendix. Brief Description of Selected Models

The Dutch ANIMO model aims to quantify the relation between fertilization level, soil management, and the leaching of nutrients to groundwater and surface water systems for a wide range of soil types and different hydrological conditions (Schoumans and Silgram, 2003). The model was developed in 1985 to evaluate N losses and later the P cycle (organic and inorganic) was added (Groenendijk and Kroes, 1999). The model ANIMO is a functional model incorporating simplified formulations of processes. The organic matter cycle plays an important role for the assessment of long-term effects of land-use changes and fertilization strategies.

APSIM, the Agricultural Production Systems Simulator (Keating *et al.*, 2001), component-based design allows individual models to interact via a common communications protocol on a daily timestep. It was produced for agricultural systems, but the models can simulate many major crop, pasture, and tree species as well as the main soil processes affecting agricultural systems (e.g., water, C, N, and phosphorus dynamics, and erosion) including denitrification and N_2O emissions. (Huth *et al.*, 2010) used APSIM to determine the likely production of N_2O emissions from leguminous crop residues when incorporating legumes into cereal crop rotations.

BASINS is a multipurpose environmental analysis system designed for use by regional, state, and local agencies in performing watershed and water quality-based studies. The model is connected to a GIS interface which links with large US databases for data input (Mohamoud *et al.*, 2009).

CNSP (McCaskill and Blair, 1990) developed for C, N, S, and P dynamics in white clover pastures is very focused on nutrient uptake, root simulation and includes mycorrhizal effects. It is a specialist model that focuses on soil nutrient dynamics.

DAISY is a soil–plant–atmosphere model (Hansen *et al.*, 1991). It is a single column model, which describes crop growth, water and heat balances, as well as the dynamics of organic matter, ammonium, and nitrate in an agricultural ecosystem. It is based on management practices as well as soil and weather data.

DAYCENT is the daily timestep version of the CENTURY biogeochemical model (Parton, 1996; Parton *et al.*, 1987). DAYCENT simulates fluxes of C and N among the atmosphere, vegetation, and soil (Parton *et al.*, 1998, 2001). Key submodels include soil water content and temperature by layer, plant production and allocation of net primary production, decomposition of litter and soil organic matter, mineralization of nutrients, N gas emissions from nitrification and denitrification, and CH_4 oxidation in nonsaturated soils. DAYCENT model considers sorbed soil P in equilibrium with a labile soil P from which leaching occurs, and P loss through soil erosion. DAYCENT accounts for soil class, daily weather, historical vegetation cover, and land management practices such as crop type, fertilizer additions, and cultivation events.

The ECOSYS model of natural and managed ecosystems is a comprehensive model with detailed processes concerning N_2O and captures the large temporal variability of N_2O at high temporal and spatial resolution, under site-specific conditions such as climate, soil type, land use, topography, etc (Grant, 1995). The model can simulate the transport and transformation of heat, water, C, O_2, N, P, and ionic solutes through soil–plant–atmosphere systems with the atmosphere as the upper boundary and soil parent material as the lower boundary (Metivier *et al.*, 2009).

The European Soil Erosion Model (EUROSEM; Morgan *et al.*, 1998) is a sediment transport, erosion, and deposition model simulating transport over the land surface by rill and interill processes in single storms for both individual fields and small catchments. Model output includes total runoff, total soil loss, the storm hydrograph, and storm sediment graph. Although a specialist model, it has the potential to be linked with other models. Compared with other erosion models, EUROSEM has explicit simulation of interill and rill flow; plant cover effects on interception and rainfall energy; rock fragment (stoniness) effects on infiltration, flow velocity and splash erosion; and changes in the shape and size of rill channels as a result of erosion and deposition.

The quantification tool EVENFLOW (Schoumans and Silgram, 2003) is a catchment model that simulates the loss of nitrate in soil drainage and the routing of leachate through a catchment system. The system uses statistical data on land use, farming practices, climate, and soil characteristics as inputs, collated at a spatial resolution of 1 km^2. The model was developed to provide a robust estimate of inorganic nitrogen fluxes and concentrations in river waters, primarily originating from agricultural land, for any catchment within England and Wales.

GLEAMS (Leonard *et al.*, 1987) was originally a chemical transport, soil erosion, and runoff model, which developed dynamic nutrient cycling, subsurface drainage flow, macropore flow, and pesticide flow.

HURLEY Pasture (Arah *et al.*, 1997; Thornley and Verberne, 1989) compartmentalizes grass into four different age categories of root and leaf; flows of carbon (C), nitrogen, and water between adjacent compartments occur in response to concentration or water potential gradients across resistances determined by compartment size; structural growth of the various compartments is governed by local substrate concentrations and temperature. Since photosynthesis varies rapidly, the fundamental timestep is short (around 15 min for stability); appropriate input data are generated from available measurements assuming sinusoidal diurnal (and, if necessary, seasonal) waves.

INCA—Integrated Nitrogen in Catchments model (Wade *et al.*, 2002; Whitehead *et al.*, 1998)—is a process-based model of the nitrogen cycle in the plant/soil and instream systems. The model simulates the nitrogen export from different land-use types within a river system, and the instream nitrate and ammonium concentrations at a daily timestep. The interface permits multiple crop and vegetation growth periods and fertilizer applications. It is able to reproduce the seasonal dynamics observed in streamwater nitrogen concentration data, and the loads associated with plant/soil system nitrogen processes (Wade *et al.*, 2002).

MACRO (Jarvis, 1994; McGechan *et al.*, 2008) is a nonsteady-state water movement and solute transport model for macroporous layered soils, which couples unsaturated–saturated flow with root water uptake and a drain system and has a separate representation of processes in "macropores" and soil matrix "micropores." In earlier versions of the model, only soluble contaminants were considered, and applications concerned mainly water contamination by pesticides. However, MACRO later (Jarvis *et al.*, 1999) included a representation of colloid-facilitated contaminant transport, a process particularly relevant to phosphorus pollution.

The MAGEC soil model (Smith *et al.*, 2006) for crop growth and yield in response to global environmental changes was adapted from SUNDIAL (Bradbury *et al.*, 1993; Bradbury and Powlson, 1994; Smith *et al.*, 1996). The soil organic matter pools were modified so that they exactly corresponded to the pools used in a well-established soil carbon model, RothC (Coleman and Jenkinson, 1996; Jenkinson and Coleman, 1994).

The timestep of the monthly SUNDIAL was altered in MAGEC to a daily timestep. Underlying physiological processes include photosynthesis, transpiration, nitrogen uptake, partitioning of biomass and nitrogen among growing organs, phenology, leaf area development and senescence, and root extension.

MODCOU is a spatially distributed hydrological model used to simulate the surface runoff and groundwater flow in multilayered hydrological systems (Korkmaz *et al.*, 2009; Ledoux *et al.*, 2002). It consists of several components, namely, surface model, groundwater model, unsaturated zone model, and the coupled model. Spatial information on the basin is extracted by using digital elevation model (DEM) analysis, and operations are carried out via a GIS interface.

The MONERIS (Venohr *et al.*, 2005) model was developed for the nutrient inputs via various points and diffuse pathways in German river basins. The basis for the model is data on runoff and water quality from river catchment studies and physical data from a GIS. There are at least four different diffuse paths to consider: direct nutrient input on the water by atmospheric deposition, nutrient input into the river by surface runoff, input via interflow which represents a fast subsurface flow component, and input via base flow (groundwater). Inputs of dissolved substances via surface runoff and entries of bound nutrients and suspended particulate matter via erosion are distinguished.

MOTOR (Modular description of the Turnover of Organic matter; Whitmore, 2007; Whitmore *et al.*, 1997) describes the transformation of organic carbon and nutrients in soil. The state of each component of the organic matter in soil is described by a vector and the transformations by a matrix of terms. Actual turnover is calculated by multiplication of these matrices, state vectors, and a rate vector. The resulting system is powerful because it is modular in construction and any one part of it may be altered simply and quickly without reference to the rest of the calculation system (Whitmore, 2007). The model derives from an earlier body of various works and an earlier version of MOTOR (Whitmore *et al.*, 1997) which incorporated the Verberne organic matter turnover model (Verberne *et al.*, 1990), and MOTOR has been influenced by SUNDIAL (Bradbury *et al.*, 1993) and the Hassink and Whitmore model of C flows (Hassink and Whitmore, 1997).

NGAUGE (Brown *et al.*, 2005) is an empirically based model of N cycling in grassland soils based on published multisite grassland data sets. It includes an optimization procedure to identify a fertilizer amount and distribution according to the criteria of herbage production and N losses to the environment. It is an improvement on existing nitrogen fertilizer 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.

NOPOLU (European Environment Agency/IFEN, 2000; Schoumans and Silgram, 2003) is an agricultural diffuse emissions module as part of a comprehensive catchment description database. It appears to avoid the issue of soil processes altogether by retrieving agricultural statistical data and processing it with land cover data to make it more relevant, and incorporating runoff data.

OVERSEER is a farmscale model that develops budgets for major soil nutrients (N, P, K, S, Ca, Mg, and Na) for most NZ farming enterprises (Ledgard *et al.*, 1999; Wheeler *et al.*, 2008). The primary purpose of the model is to prepare reports from which the user can make decisions on nutrient requirements for a farm and/or blocks of land within a farm. Of interest is the ability to calculate nitrate leaching and on farm emissions of GHGs—CH_4, N_2O, and CO_2.

The pasture simulation model, PASIM, reproduces dry matter production and energy balance of cut temperate grasslands at lowland sites (Riedo *et al.*, 2000). It is applicable to climate change, has a snow cover effects simulation, and can be used to determine long-term effects of changes in CO_2 and climate on productivity and total C in the system. It includes root system exudation and uptake. It considers grazing by dairy cows.

PSYCHIC (Davison *et al.*, 2008) is a process-based model of phosphorus and SS mobilization in land runoff and subsequent delivery to watercourses. Modeled transfer pathways include release of desorbable soil P, detachment of SS and associated particulate P, incidental losses from manure and fertilizer applications, losses from hard standings. Further, it includes the transport of all the above to watercourses in subsurface drainage (where present) and via surface pathways, and losses of dissolved P from point sources. The model can operate at two spatial scales, although the scientific core is the same in both cases. At catchment scale, the model uses easily available national scale datasets to infer all necessary input data, while at field scale, the user is required to supply all necessary data.

The Irish model, called REALTA (Kirk McClure Morton Engineering Consultants, 2001; Magette, 1998), uses a self-developed procedure for estimating losses from agriculture based on actual measurements obtained from catchment monitoring and management systems (Schoumans and Silgram, 2003). The procedure takes on board detailed knowledge of physical conditions and farming practices in the catchment. Percentage loss figures, initially derived from detailed agricultural studies at mini-catchment and subcatchment level, are linked to an agricultural risk map. Estimated nutrient percentage loss figures can be applied to the total agricultural import to produce an overall estimate for the total agricultural nutrient losses to surface waters.

RZWQM (root zone water quality model; Ma *et al.*, 2001) is an agricultural system model, simulating agricultural production and environmental quality. A nutrient module simulates carbon and nitrogen transformations in the soil profile. It comprises plant growth, water movement, heat transport, C and N dynamics, chemical transport, and management practices.

$SIMS_{DAIRY}$ (Del Prado *et al.*, 2006; Del Prado and Scholefield, 2008) is a farm scale model whose N cycling core is based on NGAUGE with strategic management operations included and an optimization procedure to maximize herbage production or minimize N losses to the environment. It has added indices for biodiversity, animal welfare, and farm economics and has an added P submodel from PSYCHIC.

SOILN (Eckersten *et al.*, 1996) was designed to simulate N transport and transformations in soils and its uptake by plants. The SOILN model includes all the major processes determining the inputs (fertilizer and manure, atmospheric deposition), transformation linked to C cycle (mineralization and immobilization), and outputs (leaching, denitrification, harvest yield). SOILN must be carried out in conjunction with the soil water and heat model SOIL (Janssen, 1998). A simulation with SOIL, which must be carried out prior to a simulation with SOILN, requires input data representing weather parameters including temperature, radiation (or sunshine hours), wind speed, and precipitation.

SOMM (Chertov *et al.*, 1995) is a specialized soil organic matter decomposition model. Originally designed for forest soils, it has since been used for Rothamsted Park Grass soil. It presents organic matter decomposition in three stages, using five mass and five N compartments. At the first stage, part of the litter layer (L pool) is set to be lost through biochemical degradation and fermentation thereby contributing to the fermentation layer (F pool). At the second stage, the fermented organic matter is lost through heterotrophic respiration and transformed into humus (H pool). At this stage, fermented matter is digested by microbial organisms, and soil mesofauna (e.g., earthworms), both producing humus. At each stage, the rates of the litter mineralization, fermentation, and humification are empirically related to the ash and N content of the decaying litter, and to local soil temperature and moisture estimates (Zhang *et al.*, 2008).

SOURCE AP (National Environmental Research Institute, 2000), the source apportionment method quantification tool, does not consider soil processes but can nonetheless serve as a tool to assess pollutant loads at catchment level if used in conjunction with another model. It quantifies nutrient losses from diffuse sources such as agricultural land, forest and pristine area, estimated as the difference between the transport and the measured emission (Schoumans and Silgram, 2003).

SPACSYS (Soil Plant Atmosphere Continuum System) is a multilayer, field scale, weather-driven, and daily timestep dynamic simulation model. It includes a plant growth component; an N cycling component; a water component, which includes representation of water flow to field drains as well as downward through the soil layers; and an energy component. Equations for soil water processes and heat transformation are almost identical to those in the SOIL model (Janssen, 1998). It is a plant growth and soil nutrient system that adds root dynamics, central to the study of plant growth and development, C and nutrient cycling, and water movement within the plant/soil system (Wu *et al.*, 2007).

UK-DNDC is inherited from the earlier version DNDC model. It was originally developed for predicting carbon sequestration and trace gas emissions from upland agroecosystems (Li *et al.*, 1997). The core of the model is a mechanistic simulation of soil C and N biogeochemistry, developed to assess N_2O, NO, N_2, NH_3, and CO_2 emissions. DNDC was modified for application to the UK and called UK-DNDC. UK-specific input data were added to DNDC's database and the ability to simulate daily C and N inputs from grazing animals and applied animal waste was added to the model. Validation of the model at the field scale shows that predictions of N_2O emission match observations well (Brown *et al.*, 2002). Since the original development of UK-DNDC, both of these models have developed separately.

The early version of DNDC (Li *et al.*, 1997) is organized as four interrelated modules for soil and climate, crop growth decomposition, and denitrification. This is the version that UK-DNDC (Brown *et al.*, 2002) uses. The soil climate submodel calculates hourly and daily soil temperature, moisture, and heat flows. The crop growth submodel simulates crop biomass accumulation and partitioning based on thermal degree days and daily N and water uptake. The decomposition submodel calculates decomposition, nitrification, NH_3 volatilization, and CO_2 production on a daily timestep. The denitrification submodel tracks the sequential biochemical reductions from nitrate (NO_3).

DNDC (Zhang *et al.*, 2002) updated to add crop genetic parameters, atmospheric CO_2 concentration, SCS curve number for surface runoff, and average water table depth.

DNDC continued in its development. DNDC (Li *et al.*, 2010) now consists of six submodels for simulating soil climate, plant growth, decomposition, nitrification, denitrification, and fermentation.

DNDC is used worldwide. The authors recognize that there are differences between UK-DNDC/the earlier and later versions of DNDC, however, the basis they are built upon and applicability are similar. To avoid repetition, they have chosen to describe one model instead of two throughout the text, referring to the UK-DNDC model (an example of how original models are adapted by researchers for specific purposes) which incorporates the earlier version of DNDC.

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