11

On the use of unsaturated flow and transport models in nutrient and pesticide management

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Abstract

Nutrient and pesticide emissions from agricultural land significantly impact surface and groundwater resources all over the world. These emissions should therefore be controlled by an appropriate management of agricultural practices. Effective agricultural management builds on a thorough understanding of the fate and behavior of nutrients and pesticides in the soil–crop system. Unsaturated flow and transport models may therefore be used as tools to predict fate and behavior of chemicals in soil, supporting decision making in the area of nutrient and pesticide management.

In this paper, we show how flow and transport models are introduced in the nutrient and pesticide management decision-making process. Examples are given of the use of flow and transport models in (i) field-scale nutrient and pesticide management; (ii) the identification and evaluation of fertilization and pesticide application practices supporting the implementation of regional-scale environmental management plans; and (iii) the registration of plant-protection products. Examples are selected across different eco-regions elucidating the generality of the presented approaches. Particular emphasis is put on (i) the limitations of the current modeling approaches for management applications, (ii) the handling of uncertainty in the data flow, (iii) the problems associated with the estimation of the required modeling data and parameters, and (iv) the transfer of scientific know-how into operational decision-making tools. Opportunities are presented for improving the process descriptions, the data generation methods, and the modeling practice. Finally, threats are summarized on the use of flow and transport models in future nutrient and pesticide management studies.

Keywords: soil water; nutrient transport; pesticide transport; regional-scale modeling; soil management

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Introduction

Globally 30 to 50 % of the earth's surface is believed to be adversely affected by non-point source pollutants (Duda 1993). Agriculture is considered to play a major role in non-point source pollution since agricultural activities result in the movement of fertilizer residues, agrochemicals and soil particles from the soil surface into rivers and streams via runoff and erosion, and into subsurface soil and groundwater via leaching (Corwin, Loague and Ellsworth 1999).

Nitrate, which is a major mobile plant nutrient, continues to contaminate surface and groundwater bodies throughout Europe. Notwithstanding the environmental protection policies adopted since the early 1990s, and in particular the implementation of the EU nitrate directive, nitrate concentrations in European rivers remained stable throughout the 1990s and there is no evidence of changes in trends of nitrate concentrations in European groundwater (Nixon and Kristensen 2003). Similar problems have been reported elsewhere in the world such as in the United States (EPA 1996; Kolpin, Burkart and Goolsby 1999).

Another issue is the contamination of water bodies by residues of plant-protection products (PPPs), generally referred to as pesticides. In contrast to the crop nutrients, PPPs are designed to have effects on plants, insects or fungi and may have toxic effects on humans. Their presence in water bodies is therefore a major concern. Residues of some PPPs in surface, groundwater and drinking water occur also at levels of concern throughout Europe (Nixon and Kristensen 2003).

To mitigate these problems, appropriate agricultural policies and management practices are needed. The European environmental legislation offers a series of instruments to reduce the nutrient and pesticide pressures on water resources. An example is the EU nitrate directive (EU/91/676) concerning the protection of water against pollution caused by nitrates from agricultural sources. Member states are required to designate nitrate-vulnerable zones, to report on any groundwater problems and to implement specific measures (such as good agricultural practices) to protect vulnerable zones. Another example is the EU/91/414 directive concerning the placing of PPPs on the market or the more recently adopted Water Framework Directive (EU/2000/60).

The agro-environmental legislation sets the environmental targets that must be reached at the larger scale, but the specific management measures should be developed at the local or the smaller regional level and should be based on the understanding of the fate and transport processes. Indeed, Clothier (1997) examined ways that soil management can be regulated to protect water quality and he concluded that science, through new technologies and alternative modeling approaches, will play a prime role in describing the link between land management and environmental quality. It should thereby be recognized that modeling is at the core of any characterization of the fate and transport processes in soil. While a conceptual model is necessary before undertaking any experimental work, it is also important to recognize that the end result of many experimental efforts is to describe how these processes will evolve in space and time through a mathematical model. In addition, modeling can further be used to optimize the characterization effort in terms of data collection quantity and quality and to evaluate different management strategies (Alvarez-Benedí and Muñoz-Carpena in press).

As the unsaturated zone controls the storage and availability of water, nutrients and pesticides in the root zone of the crops, and hence also the fluxes to surface and groundwater bodies, unsaturated-zone flow and transport models are essential components of any nutrient and pesticide management model. The basic thermodynamic principles of flow and transport are now well established, but the complexity of the processes results in different conceptualizations of flow and transport in nutrient and pesticide management models. Within this highlight paper, we will show how soil water flow and transport theories have been encoded in nutrient and pesticide management models, how some of these models have been used in nutrient and pesticide management at different spatial scales, what are the pitfalls and drawbacks with the current models, and what strategies can be identified to mitigate these. Within a first section we review shortly basic flow and transport theory and illustrate the introduction of this theory in studies supporting nutrient and pesticide management, thereby adopting a merely European perspective. In a subsequent section we perform a *SWOT* analysis illustrating the *S*trengths, *W*eaknesses (limitations) and *O*pportunities of current approaches. In the last section we illustrate the *T*hreats and give some visionary perspective on the future developments in this area. The target audience of this paper are scientists, environmental engineers and managers working in the area of nutrient and pesticide management, who do not necessarily have a basic background in soil physics but who use flow- and transport-based agro-ecosystem models to support decision making. As they will be the principal users of the models in the future, they should have a basic understanding of the functioning and pitfalls of flow and transport codes within nutrient and pesticide management-supporting tools.

The conceptualization of unsaturated flow and transport in pesticide and nutrient management models

Nutrient and pesticide management models are by definition holistic in that they deal with integrated agro-systems by decomposing them into different subsystems (e.g. the soil system, the canopy system, the farm system etc). Flow and transport models are therefore only submodels of more integrated models. In addition to flow and transport processes, nutrient and pesticide fate in the agro-ecosystem is also determined by a series of biotic and abiotic transfer and transformation processes such as the mineralization of nitrogen from, and immobilization in, soil organic material, the sorption of pesticide and ammonia on the soil matrix, the transfer of volatile ammonia and pesticides from the aqueous to the gaseous phase, etc. The transformation and phase transfer processes determine the partitioning of nutrient and pesticide components in the soil water phase. This soil water phase will be displaced in the unsaturated soil zone, and the flow and transport models will describe how these available solutes may be displaced by the carrying liquid. Submodels describing sorption and transformation processes, as well as plant uptake will be coupled to the unsaturated flow and transport models through specific sink–source and retardation terms.

The physical laws of mass, energy and momentum conservation are the building blocks for describing flow and transport in soils. Fundamental thermodynamic laws are combined with appropriate flux formalisms such as Darcy's law or Fick's law, to yield coupled equations for flow and transport in soils. The Richards equation is the most popular formalism used to describe water flow in nutrient and pesticide models:

$$\frac{\partial \theta}{\partial t} = -div\left[-k(h).\nabla H\right] - Sw \tag{1}$$

where θ is the volumetric moisture content ($L^3 L^{-3}$); H, the total hydraulic head (L); h, the matric head (L); Sw, the sink–source term for water (T^{-1}); $k(h)$, the hydraulic conductivity relationship ($L T^{-1}$); and t, the time (T). For solute transport, the most popular formalism is the convection dispersion equation (Van Genuchten et al. 1999):

$$\frac{\partial[\rho.s]}{\partial t} + \frac{\partial[\theta.C]}{\partial t} = div[\theta.D\nabla C - Jw.C] - Ss \tag{2}$$

where s is the mass of solute adsorbed on the soil per bulk mass of dry soil ($M M^{-1}$); C, the mass concentration of solute in solution ($M L^{-3}$); ρ, the soil bulk density ($M L^{-3}$); Jw, the Darcian water flux ($L T^{-1}$) and Ss, the sink-source term for solute ($M L^{-3} T^{-1}$). Many soil management models solve these flow and transport equations (1), (2) or simplifications of these such as the capacity models, subject to certain well-defined boundary conditions occurring at the soil interfaces. Alvarez-Benedí, Muñoz-Carpena and Vanclooster (in press) recently reviewed the modeling components commonly used in solute fate and transport models and how these are integrated into a holistic approach for transport characterization.

For relatively simple initial and boundary conditions and for simplified representations of the heterogeneity of natural porous media, simple analytical and semi-analytical solutions for (1) and (2) exist (e.g. Wooding 1968; Philip 1969; Šimůnek et al. 1999), resulting in explicit expressions of moisture content, pressure head or concentrations as a function of space and time. Analytical solutions are often based on the transformation of the partial differential equations in the Laplace or Fourier domain to separate variables or the application of Green's function (e.g. Leij, Priesack and Schaap 2000). When compared to numerical solutions, analytical solutions are mathematically more rigorous and exact but also much faster to implement. Analytical models are therefore often proposed in nutrient and pesticide management studies, especially when a large number of simulations need to be performed.

For more complicated descriptions of the variability of the soil properties and of the flow and transport boundary conditions, different numerical methods are used such as finite difference or finite element integration (Van Genuchten et al. 1999; Van Genuchten and Šimůnek 1996). The flexibility with which the boundary conditions and the soil variability can be described makes numerical models particularly attractive tools in nutrient and pesticide management. In a simplified form, only 1-D vertical transport in the field is considered and the 1-D forms of Eqs. (1) and (2) are numerically integrated. To deal with larger-scale applications and as such with the specific horizontal variability of soil and land use processes, a quasi 3-D approach is often implemented by linking a multiple set of 1-D solutions in a spatially distributed modeling approach. In its simplest form, there is no interaction between the vertical columns representing the unsaturated zone. In these approaches, it is not possible to distinguish between drainage fluxes to local surface waters and leaching fluxes into deeper aquifers. Examples of this approach are published by Capri, Padovani and Trevisan (2000), Tiktak et al. (2002; 2004) and Tiktak, Van der Linden and Boesten (2003). In a more sophisticated form, the vertical columns are linked with a regional-scale hydrological model, assuring a proper description of the lower boundary conditions for the 1-D model (Tiktak et al. 2002). The most sophisticated models offer a solution to the full 2-D or 3-D forms of Eqs. (1) and (2). This approach is not often used in large-scale pesticide and nutrient management practices, because it involves powerful numerical algorithms (Feyen et al. 1998).

Table 1 presents a selection of popular flow and transport codes that have been used within the context of nutrient and pesticide management. The table illustrates the diversity of flow and transport conceptualizations within these codes. For a detailed register of agro-system models the reader is referred to dedicated web sites such as the pf-models site (http://www.pfmodels.org), the CAMASE site (http://library.wur.nl/camase/), the REM site (http://eco.wiz.uni-kassel.de/model_db/), and many others.

Use of unsaturated flow models in nutrient and pesticide management studies

Nutrient management studies

Within the context of nutrient modeling, most effort has been devoted to modeling the N cycle, N being a key nutrient of agricultural crops and nitrate being a major polluter of groundwater. Initial modeling studies of nitrogen fate and transport in agro-ecosystems were conducted within an academic context to elucidate the role of the different processes and to support attempts to validate process descriptions within the simulation codes. Examples of model comparison and validation exercises are presented by e.g. Groot, De Willigen and Verberne (1991), De Willigen (1991), Vereecken et al. (1991) and Diekkrüger et al. (1995).

In the study of De Willigen (1991) fourteen simulation models of nitrogen turnover in the soil–crop system were compared using a common dataset. The simulation of the above-ground processes was less problematic than that of the below-ground processes. None of the models could account for the loss of mineral nitrogen occurring shortly after application of fertilizer in late spring and early summer. Another example is the testing of models for contrasting environments. Duwig et al. (2003) evaluated the ability of the WAVE model (Vanclooster et al. 1995) to predict the seasonal leaching of nitrate. One environment were the tropical climate and ferralitic soil conditions that exist on Maré in New Caledonia, and the other environment was a glacial terrace in the continental climate of La Côte Saint-André in France. Overall WAVE gave good predictions, even though it was used beyond its designed capacity, especially on Maré, which is characterized by variable charged tropical soil. For both sites the model gave the best results for wet conditions, which actually pose the most critical periods in relation to groundwater protection. Good results were also obtained with WAVE when modeling water and nitrogen transport in a banana field under the dry subtropical conditions of the Canary Islands (Muñoz-Carpena, Parsons and Ducheyne 1999; Ritter et al. 2003).

After validation, nutrient fate and transport-modeling codes can be used to support nutrient management at the field scale. Many studies have shown the potential benefits of nutrient fate and transport modeling for evaluating farm management policies and the implementation of agro-environmental measures at the field scale (Xu Di 1998). For example, Piñeros-Garcet et al. (2000) showed how modeling could be used to evaluate fertilizer management scenarios in mixed agricultural farms in the central part of Belgium. The efficiency of N catch crops in improving nutrient retention was evaluated for a range of different proposed land use scenarios, and the most appropriate cover crop was identified. The impact of different irrigation strategies on nutrient use efficiency and nutrient losses was modeled by Chang et al. (1994), Riga and Charpentier (1999), Hack-ten Broeke (2001), and others. The impact of the soil tillage practices on this was illustrated by Matthews et al. (2000).

Table 1. Selection of model codes used for nutrient and pesticide management applications

Code name	Management problem	Flow description	Transport description	Reference
Pesticide management				
PEARL	Pesticide registration	1-D numerical solution of Richards equation	1-D numerical solution of the Convection Dispersion equation	Leistra et al. 2001
MACRO	Pesticide registration	1-D numerical solution of Richards equation coupled to kinematic flow equation	1-D numerical solution of the Convection Dispersion equation coupled to mass-flow equation for macropores	Larsbo and Jarvis 2003
GeoPEARL/EuroPEARL	Pesticide vulnerability mapping	Quasi-3-D numerical solution of Richards equation	Quasi-3-D (ditto) numerical solution of the Convection Dispersion equation	Tiktak et al. 2002; Tiktak, Van der Linden and Boesten 2003
GROWSAFE® Calculator (SPASMO)	Pesticide management for local site and crop conditions	Meta-model of SPASMO. 1-D numerical solution of the simplified capacity model, with account of a mobile water fraction	1-D numerical solution of the simplified convective-transport model	www.growsafe.co.nz; Close et al. 2003
Nutrient management				
WAVE	Field-scale nutrient management / Precision agriculture	1-D numerical solution of Richards equation	1-D numerical solution of the Convection Dispersion equation	Droogers and Bouma 1997; Van Uffelen, Verhagen and Bouma 1997; Van Alphen and Stoorvogel 2001
WAVE	Farm-scale nutrient management	Quasi 3-D numerical solution of the Richards equation coupled to a steady-state flow model for the vadose-zone flow	Quasi-3-D numerical solution of the Convection Dispersion equation coupled to a steady-state transfer function model for the vadose-zone transport	Piñeros-Garcet et al. 2001
WAVE	Nutrient vulnerability mapping	Quasi 3-D numerical solution of the Richards equation	Quasi-3-D numerical solution of the Convection Dispersion equation	Christiaens et al. 1996
SPASMO	Nutrient management and groundwater risk assessment	1-D numerical solution of the simplified capacity model, with account of a mobile water fraction	1-D numerical solution of the simplified convective-transport model	Green et al. 2003; Rosen et al. in press
STONE	Nutrient vulnerability mapping	Quasi-3-D solution of Richards equation	Quasi-3-D numerical solution of CD equation	Wolf et al. 2003

Also nutrient balance models have been used to understand and manage land-based effluent systems in which the effluent is high in nitrogen or phosphorus, such as municipal sewage and dairy shed wash-down (Snow et al. 1999). Trees, as a sink for the effluent, can be used to mop up the nutrients in the effluent (Roygard et al. 2001), and models are used to predict the efficacy of the plant system to extract solutes from the effluent and protect receiving waters (Bond, Smith and Ross 1998).

Another application of nutrient fate and transport models at the field scale is the use of these to support site-specific nutrient management, thereby considering explicitly the impact of within-field variability of soil and land use properties on nutrient availability for plants and risks of leaching (Droogers and Bouma 1997; Van Uffelen, Verhagen and Bouma 1997; Van Alphen and Stoorvogel 2001; Lilburne and Webb 2002). In these case studies, detailed information on the within-field variability of soil properties as inferred from detailed soil sampling and soil maps was translated into site-specific susceptibility and vulnerability by means of N fate and transport codes.

At the larger farm scale, N fate and transport models for the soil–root system are coupled with other system models to evaluate alternative farm management strategies. For example Piñeros-Garcet et al. (2001) coupled a soil root-zone N fate and transport model with a simplified subsoil vadose-zone transport model to evaluate the impact of management strategies on the N load to a deep groundwater body at the farm level. The integrated model allowed to predict the N load over a time period of 30 years in terms of different nutrient management measures. In this case, the trend of the estimated N load for the 'status quo' scenario corresponded to the observed trend of nitrate concentration in the considered groundwater body.

Nutrient fate and transport models are also used to assess land management strategies at the regional scale. The availability of more detailed soil, climate and land use databases, together with appropriate information technology, allows us now to fully implement spatially distributed modeling techniques to make regional assessments of nutrient management strategies. Examples are given by Styczen and Storm (1993), Christiaens et al. (1996), Groenendijk and Boers (1999), Pudenz and Nützmann (1999), Brenner et al. (1999), Birkinshaw and Ewen (2000) and Webb, Lilburne and Francis (2001).

Pesticide management studies

As with nutrient management models, pesticide fate and transport models were first used in a purely academic context to elucidate the role of different soil and crop processes on pesticide behavior in the soil–crop continuum and the validation of flow and transport theories in this context. Examples of validation and model intercomparison of flow and transport models for pesticide fate are given by Styczen (1995), Thorsen et al. (1998), Vanclooster et al. (2000), and Close et al. (2003). An example of the use of pesticide fate and transport models to support field-scale pesticide management is given by Green et al. (2002) who used the SPASMO model (Close et al. 2003; Rosen et al. in press) to develop a leaching calculator so that pesticide choices can be made by growers to minimize the risk of both leaching and soil build-up under their specific conditions. The resulting tool, a meta-model called the GROWSAFE Calculator (www.growsafe.co.nz), provides a ranking of the leaching risk and potential for soil build-up, of those pesticides used in normal 'spray diary' practice in the growing of a range of 30 crops across 15 regions of New Zealand. The GROWSAFE Calculator uses a database of 130 pesticides (herbicides, fungicides and insecticides) plus data on 150 New Zealand soils, and the SPASMO simulations were run using 30-year records of daily weather collected in each of the regions. Another example of the use of pesticide fate and transport models to support field-scale pesticide management is given by Van Alphen and Stoorvogel (2001), who illustrate the use of a pesticide fate and transport model within a precision agriculture context.

Pesticide management studies at regional level are developed in the framework of pesticide authorization and the evaluation of policy plans. The main objective of pesticide authorization is to guarantee that individual PPPs have no harmful effects on human and animal health and no unacceptable effects on the environment. The key legal instrument at the European level is Council Directive 91/414/EEC concerning the placing on the market of PPPs (hence in the spirit of prevention at source). Strategic objectives of policy action plans include reduction of the dependency of the agricultural sector on pesticides and reduction of the emission of pesticides to groundwater bodies, surface water bodies and non-agricultural soil and the air. Examples of such policy action plans at the European level include the thematic strategy on the sustainable use of pesticides, which is part of the 6th Environmental Action Programme of the European Union. Moreover, the Water Frame Directive requires the reduction of concentrations in surface water and groundwater bodies to levels below Maximum Tolerable Concentrations (MTR values). With regards to pesticides, the present limit value (0.1 $\mu g\ L^{-1}$) in authorization is also considered the Maximum Tolerable Concentration for defining good groundwater status.

Authorization requirements at the European level led to the implementation of uniform principles for assessing the risks associated with the use of PPPs, supporting a harmonized registration. Predicting the environmental concentrations of pesticides by means of mathematical models is an essential part of such a risk assessment. To implement specific guidelines within such a context, the European Commission set up the FOrum for the Co-ordination of pesticide fate models and their USe (FOCUS). FOCUS has published general guidance documents and reports on the use of pesticide fate and transport models for Predicting Environmental Concentrations (PECs) in groundwater, surface water and soil (e.g. FOCUS 1995). A limited number of standardized worst-case scenarios for PEC calculations for groundwater and surface waters, together with guidance on selection of models, parameters, and scenarios recently became available (FOCUS 2000; 2001). Standardized scenarios are needed because they increase the uniformity of the regulatory evaluation process by minimizing the influence of the person that performs the PEC groundwater calculation. Standardized scenarios make PEC calculations and their interpretation much easier for administrators, regulators and industry (Boesten et al. 1999). A critical review of the models and scenarios used in this context is given by Vanclooster et al. (2003b; 2003a). They first proposed improvements of the pesticide-leaching models that are currently considered in this context, especially for the description of preferential flow and volatilization. They further improved the validation status of the selected models by comparing model calculations with data collected in high quality field studies. They finally made a critical assessment on the representativity of the proposed scenarios for European agricultural conditions and made some suggestions for higher tier assessments.

Also for national pesticide registration, models are being used for leaching assessments in a number of EU countries (Boesten et al. 1999). As an example, we discuss here the procedure that is currently being developed for leaching assessment for registration in The Netherlands (Van der Linden et al. 2004). In general, decision-making processes for pesticide leaching require stepwise approaches in which models are used to trigger requests for further information if the margin of safety between the estimated leaching and the regulatory upper limit is too small (going from simple and conservative approaches to more sophisticated and less conservative approaches). This is also the case in the Dutch procedure, which consists of the following steps: (i) calculate leaching at 1 m depth for the relevant crop and application using the PEARL model and the Kremsmünster scenario developed by FOCUS (2000); (ii) calculate the spatial 90th percentile leaching concentration at 1 m depth for the relevant crop and application for the whole area of use in The Netherlands using the GeoPEARL model; (iii) assess results of field or lysimeter leaching experiments (using the PEARL model for interpretation); (iv) assess results of monitoring studies in shallow groundwater; (v) assess the possible effect of degradation in the water-saturated zone; (vi) assess results of monitoring studies in deep groundwater. The basic principle is to exhaust all modeling possibilities before requiring additional experimental data because modeling studies are usually much cheaper than experimental studies. This principle is followed by using the GeoPEARL model which uses all relevant Dutch information as much as possible. GeoPEARL combines the PEARL model with geographical information about land use (based on satellite images available at a 25x25 m^2 resolution), soil profiles (based on the national soil database), meteorological conditions, groundwater depth etc. (Tiktak, Van der Linden and Boesten 2003). Note that the SWAP model is embedded within PEARL as the submodel for water flow. GeoPEARL is made accessible via a user-friendly interface in which the user has to specify only (i) the crop, (ii) the application time and dose, and (iii) basic properties of the pesticide such as half-life in soil, sorption coefficient, vapor pressure etc. Also combinations of crops are possible (relevant if the pesticide has to be registered for such a combination). Based on this, GeoPEARL calculates the 90th percentile in space (using a median value in time) for the intended area of use. GeoPEARL needs typically runs for 200 plots to obtain a 90th percentile value that is sufficiently accurate. Thus use of a sophisticated unsaturated-zone modeling tool such as GeoPEARL enables management of differentiation between crops in Dutch pesticide registration. Results from GeoPEARL will also be used in the Dutch National Environmental Indicator for Pesticides. This indicator is currently being developed to evaluate the Dutch governmental policy with respect to pesticide emissions over the period 1998-2010 (Deneer et al. 2003).

Strengths of flow and transport modeling in nutrient and pesticide management

Flow and transport modeling can be used to define suitable management options respecting a set of predefined criteria and conditions, as illustrated in the examples above. The power of modeling lies in its potential to simulate possible system responses in terms of some predefined scenarios, thereby answering typical ‘what-if’ questions. In the context of nutrient and pesticide management, a stakeholder will have the possibility to combine a given model with a given modeling scenario to generate plausible system responses. The availability of modeling data at the field, farm and regional scale makes it possible to make such assessments at different scales, thereby considering explicitly the spatio-temporal dynamics of the soil and subsoil properties, land use and climate systems, and farm management. The adoption of mechanistic and physically based models also allows such assessments to be made based on current scientific knowledge of the behavior of the system, and subject to basic physical, chemical and biological laws.

Limitations of flow and transport modeling in nutrient and pesticide management

Different drawbacks and limitations with the current approaches can be formulated which are related to the conceptual problems in the present modeling codes, problems of parameter and input estimation, problems related to an appropriate model use, interpretation of the modeling results – in brief good modeling experience and practice – and problems with the coupling of flow and transport models in integrated management tools

Conceptual modeling error

Although easily established from a conceptual point of view, it is important to realize that the governing flow and transport equations (1) and (2) rely on a series of simplifying assumptions such as i) the existence of a Representative Elementary Volume; ii) Darcy's law is valid for the soil porous system; iii) the osmotic, geostatic and electrochemical gradients in the soil water potential are insignificant; iv) the fluid density is independent of solute concentration and temperature; v) the matrix and fluid compressibilities are small; vi) the effective phenomenological properties like the hydraulic conductivity relationship k(h) can be defined; and vii) equilibrium in water pressures and solute concentrations for a Darcian scale REV. Modeling errors at the conceptual level therefore arise when processes are inappropriately described in the given model or when process descriptions are used in an application for which they were not initially conceived. The ignorance of preferential flow for instance is a major point of concern. This is a process for which a consensus exists that it is extremely relevant for describing nutrient and pesticide transport in soils (Flühler et al. 2001), yet in many nutrient and pesticide management models it remains as an example of incomplete conceptualization. The use of a small-scale validated process model to make a regional assessment is another example of model conceptual error (Beven, Schultz and Franks 1999).

Resistance to using preferential-flow models in nutrient and pesticide management has been attributed to the lack of a generally accepted model concept and the lack of robust techniques that allow prediction of preferential flow. Many preferential-flow models are bedeviled by an excess of parameters that defy measurement (Gerke and Van Genuchten 1993). Preferential-flow models are usually applied in an *a posteriori* parameter identification approach which has so far limited the range of potential applications as a management tool (Flühler et al. 2001). However, the recently developed FOCUS scenarios for pesticide exposure assessments for surface water (FOCUS 2001) represent one example of how preferential-flow models may be used in a management context. The preferential-flow model MACRO (Jarvis et al. 1997) is used to calculate pesticide inputs to surface water by subsurface drainage systems for six scenarios representative of drained land in the EU. Four of these scenarios are pre-calibrated, for example with respect to site hydrology and non-reactive solute transport, which should considerably reduce the inherent predictive uncertainty when using preferential-flow models.

The evaluation of conceptual errors in the flow and transport components of nutrient and pesticide management models is cumbersome. First, it is difficult to separate in a modeling exercise the input and parameter estimation errors from the conceptual model errors. Secondly, the observation of the 'facts' will always be limited in space and time, as compared to the number of processes and scenarios for which we would like to apply the models. Indeed, when analysing the residuals between observed system response and modeled system response, the structural model error will be lumped with parameter estimation error and observational error. Supposing that measurements are free of errors, a series of different parameter sets may lead to similar model performance, which is the core of the equifinality problem (Beven, Schultz and Franks 1999). Non-uniqueness of parameters is typically observed in inverse modeling studies and will therefore complicate the identification of conceptual errors. But even if we were able to separate appropriately model and parameter errors, the evaluation of conceptual model errors would still be complicated by the problem of scale (Beven, Schultz and Franks 1999). Indeed, the number of cases on which the theories and models can be tested will always be far fewer than the number of cases for which the models will potentially be used in a management exercise.

For pesticide leaching, the number of validation studies such as presented by Thorsen et al. (1998) and Vanclooster et al. (2000) will always be very limited as compared to the number of potential chemicals that need to be evaluated in a given environmental setting. Also, many validation studies were previously carried out in soils that were considered vulnerable, i.e. in sandy soils. This is an important limitation for large-scale model exercises, as processes in fine-textured soils like preferential flow were ignored (Tiktak et al. 2002). The scale problem further implies that the fate of each chemical in an environmental condition is unique. This also explains why transport models often perform badly in a purely predictive blind validation mode, as illustrated by Gottesbüren et al. (2000) and Trevisan, Van der Linden and Boesten (2003). Such poor performance would justify the recalibration or testing of transport models when applying them *ab initio* to new sites. However, the need for *a posteriori* recalibration would seriously restrict the use of the model in a pure extrapolation and, hence, a nutrient and pesticide management mode.

Addiscott (2003) recently provided a sagacious assessment of the potential and limitations of modeling. He cautions that modeling has a rather limited future potential unless there is a clear understanding of the limitations attached to the use of models. In discussing models, their validation and parameterization, Addiscott stresses that we need to ask first how science actually happens. Science progresses through an inductive process, which Karl Popper formalized as the hypothetico-deductive system. Popper (1992) noted that "we can never justify a theory", or therefore a model. So while we might be able to discriminate between models, we can never validate a model in the sense of proving it is entirely right (Addiscott 2003). Thus because no procedure can prove a model works, as both Popper (1992) and Addiscott (2003) lament, we have to live with understanding the bounds of the uncertainty in our predictions.

The parameter estimation problem

Extensive literature is now available to illustrate the often large variability in space and time of the material properties affecting nutrient and pesticide transport in soils. The variability is present at different spatial scales ranging from the pore scale (Cislerova 1999), the core scale (Vanderborght et al. 1999), the field scale (Mallants, Vanclooster and Feyen 1996; Jacques et al. 1998; Ritsema, Dekker and Nieber 1998; Hupet and Vanclooster 2002), to the landscape and regional scales (Roth et al. 1999). The temporal variability of material properties has often been ignored but is also clearly present. The impact of mechanical stress on the soil hydraulic properties is well illustrated in the literature (e.g. Roth et al. 1999). However, other factors may also cause temporal variability in transport characteristics. Moutier, Degand and De

Backer (1999) and Toride (1999), for instance, illustrated the temporal change of the unsaturated hydraulic properties as a function of water quality parameters. Vanderborght et al. (1997) and Javaux and Vanclooster (2003) illustrated the temporal variability of the solute dispersion length in terms of the governing flow regime. Input and parameter generation problems arise when modeling data are not available to deal with the extreme spatio-temporal variability of the system within the management application exercise.

Despite the difficulty of spatio-temporal variability in the key properties that determine flow and transport through soil, new measurement technologies are being developed to provide direct measures of the parameters required for modeling nutrient and pesticide transport through field soils. The hydraulic properties of topsoil can be measured, reasonably easily, *in situ*, using disc permeameters, or as they might be known 'tension infiltrometers' (Perroux and White 1988). With these devices, the spatial and temporal changes in the topsoil's transport properties can be quickly resolved (Messing and Jarvis 1993). Furthermore, using tracers in disc permeameters, the preferential-flow properties of the mobile water fraction in structured soils can now be resolved (Clothier, Kirkham and McLean 1992; Jaynes, Logsdon and Horton 1995) to provide direct parameter input into preferential-flow models (Jarvis et al. 1997). By using multiple tracers, including reactive compounds, the adsorption isotherm of invading solutes that exchange with the soil's matrix can now be determined (Clothier et al. 1996). Measurement technologies for direct parameterization of the soil's hydraulic and transport properties are now available, albeit there is a certain degree of effort required to establish the spatio-temporal pattern in these parameters at the pedon scale.

At the regional scale, other means of parameterization are required. A typical example is the evaluation of large-scale non-point source pollution with spatially distributed modeling approaches, which very often rely on the availability of the soil's physico-chemical properties at the scale of each grid of a constructed soil information system. Unfortunately, only limited hard data are available in most soil information systems. Grid-scale modeling parameters need to be generated by interpolation, extrapolation, geo-statistics, pedo-transfer functions and the like. In such up-scaling procedures, one is confronted with the core of the scale problem, i.e. the uniqueness in time and space of a transport event and the non-linearity of the transport process. Indeed, each nutrient and pesticide transport event is unique in place and time and a perfect repetition of this event can never occur. Hence, a model inferred from an observation in a given space and time framework can never be tested since this observation is unique. The non-linearity of the transport process further suggests that the transport parameters cannot simply be averaged at the grid or time step scale.

Another aspect of data availability is related to the definition of the scenarios that will be used in a management exercise. Due to limited computing and data resources, the model will only be calculated for a limited series of 'sensitive' scenarios which, in comparison with what may occur in reality, will only yield a small sample of possible behaviors. An example is the use of scenario analysis with a pesticide-leaching model as support for the lower-tier registration of PPPs in Europe (FOCUS 1995; 2000). Boesten et al. (1999) proposed 9 'worst-case scenarios' in a first-level screening of the risk of pesticide leaching to groundwater at the pan-European scale to represent a nearly infinite number of potential scenarios. The definition of the parameters of these 9 'worst-case scenarios' was largely based on expert judgment. Hence, from a statistical point of view, it is difficult to evaluate if this limited sample will be an unbiased sample of the unknown population of 'worst-case scenarios' (Vanclooster et al. 2003b).

Model user experience and good modeling practice

A lack of good modeling practice restrains the advanced use of modeling for soil management. In the past, most modeling work was performed within an academic context. The modeling codes were often poorly documented and limited in pre- and post-processing capabilities. The lack of appropriate interfacing and advanced pre- and post-processing capabilities introduced an additional and often insurmountable burden for the soil manager. The complexity of the modeling process and the lack of operational modeling guidelines further hamper the introduction of advanced transport codes in operational nutrient and pesticide management. This also introduces an additional risk of modeling error due to user subjectivity, as was clearly illustrated by Brown et al. (1996) Jarvis, Brown and Granitza (Jarvis, Brown and Granitza 2000) and Boesten (2000). Boesten (2000) compared the estimation of the pesticide half life at 10°C of ethoprophos and bentazone as estimated by 20 model users using a common laboratory degradation study at reference temperature. The coefficients of variation of estimated half life were 29% and 46 % for ethoprophos and bentazone, respectively. The principal cause of this important user-subjective variability was the lack of guidance on the transformation rate dependency on soil temperature. Brown et al. (1996) compared the outputs from three models operated by five modelers. Differences between the output data from the five modelers using the same model were of a similar magnitude to the variation associated with field measurements. They concluded that model development should seek to reduce subjectivity in the selection of input parameters and improve the guidance available to users where subjectivity cannot be eliminated.

Coupling of flow and transport models in integrated nutrient and pesticide management models

As suggested above, nutrient and pesticide management models are holistic and transport models must be coupled to other components describing the behavior of complete agro-systems. Such coupling may suffer from a series of inconsistencies and incompatibilities, which is a typical problem when dealing with integrated system models. Indeed, the different submodels of holistic nutrient and pesticide models are traditionally developed by different scientific communities. Soil nutrient turnover models tend to be developed by soil biologists and chemists, with nutrient uptake models built by crop physiologists, and the nutrient management schemes created by general agronomists, with transport modules developed by soil physicists. Each community has its own standards and reference methods which may result in different notions of agro-system analysis, different traditions and methods in numerical modeling, and different scales of conceptualization and model implementation. As an example, the representative volume for which macroscopic soil flow and transport equations are developed is of the order of magnitude of $10^{-3} – 10^{0}$ m^3, corresponding to the scale at which soil properties can still be characterized. The representative volume for which crop growth components in agro-system models are developed is typically of the order of 10^2 m^3, corresponding to an ensemble of crop plants. This scale discrepancy between reference crop growth models and soil flow and transport models makes this coupling a difficult task.

Opportunities for flow and transport modeling in nutrient and pesticide management

Improved knowledge of the transport process and process description in current nutrient and pesticide management models

Much to the chagrin of soil scientists, convective flow through and diffusion within field soils do not behave in the uniform and isotropic way that their models demand. Rather, soil structure in the form of either aggregates, cracks or bio-pores, serves to create an apparently chaotic flow regime that is rapid and far-reaching. Better observations of this preferential flow, made by means of new techniques such as soil tomography, dye tracing and hydro-geophysics such as TDR or GPR (Lambot et al. 2003), will lead to better understanding of the processes and patterns of preferential flow (Clothier 2002). This knowledge might even lead us to develop alternative schemes for describing by-pass flow, such as network models (Deurer et al. 2003).

Roots are the big movers of water and chemicals in soil (Clothier and Green 1997). In a landmark paper, Gardner (1960) modeled capillary flow to a single root using a simplified cylindrical co-ordinate system. This paper was referenced in over 200 publications between 1960 and 1985, and Wilford Gardner thought it was "… so frequently cited because the approach is essentially the same that all computer models now follow". However Gardner (1985) lamented that "… while this was probably a useful start, I think it has eventually led us to a dead end!". Green et al. (2002) used an intensive array of 60 TDR wave guides around an apple tree to determine the spatio-temporal patterns of root water uptake, and they were able to model these patterns using the scheme of Feddes, Kowalik and Zaradny (1978) for root water uptake. Green et al. (2003) concluded that the measurement-modeling dualism will ultimately improve our ability to predict the fate of surface applied water and nutrients. However, Hupet et al. (2003) sound a cautionary note for those who would seek to use inverse modeling to infer root water-uptake parameters for models. They noted that this was not feasible for medium- to fine-textured soils due to the compensating effect of vertical unsaturated water flows. They concluded that the feasibility of estimating root water-uptake parameters was improved if it was carried out simultaneously with optimization of other parameters. This will of course invoke the spectre of Beven's equifinality!

Improved methods for local-scale model input and parameter estimation

As noted above, the lack of acceptable and reliable indirect methods for estimating model parameters that cannot easily be measured hampers the widespread adoption of flow models in the policy and management arena. Inverse modeling techniques may prove useful in estimating flow and transport parameters, but the data requirements for a well-posed solution may not always be fulfilled. Using an advanced global search algorithm, Lambot et al. (2002) studied the conditions where a global optimum for single-domain unsaturated flow parameters can be obtained from transient flow experiments in soil columns using only soil moisture data. They showed that a global estimation of the hydraulic properties was sensitive to measurements of soil moisture close to the column boundaries. Hence, if such data can be collected, then soil hydraulic properties can be retrieved from soil moisture time series collected during a transient flow experiment. These theoretical considerations were experimentally validated for sandy and sandy loam soils by Lambot et al. (2004) and for volcanic soils by Ritter et al. (in press). For dual porosity models, Schwartz et al. (2000) encountered difficulties in obtaining physically realistic parameter estimates using bromide breakthrough curves measured in a variably charged tropical soil, where the Br^- ion could be considered as a weakly sorbed reactive solute. In contrast, Kätterer et al. (2001) used a global search method (SUFI, Abbaspour et al. 1997) to estimate the parameters of a dual-permeability model using column breakthrough experiments for multiple non-reactive tracers (deuterium, bromide and chloride) and two soil-indigenous solutes (sulfate and nitrate). The model parameters were first estimated from effluent breakthrough curves for bromide and chloride, where bromide was applied at the surface, and chloride was injected at 5 cm depth in the soil columns, and then successfully validated by comparing model predictions against the elution curves of deuterium, sulfate and nitrate and the resident concentration profiles of four of the solutes in the columns. Using generated data, Roulier and Jarvis (2003a) confirmed the crucial role of data quantity and quality in determining the likelihood of achieving reliable inverse parameter estimation for dual-permeability pesticide-leaching models, and proposed a methodology for micro-lysimeter experiments based on the SUFI program (Abbaspour et al. 1997). Roulier and Jarvis (2003b) successfully applied this methodology to breakthrough experiments for a tracer and the herbicide MCPA carried out in a macroporous loamy soil. Despite an acceptable model performance, significant uncertainties remained for key parameters controlling macropore flow, even after calibration. It was suggested that the posterior uncertainty ranges could have been reduced with a more exhaustive sampling of the parameter space and improved experimental designs.

Improving pedotransfer functions

Notwithstanding the availability of soil data in soil information systems, there is still a gap between the parameters that are needed in physically based chemical-transport models, and the parameters available in the soil data bases. Pedotransfer functions allow us to bridge this gap by translating the basic soil data into functional data. Most available pedotransfer functions, however, have been developed using data from small-scale samples. Given the scaling problem, it would be unsound to consider a pedotransfer approach as a way to obtain effective functional model parameters of, for example, a grid in a spatially distributed model. The role of pedotransfer functions is not to give an exact effective parameter, but rather to generate a realistic *a priori* parameter that constrains the parameter space in a more generic Bayesian type parameter estimation framework. Many pedotransfer functions have been described in the literature. Good reviews of the use of pedotransfer functions in hydrology are given by Pachepsky, Rawls and Timlin (1999) and in a series of papers in Van Genuchten, Leij and Wu (1999).

For the hydrological component of the transport codes (Eq. (1)), a series of well-performing approaches exist to estimate the matrix hydraulic properties such as the moisture retention and hydraulic conductivity relationships. Several empirical and quasi-physical methods exist, but the vast majority of these methods are empirical, and are based on linear-regression models, non-linear-regression models or even artificial neural networks (e.g. Schaap and Bouten 1996). However, these approaches are not appropriate for well-structured soils. In general, structure is much less well quantified in soil data bases, and therefore considerably more difficult to account for in a pedotransfer approach (Jarvis et al. 1999). In dual-porosity models, the matrix and macropore hydraulic properties need to be predicted. Whereas the saturated conductivity of the matrix can likely be predicted by a pore size distribution model (Jarvis et al. 1999) or from soil texture (e.g. Smettem and Bristow 1999; Jarvis et al.

2002), the saturated conductivity of the complete soil, including the macropores, is best predicted using pedotransfer functions based either on field survey descriptions of soil structure or measurements of drainable or effective porosity (Rawls, Brakensiek and Logsdon 1993; 1996; Jarvis et al. 1997; Rawls, Pachepsky and Lin 2001), but concern should be raised about the robustness of these procedures.

In principle, the strength of macropore flow should be regulated by soil structural development, but this is a difficult concept to quantify. However, the few studies published in the literature that have attempted to relate leaching characteristics to observed soil structure have met with some success. For example, early work on aggregated fine-textured soils showed that strongly developed structures resulted in more pronounced macro-pore flow than weaker structures (Anderson and Bouma 1977). In field dye-tracing studies, marked preferential flow behavior was found in thirteen out of fourteen Swiss agricultural soils and the observed flow patterns were shown to be, at least qualitatively, strongly correlated with the texture and visible structural development in individual horizons and profiles (Flury et al. 1994). Shaw et al. (2000) developed simple estimation routines for the parameters of the mobile–immobile dual-porosity model (MIM) model based on clay content, cation exchange capacity, and the size of structural units. Similarly, Gonçalves, Leij and Schaap (2001) developed neural-network pedotransfer functions for the parameters of the MIM model for structured clay soils in Portugal based on soil water retention and hydraulic-conductivity parameters. The MIM concept is, however, limited in its applicability to field conditions, and no suitable parameter estimation routines are available for parameters in more state-of-the-art dual-permeability models. However, in one preliminary study, Roulier and Jarvis (2003b) showed that mass exchange coefficients of loamy soils estimated from transient tracer experiments in micro-lysimeters sampled at three landscape positions could be qualitatively related to basic soil properties such as the clay and organic-matter contents.

In contrast to the extensive literature available on pedotransfer functions for the soil hydraulic properties, less work has been carried out to develop pedotransfer functions for the solute transport properties of Eq. (2), or other chemical-transport models. This is a little surprising since the flow properties will directly influence the solute transport, so that tracer studies yield direct information on the effective flow behavior in soil. This is partially due to a lack of appropriate measuring techniques, which makes the characterization of chemical transport in soils a difficult task. However, recent advances in chemical tracing with techniques such as TDR (Kachanoski, Pringle and Ward 1992; Vanclooster et al. 1995; Vogeler, Clothier and Green 1997; Gaur et al. 2003), dye tracing (Gähwiller et al. 1999), or the use of anionic tracers (Clothier, Kirkham and McLean 1992), now allow us to quantify solute transport at the field scale with a high spatial and temporal resolution. It also allows the exploration of the relationships existing between macroscopic water flow and solute transport. In this way, we can infer solute transport properties from observed flow properties and patterns of tracer infiltration.

Lennartz (1999) showed that the parameters in a convective log-normal transfer function model of solute transport derived from breakthrough experiments carried out on 99 core samples of loamy moraine soil were significantly correlated to soil-textural fractions. Thus, the mean convective transport time for a bromide tracer and the adsorption retardation factor for the herbicide IPU both decreased as the clay content increased, indicating stronger preferential flow and transport in the finer-textured core samples. Perfect, Sukop and Haszler (2002) could explain 50% of the variation in observed solute dispersivity during saturated steady flow through small cores from measured water retention parameters, which in turn could be related to clay content. Roulier and Jarvis (2003b) also inferred larger solute dispersion in the matrix of a loamy soil in columns with larger clay contents. Vanderborght et al. (2001) described a series of tracer experiments carried out in Belgium at the scale of soil monoliths (ca. 1 m^3) under controlled boundary conditions to identify relationships between basic soil properties, flow properties and transport properties. The relationship between the flow and transport velocities was evaluated using the multi-domain transport model of Steenhuis, Parlange and Andreini (1990). In cases where matrix-driven flow was expected, solute properties could be well predicted from the flow properties. However, such predictions did not work at all in cases where preferential flow was expected to occur. Similar conclusions were obtained from field-scale studies. Using matrix based stochastic continuum modeling approaches, Kasteel (1997) and Vanderborght et al. (1997) predicted solute transport from a statistical description of the flow properties at the field scale in a macroporous soil. Although partially successful in the unsaturated range, important underestimations of the solute fluxes were observed when the soil reached saturation such that the macropore domain contributed significantly to chemical transport. Similar problems were reported by Javaux (2004), who predicted water and chemical transport in an unsaturated sandy subsoil.

Scale-dependent modeling approaches

Following the recent developments in hydrology as presented by Beven (1995) and Beven, Schultz and Franks (1999), we propose to use a pragmatic approach. We are of course interested in knowing the functional response of the system, i.e. how nutrients and pesticides will behave at different scales (the field plot, the field, the farm, the region) subject to alternative management practices. Hence, the representation of the large system by means of an ensemble of small-scale modeling systems is one of the many ways for describing the functional response of the system. If the small-scale modeling system is based on governing transport models like Eqs. (1) and (2), it has the merit of being based on physical concepts, since it considers some process knowledge in the modeled system. But this is not necessarily the most appropriate way of conceiving the small-scale process. Similar functional behavior at the small scale could equally well be described with a purely empirical model.

We have accepted a given model formalism for the small-scale processes, such as a solution of Eqs. (1) and (2), and we assume that a spatially distributed model can be constructed. Given the issue of equifinality, it is probably true that a range of parameter sets in the spatially distributed model will yield a similar model performance at the larger scale. If indeed such a functional similarity exists, then we propose to accept this and consider a range of equifinal parameter sets in a predictive (soil management) mode. Hence, we suggest to move towards a stochastic ‘Monte Carlo’ type of modeling approach where a range of plausible functional responses are predicted using a range of equifinal model parameters. Weights to the individual model responses can be assigned in terms of their previous functional behavior, so that statistics on the most likely system response can be generated. However, given the possible large ranges of model parameter sets, important predictive uncertainties will be generated. Still, as more information on the real system behavior is obtained, for instance when monitoring of the system continues, the functional behavior of the different model and parameter sets can be re-evaluated using Bayesian rules, so that inappropriate parameter sets can be rejected. In this case, the uncertainty in the model predictions will be reduced as the model is conditioned on the observed data, and more unlikely modeling parameter sets are rejected.

We may now question in which form we should represent the small-scale processes in a spatially distributed model and whether solutions of equations like Eqs. (1) and (2) are an appropriate basis for modeling large-scale processes. As discussed above, it is likely that no single model, or parameter set can be considered as ‘valid’ for describing small-scale processes in a large-scale management application. However, it could be that the solution of (1) and (2) is one of the valid solutions, one among many others. However, if so, will it also be the most efficient one? Or, in other words, do we start with detailed numerical solutions of Eqs. (1) and (2) if we are indeed faced with a large-scale soil management problem? We can consider the example of the use of pesticide-leaching models to support pesticide registration. Some advanced (and probably also well-performing) numerical process-based pesticide-leaching models based on the solution of Eqs. (1) and (2) are available. However, their use in a European spatially distributed risk management context as illustrated by Tiktak et al. (2004) is limited given the computational burden and the lack of available input data. Therefore, at the pan-European scale, a much ‘simpler’ modeling approach is needed which on the one hand can be parameterized based on the data available in European data bases, but which on the other hand respects as much as possible the functional behavior of the system, and therefore mimics as closely as possible the more detailed process-oriented numerical model.

One way to do this is to perform a model reduction, in which the complex numerical model is synthesized in a meta-model, thereby retaining only the most sensitive parameters that are available in spatial databases. Meta-modeling is a way to develop robust models consistent with the complex system models (Barton 1998). Meta-models were first used in other earth-science modeling disciplines such as global-climate modeling (Bowman, Sacks and Chang 1993) and hydrology (Vanclooster et al. 2002), but were recently also introduced in nutrient and pesticide fate modeling. For example, Bouzaher et al. (1993) presented pesticide meta-models, while Bouzaher et al. (1995) described the use of regression meta-models inside an integrated model of soil degradation and agricultural policies. Akkermans (2000) presented a neural network meta-model to predict nitrate concentrations in water bodies. Børgesen, Djurhuus and Kyllingsbaek (2001) describes a linear-regression meta-model for nitrogen leaching from different soils and with different irrigation, climate and farm types. Piñeros-Garcet et al. (2003) described a meta-model for the EuroPEARL model of Tiktak et al. (2004) to assess the validity of the EU FOCUS modeling scenarios (FOCUS 2000), thereby incorporating the uncertainty in modeling data. The GROWSAFE Calculator that can be used by growers to improve their selection of pesticides so as to match their local conditions, is a meta-model of the detailed SPASMO model of water and chemical movement through soil of Green et al. (2003).

In any of these modeling approaches, whether it is now an empirically based meta-model or a physically based reduced model, it is indicative that most model parameters or proxies of them can be identified at the scale of interest. In the case of the EuroPEARL meta-model (Piñeros-Garcet et al. 2003), most parameters were identified directly from the European soil map and associated soil data base (Jamagne et al. 1994). The remaining unknown model parameters were calibrated using simulations of the EuroPEARL model. Calibrating against a more detailed numerical model, rather than against real data, adds additional uncertainty to the original model. However, given the existence of previous validation studies of the detailed numerical model, this uncertainty can be quantified. Calibration of the model using real-world data is currently impossible since reference data on groundwater quality at the pan-European scale are not available. However, it is expected that the implementation of a groundwater-monitoring network in the context of the Water Framework Directive will yield the necessary data, which will allow effective model calibration in the future. In this case, effective model parameters will be upgraded and conditioned to new observations, thereby reducing the uncertainty in the modeling predictions (Freer, Beven and Ambroise 1996).

Therefore, it is of paramount importance to invest in environmental measurement and monitoring, and not just model development. Current information technology allows the storage and representation of remote data related to non-point-source pollution. Yet still, there is a strong need to improve the quality of the large-scale data sets. Particular attention should be paid to remote-sensing technology which, by definition, has the capability to monitor environmental variables at the larger scale. Satellite remote-sensing techniques are now available to characterize land cover and land use, drainage patterns and topography, surface temperature, snow and surface soil moisture. But most of these techniques only sample the soil at the surface, while chemical transport in soils is significantly affected by what happens deeper in the soil profile. Hence, methods need to be developed which allow characterization and monitoring of the subsoil at larger scales. In a recent study, Hoeben and Troch (2000) showed how information on subsoil moisture profiles could be inferred from radar images using a data assimilation framework. Similar information can be obtained by using new applied geophysical techniques such as subsurface resistivity measurements (Kemna et al. 2002) or ground-penetrating radar tomography (Annan 2002; Huisman et al. 2003; Lambot et al. 2003). However, more research is still needed to improve the interpretation of the signature of these devices in terms of transport properties of soils.

Development of good modeling practice guidelines

The appropriate use of transport models in nutrient and pesticide management is only possible if the different actors in the soil management process receive appropriate training. Often the surprisingly poor modeling leads to a user inter-comparison ring test (e.g. Boesten 2000), which clearly elucidates the need for advanced education and training in chemical-transport modeling, as well as the implementation of strict guidelines for good modeling practice. The model user is responsible for understanding the model and its appropriate use. He is also responsible for estimating the model parameters and the input for the selected scenarios. He must further keep in touch with the evolution of the different model versions and documentation. He is further responsible for developing modeling reports that contain sufficient and reliable information. Most of the state-of-the-art modeling approaches are developed by the research community and need to be disseminated to soil professionals. In many cases, a tremendous gap still exists between models available in the research community and those used in management applications. However, some progress is being made. The FOCUS modeling tools and scenarios developed for EU-harmonized pesticide registration (FOCUS 2000; 2001) represent a good example of how this gap can be bridged. Models originally developed in the research arena have been equipped with user-friendly interfaces to improve their usability for this specific purpose. Therefore a plea is made to upgrade existing scientific models further into useful engineering tools, to improve the training of the potential model user, and to implement strictly the concepts of 'Good Modeling Practice' (Van

Genuchten et al. 1999). The latter idea is to make the modeling process completely transparent by documenting each step of the modeling process such that it can be independently executed by any other model user (Van Waveren et al. 1999).

The future

For the immediate future, enhanced knowledge will arise first through interpretation of the improved observations that we will obtain using new and developing technologies. Despite impressive software developments in modeling, we are still in a period of data-led discovery. From the breadth of this new information, we will then be able to use the comprehensive modeling schemes to deepen our understanding of the exchange and transport processes and of the pathways of water flow and the fate of chemicals in the terrestrial environment. Tools and models together will be the key. Improvements in our ability to describe mathematically the dynamics of the linked underlying mechanisms demand that we can parameterize these quantitative representations, in order that the models be run appropriately. So, as we develop more sophisticated codes, we must have better means of observing and monitoring processes in the field so that these schemes can be aptly parameterized, and the predictive results corroborated.

The models that we will develop to enhance our understanding of chemical transport, fate and exposure in the environment will come under critical scrutiny not only from fellow scientists, but also from policymakers and regulators. This will generate non-scientific challenges that must be tackled.

Corwin, Loague and Ellsworth (1998) considered that "… even though policymakers and environmental modelers are converging, the policy-making process is clearly about politics. Models used in this realm are most likely to be applied as political weapons, not unbiased tools. The notion that science and technology will mitigate environmental problems on a 'truth wins' basis is probably illusory".

Nonetheless, scientists need to participate actively in dialogue with policy analysts, politicians, economists, sociologists and the agricultural industry, so that sustainable outcomes are achieved for nutrient and pesticide management. The scientists' observations, along with their flow and transport models will be key tools in these discussions, as well as in the implementation and verification of sustainable practices.

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