NATIONWIDE ASSESSMENTS OF NON-POINT SOURCE POLLUTION WITH FIELD-SCALE DEVELOPED MODELS: THE PESTICIDE CASE[1]

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Abstract

The use of nationwide models of non-point source pollutants in soils is now common practice. Most of these models have originally been developed at the field-scale. An integrated approach (a 'research chain') is presented, and applied to the modelling of pesticide leaching in the Netherlands. The research chain consists of five steps, i.e. (i) problem definition, selection of model approach and model building, (ii) application of the model to a number of field-plots, (iii) scale transfer, including process aggregation and data aggregation, (iv) regional-scale model application, and (v) analysis and presentation of results. It was shown that some of the steps of the research chain could not be completely carried out. In this particular study, regional-scale model validation and uncertainty analysis were hampered by lack of data. Probably the most important part of the research chain is the phase of scale transfer. It was shown that in the pesticide leaching study data aggregation was more appropriate than process aggregation (model simplification). Data were aggregated by stratifying the input-data and by setting up procedures in which specific model-inputs were derived from generally available data sources.

Key words: Regional-scale modelling; Pesticides; Research chain; Data aggregation; Process aggregation; PEARL.

1 INTRODUCTION

Because of their widespread occurrence and potential chronic health effects, non-point source pollutants have become a focal point of attention world-wide. Problems that receive particular attention are pesticide, nitrate and phosphate losses to surface- and groundwaters, and heavy-metal accumulation in soils. To prevent further build-up of these pollutants in soils and waters, policy makers need information about the current state of the environment and the response to reduced pollutant loads. Dynamic simulation models are indispensable tools in making quantitative predictions.

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[1] To be referred to as follows: Tiktak, A., J.J.T.I. Boesten, and A.M.A. van der Linden. 2002. Nationwide assessments of non-point source pollution with field-scale developed models: The pesticide case. In: G.J. Hunter and K. Lowell (eds). Proceedings of the 5th international symposium on spatial accuracy assessment (Accuracy 2002). Melbourne, July 2002, pp. 17-30.

Most models for simulating the fate of non-point source pollutants in soils have originally been developed for field-plots. The reason is that often at this scale, direct measurements of model inputs and time-series to evaluate model performance are available (Van Grinsven et al., 1995). Due to the ubiquitous nature of non-point source pollutants, decision makers are usually not satisfied with results from a model application at a specific plot, but rather are interested in larger scale model applications. This is, however, not without risk. The field experiments may not cover the full range of conditions encountered at the regional-scale, so that important processes are overlooked. Also, the effect of data-aggregation and the use of pedotransfer functions on the final model results cannot be tested by applying the model to field plots only.

To avoid these problems, an integrated approach (a 'research chain') is advocated when applying or developing models. A research chain consists of a number of research steps to be taken when developing models (Bouma et al., 1998). The general set-up of a research chain for developing non-point source pollutants in soils will be shortly presented. The major objective of this paper is to review the applicability of the research chain to the modelling of pesticide leaching to surface- and groundwaters with the PEARL model (Tiktak et al., 1996; 2002). The paper focuses on the effects associated with scale transfer by process aggregation (model simplification) and data aggregation.

2 THE RESEARCH CHAIN

Both De Vries et al. (1998) and Tiktak (1999) published an integrated approach for developing regional-scale models of non-point source pollutants in soils. This procedure consists of the following major steps (figure 1):

1 *Problem definition, selection of model approach and model building.*
Not enough time is being spent in many projects on problem definition and interaction with stakeholders (Bouma et al., 1998). The proper modelling approach is a compromise between practical issues such as the aim of the model and the associated temporal and spatial resolution of the model outputs, and theoretical issues, which are governed by the inherent nature of the system to be modelled. Testability of the model concepts often requires that a comprehensive model is developed, which can be applied to intensively monitored field-sites.

2 *Application of the model to the field-scale.*
During this stage of the research chain, the model is applied to a broad range of field-studies. The primary reason for performing this step is to evaluate the model concepts (i.e. model validation in weak sense cf. Leijnse and Hassanizadeh, 1994). This step includes a sensitivity analysis to determine the most important model parameters.

3 *Scale transfer.*
This is the central step in developing regional-scale models. Both process aggregation and data aggregation may be carried out. Possible simplifications are: (i) the reduction of temporal resolution, (ii) reduction in vertical resolution, (iii) reduction of spatial resolution, and (iv) exclusion of processes that are not relevant. Data can be further aggregated by organising the data in such a way that specific model inputs can be derived from generally available data sources. It is clear

that the number of model inputs that cannot be directly or indirectly obtained from measurements should be minimised.

4 *Regional-scale model applications.*
In this step, the model is compared with data from national monitoring networks. During the field-scale model applications, the conceptual part of the model was evaluated. For a model to have predictive abilities, however, this is not enough. It is also required to have a good knowledge of the boundary conditions, parameter values and their spatial and temporal variation for the system to be modelled (validation in a strong sense cf. Leijnse and Hassanizadeh, 1994). It is therefore important to evaluate the model at its final scale of application.

5 *Analysis and presentation of results.*
All environmental model assessments are laced with uncertainty (Loague and Corwin, 1996). It is important that this uncertainty is communicated to decision makers, who may make a wrong decision based on a single model calculation. Also, the underlying model concepts, model limitations and possible alternative approaches should be communicated.

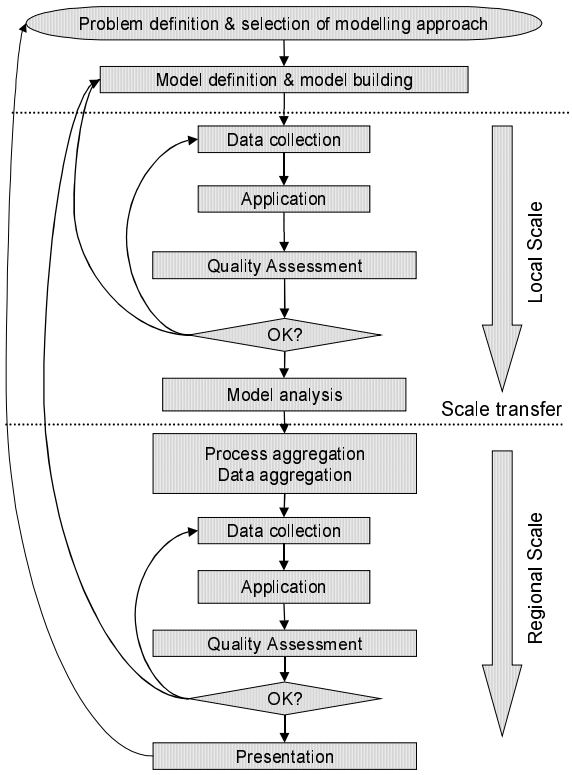

Figure 1. Diagram showing the sequence of research steps ('research chain') to be followed when calculating non-point source pollution on a regional-scale. After Tiktak (1999).

Figure 1 contains a number of backward lines. Regional-scale model applications should not be considered end-products, but should be considered as part of an ongoing process. To prevent obsolete model applications, stakeholders must be prepared to continuously invest in further model development, data-collection and basic research.

3 MODELLING PESTICIDE LEACHING AT A NATIONWIDE SCALE

In this section, the research chain approach is applied to the modelling of pesticide leaching at a regional-scale in the Netherlands. Particular attention will be given to the selection of a proper model approach, scale-transfer and model evaluation.

3.1 Problem definition and selection of model approach

The leaching of pesticides has become a focal point of attention in the Dutch Decision Tree on pesticide registration (Brouwer et al., 1994). One of the considerations is to protect the groundwater as a source of drinking water. As the extracted water is a mixture of many years, it is more preferable to protect a large area on long-term, than a small area against peak concentrations. These considerations have led to the development of a new procedure (Van der Linden et al., 2002), in which a pesticide can only be registered if the long-term average concentration meets the EU drinking water limit (0.1 $\mu g\ L^{-1}$) at more than 90% of the area of usage[2]. Models play an important role in the evaluation of this criterion. The models should (i) be applicable to a large number of pesticides with different properties, (ii) be able to predict the *long-term average* concentration of pesticides in the groundwater, and (iii) be able to produce *spatial patterns* of pesticide leaching. The latter is important, because stakeholders become more and more interested in areas of 'safe usage' and areas where problems may be expected.

The simulation of spatial patterns requires that the model is applied under different conditions. Maloszweski and Zuber (1992) state that models with a large number of parameters provide greater conceptual resolution than models with few parameters; however, the most complex model may not be the best model in terms of accuracy and precision due to poor parameter identifiability in a data scarce environment (Van Grinsven et al., 1995; De Vries et al., 1998). Taking this dilemma into account, the optimal model meets two criteria: (i) the model must have sufficient conceptual resolution to be applicable to the entire area for which it is developed, and (ii) the number of model inputs that cannot be directly or indirectly (through pedotransfer functions) be obtained from measurements should be minimised. How to deal with this dilemma is illustrated with the selection of the model of soil water flow as an example. Soil water flow can be simulated with the capacity type of model (Mullins et al., 1992), or with the mechanistic Darcy type of model (Van Dam, 2001). In the Netherlands, the groundwater table is close to the rooting zone at 50% of the total area (Tiktak et al., 1996). The capacity type of model was considered inappropriate, because it has been shown that it is restricted to sandy soils with deep groundwater tables (Vanclooster and Boesten, 2000). As pedotransfer functions are now commonly available to describe the hydraulic properties that are required for mechanistic models of soil water flow (Wösten et al., 1994), there is no reason to use the simpler approach.

The philosophy of conceptual flexibility in combination with the possibility of deriving all model-inputs directly or indirectly from observations, has led to the development of the PEARL[3] model (Tiktak et al., 2000). PEARL is a one-dimensional, dynamic, multi-layer model of the fate of a pesticide and relevant transformation products in the soil-plant system (figure 2). Soil water flow is described with the SWAP model (Van Dam, 2001). An important feature of PEARL is that it can be

[2] The exact percentile is still a matter of political debate.
[3] The PEARL model is the follow-up of the PESTLA and PESTRAS models.

linked with a regional groundwater model (Kroon et al., 2001). This feature allows to distinguish between fluxes into the deep groundwater and local drainage fluxes into local surface waters. This distinction was considered relevant, because the Dutch policy is aimed at protecting the deep groundwater (Van der Linden et al., 2002).

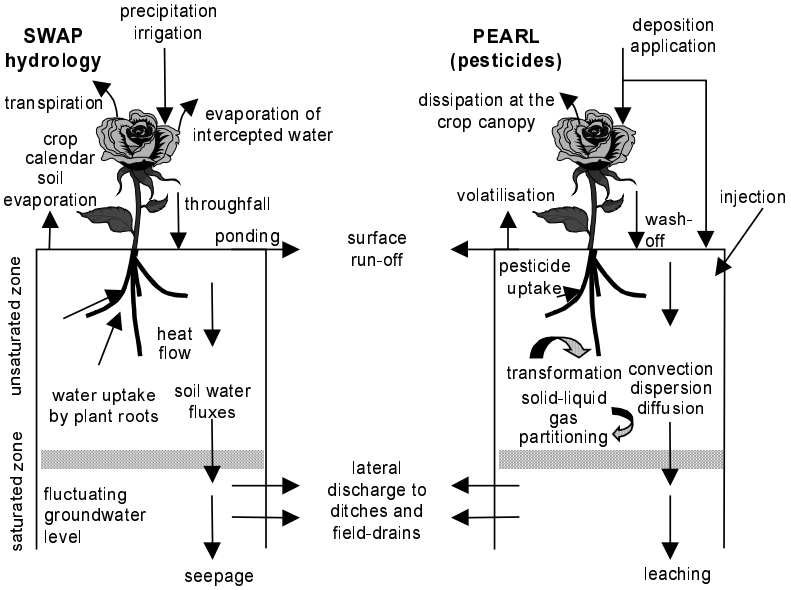

Figure 2. Overview of processes included in the PEARL and SWAP models.

3.2 Field-scale model applications

Model application at the field-scale is a crucial step in the development of models of non-point source pollutants in soils. The reason is that usually at this scale, direct measurements of model inputs and time-series to evaluate the model concepts are available (De Vries et al., 1998; Van Grinsven et al., 1995). To evaluate the concepts of the PEARL model, field-studies have been carried out throughout the country (Boekhold et al., 1993; Tiktak et al., 1998). An example of the application of a precursor of the PEARL model to a field-study is shown in figure 3. This figure shows a fast decrease of the pesticide content directly after application. Further analysis showed that this was caused by volatilisation of this surface applied pesticide. The model could reproduce this fast decrease, but only after calibration. It was therefore decided that this process could not (yet) be introduced into the regional-scale version of the model. The left-hand side of the figure shows that the movement of the pesticide was slightly overestimated. This was due to not considering non-equilibrium sorption. This process was included in a later version of the model, because it is significant and can be parameterised on the basis of standard experiments (Boesten and van der Linden, 2001). To get insight into the most important processes, the field-scale model applications were completed with sensitivity analyses (Boesten and van der Linden, 1991; Tiktak et al., 1994). The effect of data aggregation and the use of generic soil data on the quality of the model outputs was evaluated by Tiktak et al. (1998).

Until now, all field experiments have been carried out in sandy soils. The risk is that processes that occur in other soil types are overlooked. The most obvious example is the effect of preferential-flow on pesticide leaching, which is important in cracking clay soils. For this reason, PEARL is now applied to a broad range of soil types, including cracking soils. This research is accompanied by methodologies to derive pa-

rameters of hydraulic properties of cracking clay soils from generally available soil data.

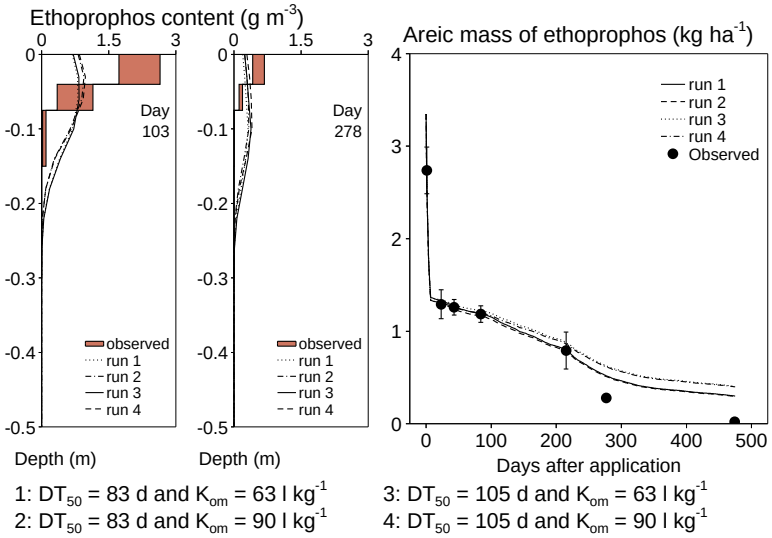

Figure 3. Application of the PEARL model to a field study in Vreedepeel, the Netherlands (after Tiktak et al., 1998). Left: Simulated and observed concentrations of ethoprophos as a function of depth. Right: Areic mass of ethoprophos as a function of time.

3.3 Scale transfer

To reduce the data requirements of a regional-scale model, both process aggregation and data aggregation can be carried out (De Vries et al., 1998). These two aspects will be elaborated further.

Process aggregation

De Vries et al. (1998) describe three possible pathways to get a simpler model, i.e.: (i) reduction of the temporal resolution, (ii) reduction of the vertical resolution, and (iii) exclusion of processes that are less relevant.

The simulation of long-term average concentration levels may require less temporal detail of the model outputs than the simulation of peak concentrations. Unfortunately, the leaching of pesticides is an extremely non-linear process (Tiktak et al., 1994), so variability of weather conditions has an extreme impact on leaching rates (figure 4). This implies that the reduction of the temporal resolution of the model inputs is not acceptable. Also the reduction in vertical resolution offers no true alternative. There are several reasons for this. The first is that the solution of the convection-dispersion equation requires the satisfaction of the so-called Peclet condition, which requires a maximum thickness of the computation layers (Tiktak et al., 2000). The second reason is that virtually all processes depend on soil properties. The sorption of pesticides, for example, is usually dependent on the organic matter content. It can be shown that the leaching of pesticides is underestimated if vertical heterogeneity was ignored (Figure 4).

The third method for process aggregation is exclusion of less relevant processes. Tiktak et al. (2002) performed simulations for four pesticides with different properties, and concluded that the relative importance of the underlying processes differed. This resulted in the prediction of completely different spatial patterns for the individual pesticides (figure 5). It can be concluded that the fact that the model must be applica-

ble to a large number of pesticides with different properties, hampers the possibility of model simplification.

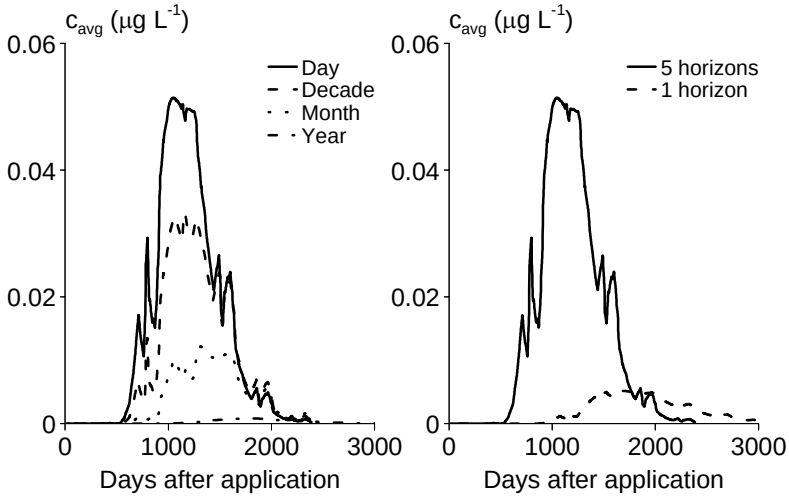

Figure 4. Effect of temporal resolution of the weather data (left) and effect of ignoring vertical heterogeneity (right) on the average concentration of atrazine in the upper meter of the groundwater (c_{avg}).

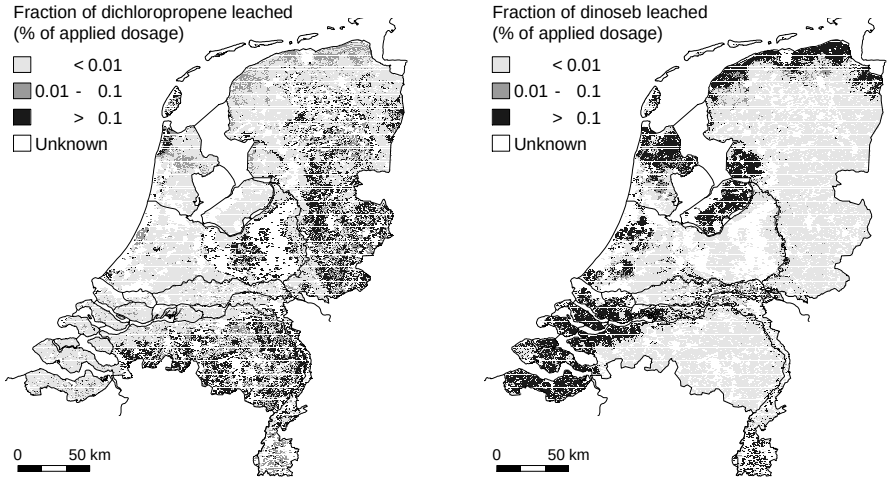

Figure 5. Leaching of a volatile pesticide (dichloropropene) and a pesticide showing *p*H dependent sorption (dinoseb) into the regional groundwater as predicted with the PEARL model (Tiktak et al., 2002). Notice the opposite spatial patterns.

The above considerations also limit the applicability of the so-called attenuation factor model (AF model), which was originally developed by Jury et al. (1983). This model has been used in pesticide leaching assessments (Loague and Corwin, 1996). The attenuation factor model is a simple analytical model, which tries to describe the most relevant processes with minimal computation time and data requirements. Analytical models do not account for vertical heterogeneity and assume steady-state flow,

leading to a strong underestimation of the leaching fraction (Van der Zee and Boesten, 1991). Van der Zee and Boesten also showed that this difference could be overcome by introducing effective model parameters. The problem with this approach is, however, that these parameters are site-specific, and can only be obtained by calibration

The conclusion of this section is that model simplification was not the most logical step when going from the local to the regional-scale.

Data aggregation
There are two methods of reducing the data requirements of comprehensive models. The first is to set-up procedures in which specific model-inputs are derived from generally available data sources. The second is to stratify the model inputs, so that the number of unique combinations for which the model has to be run is reduced. Full details of this procedure are given in Kroon et al. (2001) and Tiktak et al. (2002).

To establish the relationships between the model-inputs, and to avoid data redundancy, a relational database has been set-up (Tiktak et al., 1996; 2002). This database contains a hierarchy (figure 6). At the highest level, a distinction can be made between spatially constant parameters and spatially distributed parameters. Parameter values for the bottom boundary condition and drainage characteristics are given for each unique combination, and are obtained from the linkage between PEARL and the regional groundwater model (Kroon et al., 2001). All other spatially distributed parameters were related to four basic parameters, i.e. soil profile, weather district, land-use type and groundwater depth class.

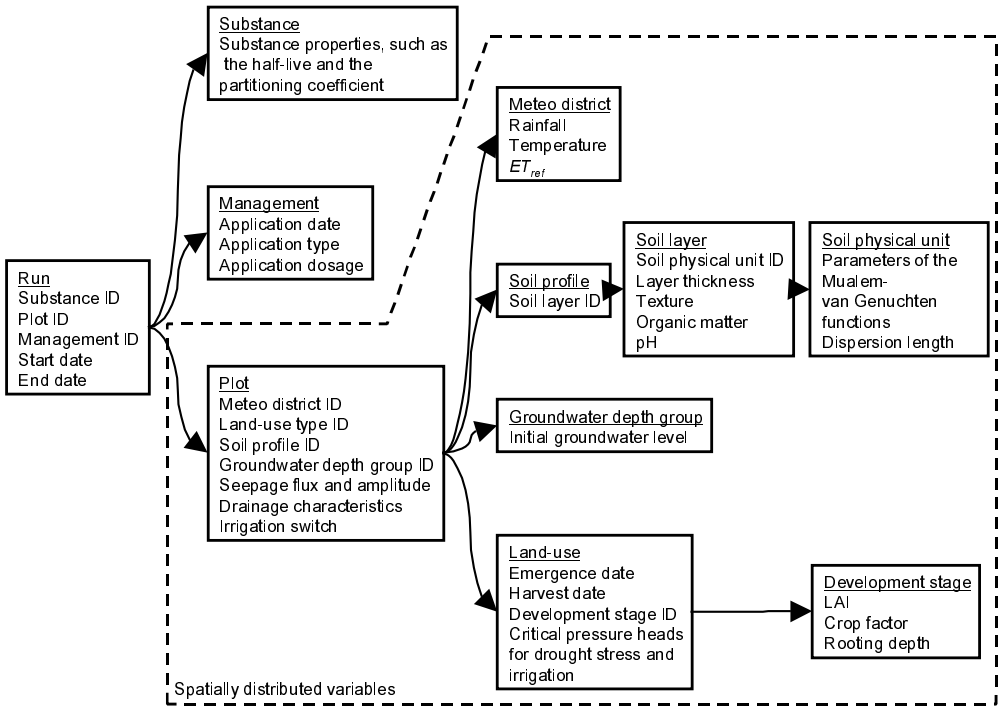

Figure 6. Structure of the PEARL database.

To reduce the number of unique combinations for which the model has to be run, the input data were stratified. The so-obtained stratified maps were combined in a GIS. The result was a map of almost 100,000 unique combinations. Application of PEARL to all these combinations would require too much computation time. For this reason,

so-called relation diagrams (Kroon et al., 2001) have been set-up, which defined analogous properties and allowed elimination of small sized units. A way to judge the quality of the obtained schematisation is to look at the frequency distribution of the model outputs. Figure 7 shows that the frequency distribution of the leaching fraction was almost unaffected as long as the number of unique combinations exceeded 250. We therefore concluded that spatial aggregation is an appropriate step when going from the local to the regional-scale.

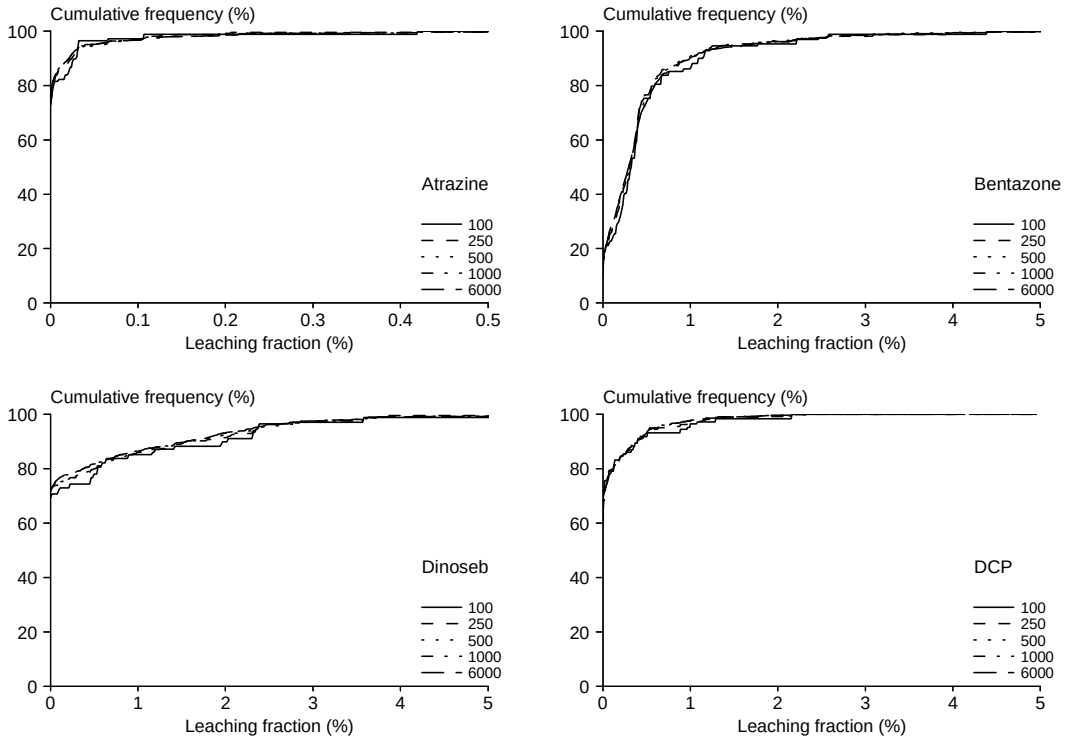

Figure 7. Cumulative frequency distribution of the leaching fraction of four pesticides calculated with 100, 250, 500, 1000 and 6000 unique combinations, respectively.

Meta-models

Another pathway to go from the local to the regional-scale is the use of so called 'meta-models'. These models give a statistical summary of complex mechanistic models. Because they are computationally inexpensive and easy to use, these models have become popular in larger scale pesticide leaching assessments (Douven, 1996). Existing meta-models are based on a limited number of parameters, i.e. the half-live and the sorption coefficient. These parameters were considered most important in the beginning of the nineties (Boesten and van der Linden, 1991). Tiktak et al. (1996; 2002) showed, however, that the spatial pattern of pesticide leaching was affected by more parameters, and that the relative importance of these parameters differed between individual pesticides (see also section 3.3). This resulted in opposite spatial patterns for two pesticides (figure 5), which could never have been described with the meta-model, where the sorption constant depends only on organic matter.

This example, where information from the beginning of the nineties is still being used in environmental model assessments, shows that the development of meta-models is not without risk. Meta-models models summarise one given set of model outputs generated with one model version, so they are the ultimate tools for creating a 'fixed body of knowledge' (Bouma et al., 1998), potentially even frustrating further research.

There is another often overlooked aspect with meta-modelling, which pertains to the model error. By using a meta-model, an additional error is introduced on top of the model error of the original model. Yet, no studies have been carried out to quantify the error propagation in the chain original model – meta-model.

3.4 Regional-scale model applications

During the field-scale model applications, the conceptual part of the model was evaluated. For a model to have predictive abilities, however, this is not enough. It is also required to have a good knowledge of the boundary conditions, parameter values and their spatial and temporal variation for the system to be modelled (Leijnse and Hassanizadeh, 1994). It is therefore important to evaluate the model at its final scale of application. For this purpose, results from regional-scale models are usually compared with data from national monitoring networks (De Vries et al., 1998; Tiktak et al., 1999; Overbeek et al., 2001). Regional-scale data on pesticides in the groundwater are, however, virtually non-existing. The primary reason is that the concentration of pesticides in the shallow groundwater shows strong temporal dynamics. Combined with the high costs associated with pesticide analyses and the large number of pesticides admitted, it becomes clear that true regional-scale monitoring of pesticides is not feasible. This means that evaluation of PEARL could not be carried out at its final scale of application. Statements about the performance of PEARL on the regional-scale were therefore limited to qualitative remarks, such as 'Pesticides were only found in the groundwater in regions that were classified vulnerable' (Tiktak et al., 1996).

If true regional-scale monitoring is not possible, the only alternative is to apply the model to a broad range of field-experiments. The pitfalls associated with this approach have already been described in section 3.2. An interesting addition to the application of models to the field-scale was mentioned by Loague and Corwin (1996). They advocated to quantify the overall model performance of a model for a number of field-sites at once, instead of employing the usual one-to-one field-tests. In this methodology, the observations are treated simultaneously and common values for field-specific data are optimised using inverse modelling. Unfortunately, this procedure has not yet been brought into practice.

The model application should be completed with an uncertainty analysis at the final scale of application (in this study the regional-scale). Probably the most important results from such an analysis are contributions of individual error sources to the total variance (Tiktak et al., 1999). This information can be helpful in prioritising further research. Until now, only a limited uncertainty analysis of the PEARL model has been carried out (Tiktak et al., 1996). As with many environmental assessments, a thorough analysis is still hampered by the lack of information on input errors (Heuvelink, 1998).

3.5 Presentation of model results

Too often, presentation of model results is regarded a trivial step, coming down to just producing multicoloured maps. Recent experiences during the development of the PEARL model have shown that this is not the case. The proposed new Dutch registration procedure states, for example, that a pesticide can only be registered if a pesticide meets the concentration limit *at 90% of the area of usage* (Van der Linden et al., 2002). What is meant by 'area of usage'? Is the actual area of usage intended, should

all crops where a pesticide is potentially used be included, or should the predictions even be made for the entire country? The answer to this question can make a big difference for the 90th percentile (figure 8). Communication with stakeholders, preferably in interactive sessions, is important to deliver the appropriate model outputs.

Another aspect that has to be mentioned deals with Good Modelling Practice (GMP). GMP practice requires clear communication of the underlying assumptions, uncertainties and limitations. New technologies, such as an on-line help function and a website (http://www.alterra.nl/models/pearl) offer prompt communication, and proved to be indispensable. GMP also requires that the modeller does not pretend more than justified. The hydrological component of the PEARL model has been parameterised for nationwide assessments, predictions for areas smaller than 12 km^2 are not allowed (Kroes et al., 2002, this volume). The User Interface, which is now under developnt, will therefore not have zooming possibilities.

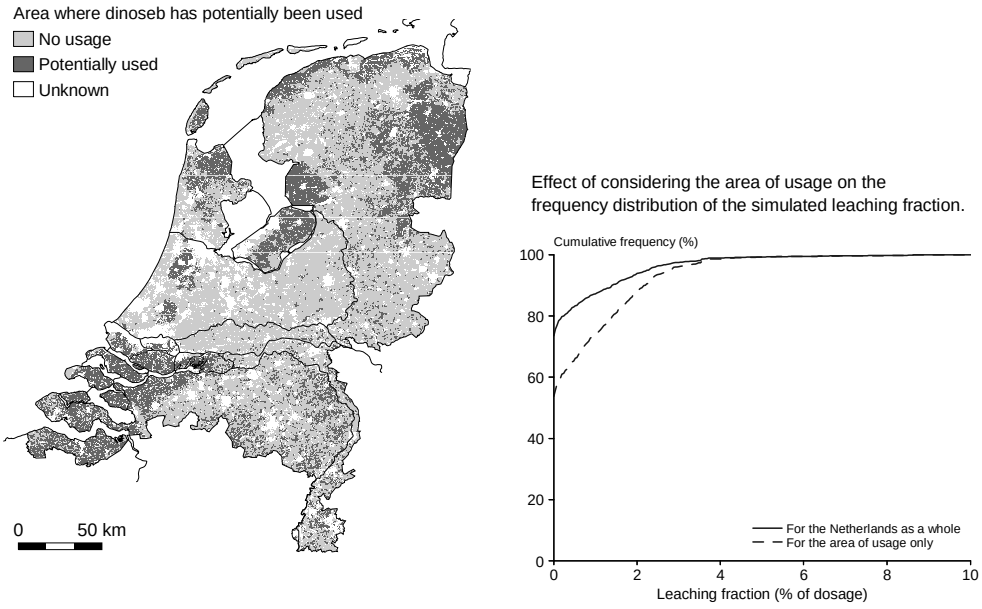

Figure 8. Effect of considering the area of usage on the calculated frequency distribution of the leaching fraction. To be interpreted in combination with the right-hand side of figure 5.

4 CONCLUSIONS

A general research chain for developing models of non-point source pollutants in soils has been developed. In this procedure, models are first applied to the field-scale. Model and data are then aggregated and applied to the regional-scale. The research chain approach was applied to the modelling of pesticide leaching on a regional-scale. It was shown that some of the steps of the research chain could not be completely carried out. In this particular study, regional-scale model validation and uncertainty analysis were hampered by lack of data. The largest benefit of the research chain is that it pinpoints the gaps in knowledge and data; it helps to prioritise further research.

Probably the most important part of the research chain is the phase of scale transfer. In this phase, both process aggregation (model simplification) and data aggregation

can be carried out. It was shown that in the pesticide leaching study data aggregation was more appropriate than process aggregation. Data were aggregated by stratifying the input-data and by setting up procedures in which specific model-inputs were derived from generally available data sources. Nevertheless, finding the proper balance between model detail and parameter identifiability is an important challenge to model builders, requiring more quantitative assessments (Heuvelink, 1998). It is the subject of a PhD study financed by the Dutch Institute of Public Health and the Environment.

Acknowledgements
Part of the work was carried out within the framework of the APECOP project, which is sponsored by the European Union. The spatial schematisation used for PEARL was originally derived for the Dutch Nutrient Emission model 'STONE', which is a joint product of three Dutch research institutes (RIVM, Alterra and RIZA). More information about PEARL can be found at the address http://www.alterra.nl/models/pearl.

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