Modeling non-point source pollutants in soil: Applications to the leaching and accumulation of pesticides and cadmium

Tiktak, A.

Citation for published version (APA):
The general objective of the present study was to contribute to a justified application of plot-scale developed models of non-point source pollutants on a regional-scale. Two environmental issues were studied, i.e. the leaching of pesticides to the shallow groundwater and the accumulation of cadmium in the topsoil and leaching into the groundwater. These two issues were chosen because they required entirely different model approaches. Pesticide leaching was calculated with a detailed, numerical, multi-layer model with a high temporal resolution (PESTRAS). Processes included were transient flow, convection, hydrodynamic dispersion, equilibrium sorption, degradation, uptake by plant roots and volatilization. In the heavy metal accumulation study two models were used: A comprehensive, multi-layer, numerical model (METRAS), which was applicable at the plot-scale, and a simple analytical, one-layer model with a lower temporal resolution (SOACAS), which was used for the regional-scale assessments. Processes included in SOACAS are steady-state waterflow, convection, equilibrium sorption, complexation, and plant-uptake.

A general procedure was outlined for the development and evaluation of regional-scale models of non-point source pollutants in soil (chapter 1). The following major stages were distinguished: problem definition, selection of model approach and model building (chapter 1), application and evaluation of the model at a number of field-plots (chapter 2), change in spatial-scale, including upscaling, data-aggregation and process-aggregation (chapter 3), regional-scale model application and evaluation (chapters 3 and 4), and presentation of results (chapter 3).

Plot-Scale Model Applications

Chapter 2 consists of three papers dealing with plot-scale model applications. There are two central questions. First, the performance of the models is evaluated using on-site measured monitoring data. Secondly, the effect of using literature data or pedotransfer functions was evaluated. The second issue is im-
important if the model is intended to be used for regional-scale assessments.

Chapter 2.1 deals with the application of the PESTRAS model to a field-study with bromide, bentazone and ethoprophos in a humic sandy soil in Vredepeel, the Netherlands. Model predictions were generally within the 95% confidence intervals of the observations when site-specific model inputs were used. However, when generic parameter values were used, the model predictions sometimes deviated strongly from the observed data. This was particularly the case for pesticide degradation properties. The need for calibration is a problem when extrapolating the model results for policy-oriented applications.

In chapter 2.2, the performance of nine pesticide leaching models with different complexity of the included process descriptions (including the PESTRAS model) was compared using the same data set. All modelers received an extensive description of the experimental data. Despite this fact, the interpretation of the experimental data was ambiguous, leading to tremendous user dependent variability of selected model inputs. Together with the fact that most modelers calibrated at least part of their model, the possibility for evaluating model concepts was limited. Nevertheless, it could be concluded that models lacking volatilization, kinetic sorption and adaptation of the microbial population were not able to reproduce the fate of the strongly sorbing, moderately volatile compound ethoprophos.

Chapter 2.3 describes the application of the METRAS model for cadmium to three field plots under natural land-use in the vicinity of a zinc-smelter in the Dutch-Belgian Kempen region. In this study, basic soil properties were measured on-site, all other model-inputs were derived from pedotransfer functions, or were obtained from the literature (generic data). This implies that the model was parameterized in the same way as was done for the regional-scale model SOACAS. With this combination of on-site measured data and generic data, the model could generally reproduce the currently observed depth-profiles of cadmium. This indicates that the generic sorption isotherms, which were based on batch experiments, were appropriate. It could also be concluded that biocycling was indispensable to describe the currently observed high cadmium contents in the ecto-organic soil layer.
Regional-Scale Model Applications

Chapter 3 presents the regional-scale model applications. The PESTRAS model in combination with a Geographical Information System was used to predict the leaching of pesticides on a regional-scale (chapter 3.1). A procedure was developed to reduce the number of unique combinations of the major spatially-distributed model inputs (soil texture, organic matter content, groundwater-depth-class, land-use and climate). Specific model inputs were derived from these basic properties by (pedo)transfer functions. Results showed considerable leaching of four commonly used pesticides to the shallow groundwater.

Chapter 3.2 introduces ‘hind-cast simulation’ as a methodology to evaluate the performance of the SOACAS model. In this procedure, it was tested whether it was possible to reconstruct the presently observed geographical distribution of cadmium using historical data on metal loads in atmospheric deposition, fertilizers and animal manure. 2544 Point observations of cadmium were available for this purpose. These data were interpolated onto the 500x500 m² grid used by SOACAS by means of a Generalized Additive Model (GAM). An attractive aspect of the GAM was that it is based upon the data, instead of being model-based. The model predictions were within a factor of 2 from observed cadmium contents at 90% of the total area. The simulations further showed that cadmium contents in the topsoil currently decrease in highly polluted areas around industrial plants, but still increase in arable land.

Sensitivity and Uncertainty Analyses

Chapter 4 deals with sensitivity and uncertainty analyses. In chapter 4.1, Monte Carlo simulations were used to gain insight into the sensitivity of an early version of the PESTRAS model to changes in its parameters. Results were strongly dependent upon the value of the model inputs, indicating that overall conclusions about the behavior of the model should be made with care and could not be based upon results obtained for a single pesticide. It could, however, generally be stated that the model was extremely sensitive to changes in pesticide degradation properties and to changes in the sorption coefficient.
In chapter 4.2, the uncertainty in the regional-scale cadmium accumulation assessment was quantified. From a Monte Carlo analysis carried out for a number of characteristic cases we concluded that the model behaved virtually linear within the range of model inputs considered, and concluded that First-Order Uncertainty Analysis (FOUA) was appropriate for mapping prediction uncertainties. The maps created by FOUA indicated that the contribution of individual model parameters to the total uncertainty was soil dependent, and that the pedotransfer function for cadmium sorption gave the largest contribution to the total uncertainty. The analysis further showed that ignoring uncertainty may result in misleading interpretations when the model is compared to field measurements.