Ministère de l'Agriculture et de la Pêche
Commission d'étude de la toxicité des produits antiparasitaires à usage agricole et des produits assimilés
Groupe de travail "Comportement des pesticides dans le sol"

Good Practices for the Use of Modeling in Environmental Chemistry

Application to Crop Protection Products General Principles and Codes of Good Practices

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Contents

1 - Modeling in Environmental Chemistry

1.1 - Objectives of Modeling

Like many other disciplines, environmental chemistry makes an increasing use of modeling for the study of organic substances behavior in the environment. In particular, modeling is applicable to the assessment of risk for environment posed by the use of plant protection products, using the capabilities of mathematical models as instruments to help formalize, understand and predict the environment response. This function also contributes to the provision of information usable in a regulatory context for pesticide registration; for instance, the calculations of predicted environment concentrations (PECs) in various compartments [2].

1.2 - Objectives of a Document on Good Practices for the Use of Modeling

Modeling, now frequently proposed in replacement of certain costly experimental studies, is favored by an increasing computing power at decreasing costs. Actually, mathematical models should be considered more as a complement of experiments and, whatever the reasons of their use might be, they must be run with certain precautions. These are necessary to guarantee the scientific validity and formal quality of the results in a similar way as for experimental work in the laboratory or in the field. Based on the state of the art in modeling and the users' experience, this document pursues the objective to determine the conditions where mathematical models can be used to predict environment concentrations (PEC) in soil, water and air in the framework of pesticide registration. The principles to follow for the good use of environment oriented models are mentioned in the first part. Other chapters are devoted to relevant information relative to each type of PEC and related compartments.

1.3 - PEC Calculation

First, the various environment compartments concerned by the PECs should be clearly defined to maintain the coherence between the spatial dimension of data needed by models and the environment domain of interest for the PEC.

1.3.1 - Soil

The soil layer related to the PEC_S is determined according to the type of PEC (short or long term) and the organisms potentially exposed to biological effects.

1.3.2 - Water

Two distinct compartments must be considered, in relation with two different PECs:

With regard to PEC_{GW}, groundwater corresponds to water in unconfined aquifers. The volume of interest corresponds to the treated zone with a sufficient depth to encompass the residues.

Eventually, the whole aquifer should be taken into account to assess the risk for potable water abstracted from groundwater.

With regard to PEC_{SW}, surface water corresponds to the permanent hydrographic network next to the treated field or at the watershed scale.

Concentrations in drinking water can be estimated using raw water concentrations as a function ør their origin (surface or groundwater) and the nature of treatment process used to produce drinking water.

1.3.3 - Air

PEC in air is not considered in this draft document.

2 - General Considerations on Modeling

2.1 - Choice of Models

Screening models, mainly developed to assess leaching potential, are not considered in this document [9]. Easy to use, they are very helpful in preliminary assessments of risk, but they are unable to predict concentrations. Only models suitable for PEC calculations are considered in this document [12].

Theoretical classifications of models have been proposed according to various criteria [8]:

- the knowledge of input and output data and of the functions which link them in the modeling system (models for identification, prediction or detection),

- the knowledge of causal relationships between sensitive factors (deterministic or stochastic models),

- the nature of the functions linking inputs and outputs in the system (mechanistic, conceptual or empirical models),

- the spatial distribution of information used by the model for the system variables (global, local, distributed or semi-distributed models),

- the time dependence or independence of the system evolution (static or dynamic models).

From a practical point of view and with regard to model use, one can identify:

Operational or routine models call for a relatively simple representation of reality. They are easy to use (users' training and computing power) and are applicable to most of the situations (availability of input data). Performances are approximately in proportion to the sophistication level of the representation of relationships linking the various elements of the reality. They are widely used by the scientific community worldwide.

Research models, at the opposite, are likely to exhibit good performances but their scope is frequently restricted by several requirements regarding the availability of input data, the computing power needed or the required user level of competence. Used by a limited number of people, they are privileged tools for progress in the state of the art but are less suitable for industry or regulatory concerns.

Irrespective of a somewhat arbitrary distinction between routine and research, models can be used correctly only by people with a sufficient level of competence in the areas of environment and modeling. Consequently, a model should be considered, in complement of experimental work, as a research tool to be used in this very context, even if the purpose is simply the determination of values useful for registration purposes. Modeling cannot be likened to carrying out standard experiments.

Choice of model type is mainly driven by the spatial scale of the compartment of interest. For instance a mechanistic, deterministic, local, dynamic and predictive model is suitable for the soil compartment at the field scale.

Except for a few infiltration models such as LEACHP, PRZM or PESTLA for instance, no model has been specifically designed as a decision making tool in the framework of registration of plant protection products. Users' needs for regulatory modeling do not necessarily correspond to those of researchers and of model developers [3]. Before models are specifically developed in this intent, the user takes his choice among a set of available models according to the following criteria:

- the defined objectives (spatial scale, model variables),
- the model availability (accessibility, performances, adequacy with available input data),
- the own users' experience.

Among others, the following qualities of models are particularly important [10]:

- rational coherence,
- capacity to match experimental data,
- prediction capacity.

For a defined problem, users can make different choices according their own constraints. The application domain of models should be kept unrestricted by allowing the users a sufficient freedom of choice and of application conditions, with the responsibility to justify formally and scientifically his decision [7]. Consequently, the choice of a model in a regulatory context should be based on objective arguments and, in the future, on a consensus.

2.2 - Validity and Limits of the Use of Modeling

When using models as a tool for decision making in a regulatory setting, the quality of the results must offer certain guarantees, often covered by the term validation. One has to make a clear distinction between validation of the model itself (simulator validation) and model validation in a specific application.

Validation tends to verify that the model faithfully performs the functions that have been assigned to it. This task is done by model developers and is implicit for the user.

Validation in a specific application tends to verify that, in a known evolving situation of the real system which is different from the calibration conditions, the values of variables computed by the model are close enough to the measured values.

Model calibration consists in adjusting uncertain parameters of the model in this intent. This operation is different from the validation in a specific application and both must be carried out using independent data sets.

Quality of calibration or of system validation may be assessed using adjustment criteria [1]. A model can be granted a predictive value inasmuch it has been calibrated and validated in configurations which are representative of application conditions. Confidence of predictive values decreases as the conditions of model operation differs from these configurations. At the present time, available data suitable for validation are scarce. After calibration in a set of conditions, a model is not necessarily equally accurate when used with other scenarios, because of the large number of parameters for which relevant information is frequently lacking. The

model can still be used in acceptable conditions if it is not too sensitive to the modified parameters.

Errors in predictions of mechanistic models originate from the various assumptions included in the model, the methods used in solving equations and the selection of input parameters. The user keeps control of these errors by choosing a model adapted to the application of interest and the specification of correct input parameters. Model assumptions should be know by the user and their pertinence in each specific application should be considered. The validity of each input parameter must be also taken into account, especially in the relatively frequent case when data generated in conditions different from the application or with different products are used.

2.3 - Risk Assessment for the Environment and Modeling Strategy

There is an obvious connection between the use of models and the experiments which generate relevant information regarding the environmental fate of plant protection products, particularly persistence and mobility [4]. Because of its versatility, modeling can be used both in the primary assessment of risk using laboratory data and the calculation of PECs as well.

Despite a right choice of models and the full awareness of their limits, there is a risk that modeling results could be given too much credit. A decision cannot be based exclusively on model predictions. A good understanding of the environmental behavior of a product, and the corresponding decision on use by expert judgement, is obtained using the whole set or results from laboratory and field data, and from adequate modeling.

One has to admit that modeling results are neither exact nor unique. Hence the goal to estimate the errors of models, for instance by combining a stochastic approach with the interpretation of results produced by a deterministic model. If possible, the objective should be to express the results in terms of confidence intervals, taking into account the uncertainties from input data, calibration, limit conditions, etc. Expressing the results in this way will certainly contribute significantly to model credibility [4].

An alternative method to the model validation "at all cost" consists in using a library of different and complementary models (multi-model strategy). For each model, the limitations and the application domain must be clearly outlined in a guide. This approach is in agreement with the restrictions resulting from unavailable data and related assumptions.

Interpreting the modeling results in a comparative manner using determined scenarios specifying all necessary parameters (soil, climate, crop data, etc.) but those relative to the plant protection product is a way round the problem [13]. Inasmuch as the scenarios are available and remain realistic with respect to the product use, this approach, already used in a few countries (Germany, The Netherlands, United States), tends to compare the environmental fate of a product with those obtained for other products in the same conditions. In return, a hampered versatility of modeling is the price to pay for the gain in accuracy offered by standard scenarios.

Modeling in a regulatory setting has to follow the state of the art. User needs should be taken into account by model developers so that models could become effective regulatory tools.

3 - General Principles for the Good Use of Modeling

General principles for the good use of modeling concern several domains like the knowledge of model operation, the definition of clear objectives, the selection of input parameters, and the critical examination of simulation results.

3.1 - Knowledge of Model Operation

Without having a detailed knowledge of the model structure, the user should know enough about the nature of the simulated processes, the assumptions made in the model and the resulting mathematical representation. Among other influential factors, performance of a model is affected by its level of sophistication. A description of model structure and a detailed user manual are essential.

3.2 - Specification of Model Application

Definition of objectives is a critical step when choosing a model for which a specific application has been selected and validated at a known level of prediction accuracy [4]. Assessment of leaching potential in unfavorable conditions (sandy soils, wet climate), simulation of product behavior in soil in standard scenarios, or prediction of residue concentration in groundwater are ordinary examples of model applications.

The selected application is closely related with constraints of input data availability and quality. Actually, uncertainties of sensitive parameters make a faithful representation of reality merely conjectural. However, application of models in conditions minimizing those constraints is still possible. For instance assessment of behavior in soil using conventional situations (scenarios) or worst case conditions may alleviate the effects of model sensitivity to uncertainties of input parameters.

Model validation in a specific application is based on the good agreement between predictions and measurements. It must be primarily obtained in the application domain, not only for the predicted variables which directly involved in PEC calculations, but also for a relevant set of variables considered as indicators of good operation of the model. For a valid application of a model, those variables must be specified with their limits of variation, particularly the lower limit when the model is used to assess the possibility for predictions to exceed a legal value.

3.3 - Selection of Model Input Parameters

Mechanistic models require a large number or input parameters, mainly weather data, soil and product characteristics, conditions of crop and product use. The objective of this chapter is to document which information in the input parameters cannot be compromised by assumptions supposed to replace missing or inaccurate data.

3.3.1 - Availability

The choice of site to be simulated is mainly a function of the objectives of model application. However restrictions can result from the unavailability of descriptive information about the site. One of the limiting factors in good use of models is the availability or data representative of the situation to be simulated. Use of scenarios may restrict this problem to product characteristics.

3.3.2 - Selection

Selection of input parameters is a critical step in modeling since simulation results are largely affected by their quality. Many unknown or uncertain parameters of variable influence must be selected. Estimating unknown values or choosing them among a set of possible values is a typical selection procedure. Selection efforts should focus primarily on parameters with determinant roles:

- product characteristics (affinity for soil and degradation rate),
- soil properties affecting hydrologic behavior (density, texture, etc.) and residue retention (organic matter),
- climatic data and parameters of interest for the calculation of evapotranspiration.

For many other parameters of minor importance, a coarse calibration or model default values can be sufficient. The PRZM user manual [11] describes the techniques for estimating the parameters used by unsaturated zone models. The relative importance of those parameters for infiltration models has been assessed in a document of the FOCUS group on necessary data for model validation [5].

Generally, the user should run a set of simulations including a likely interval of variation for influential input parameters. Their selection has usually more influence on prediction quality than the accuracy which results from model sophistication. As far as possible, information related to the simulated site should be used and the assumptions made for estimating unknown parameters minimized. The procedures used and the assumptions made should be carefully documented with the results. All relevant information for the result interpretation should be accessible.

3.4 - Validity and Acceptability of Simulation Results

Results are generally optimized by adjusting certain input parameters in successive simulations. A more complex procedure should be followed when parameters of influence are uncertain and must be estimated under certain assumptions: degradation rate, soil sorption coefficient, organic matter profile in soil. This case occurs when half-life measurements on a site or on different sites exhibit a large variation or when distribution coefficients have to be estimated using other parameters like the water solubility. Without a need for a comprehensive sensitivity analysis, a sufficiently wide domain of variation must be covered for these parameters and the simulation results should be examined and interpreted accordingly.

3.4.1 - Examination of Simulation Results

Simulation models generate data in large number, only a part of which being relevant for the objective pursued. Usually, if the program does not perfom it by itself, it is necessary to organize the outputs in the form of synthetic tables so that they could be examined easily. From a practical point of view, the acceptability of each simulation is based on the critical examination of relevant outputs.

3.4.2 - Expression of Simulation Results

Modeling requires information regarding soil, climate, crop and product properties obtained from various sources or estimated if not available. For a correct interpretation of the simulation results, information should be correctly documented in order to make a clear difference between data directly related to the simulated site and data extrapolated from other areas under certain assumptions.

4 - Codes of Good Practices for the Use of Modeling

Common problems encountered in modeling include the limited accuracy of models, the use of models without defined objectives and the use of models by untrained personnel [13]. To guarantee a formal and scientific quality of results, it is necessary to respect general principles on the good use of models which are applicable to the diversity of environmental risks. From a practical point of view, these principles are materialized in codes of good practices for the use of modeling. The objective of these codes is to provide guidance to the model user with a set of precautions and recommendations adapted to each model type. Because of the close relationships between modeling and experimentation, the scope of these codes should extend to the design of experiments for validation of model applications and the establishment of simulation scenarios.

A number of unsaturated and saturated zone models has been used at the field scale to asses the potential for groundwater contamination [6]. Unsaturated zone models are primarily concerned inasmuch the mechanisms in this compartment largely determine the occurrence of residues in the aquifer. Saturated zone models can be linked to the former to predict the movement of residues in the aquifer and assess the potential impact on drinking water quality.

Run-off and erosion models have been developed in lesser number for the prediction of residue transfer to surface water. They operate at different geographic scales, from field size to the catchment.

Appendices A and B are an attempt to define codes of good practices for these models respectively.

5 - Bibliography

[1] A.E. Boekhold
Validation of the PESTLA Model: Definitions, Objectives and Procedure.
National Institute of Public Health and Environmental Protection, The Netherlands.
Draft Report, 1994

[2] Commission of the European Communities - Directorate General for Agriculture
Directive 91/414/EEC; Annex II (Data Requirements for Active Substance), § 7.4 (Predicted Environmental Concentrations).
Working Document, July 20 1993

[3] A.S. Donigian Jr., R.F. Carsel
Developing Computer Simulation Models for Estimating Risks of Pesticide Use: Research vs. User Needs.
Weed Technology 6, 677-682, 1992

[4] European Crop Protection Association asbl
The Regulatory Use of Lysimeter Studies and Computer Modeling for the Evaluation of Pesticide Mobility in Soil.
Technical Monograph n°16, March 1993

[5] FOCUS
Input and Ouput Data needed for Validation of Pesticide Leaching Models.
April 1994.

[6] FOCUS
Assessment of various Leaching Models
March 1994.

[7] G. Görlitz
Rules for the correct Performance and Evaluation of Model Calculations for Simulation of the environmental Behavior of Pesticides.
Fraunhofer Institut für Umweltchemie und Ökotoxikologie

[8] ISMAP - Groupement des partenaires français
Phase de définition - Sous-projet 4 - Modélisation et aide à la décision.
Rapport final, février 1993.

[9] R.L. Jones
Assessing Movement of Pesticides in Agricultural Environments - Hazardous Waste Containment and Treatment.
Encyclopedia of Environmental Technology, Vol. 4, P.N. Cheremisinoff Ed., Gulf Publishing, 1990.

[10] L.A. Kauark Leite
Réflexions sur l'utilité des modèles mathématiques dans la gestion de la pollution diffuse d'origine agricole.
Thèse doctorat, Ecole Nationale des Ponts et Chaussées, 26 octobre 1990

[11] J.A. Mullins, R.F. Carsel, J.E. Scarbrough, A.M. Ivery
PRZM-2, A Model for Predicting Pesticide Fate in the Crop Root and Unsaturated Soil Zones: Users Manual for Release 2.0
Environmental Research Laboratory
U.S. Environmental Protection Agency, Athens, GA 30605-2720 USA

[12] OECD Environment Directorate
Report of the OECD Workshop on the Application of simple Models for environmental Exposure Assessment.
Environment Monograph n°69, OECD Paris 1993

[13] M.H. Russell, R.J. Layton
Models and Modeling in a Regulatory Setting: Considerations, Applications, and Problems.
Weed Technology 6, 673-676, 1992

[14] R. D. Wauchope
Environmental Risk Assessment of Pesticides: Improving Simulation Model Credibility.
Weed Technology 6, 753-759, 1992

6 - Glossary

[Include the definitions used by the FOCUS Regulatory Modeling Workgroup]

Appendix A

Unsaturated Zone Models
Concentrations in Soil and Groundwater

Contents

Unsaturated Zone Models
Concentrations in Soil and Groundwater

There is a large number of unsaturated zone models, differing in the number of elementary processes simulated, the way these processes are mathematically represented, the methods used to solve the equations (and the computing power required), and the amount input and output data needed. Irrespective of detail differences, they fulfil the same function, i.e. they represent the same processes according to a mechanistic approach. They predict the movement and the degradation of plant protection products in the soil unsaturated zone in specified conditions. In principle, their use is general and not restricted to specific applications. The FOCUS group carried out an evaluation of leaching models commonly used [1].

1 - Model Operation

Leaching models generally include two parts: the first one is devoted to the description of water movement (hydrologic sub-model), the second is dealing with pesticide behavior (chemical sub-model).

The hydrologic sub-model has a key position in the model and computes the water balance between supplies by precipitation and irrigation, and the losses by run-off, evapotranspiration and infiltration. Water movement, generally represented in one single vertical dimension, is calculated using a simple representation of infiltration or more complex equations involving soil characteristics. According to the algorithm used, water is supposed to move exclusively downwards or capillary ascension may be simulated also.

The chemical sub-model is built on the hydrologic sub-model to determine the movement of residues in the soil profile as a function of product properties (sorption coefficient, degradation and volatilization rates) and of product use (application mode and rates, treatment dates).

One of the major factors driving the movement of residues in the soil profile is the quantity of water infiltrated below the root zone. All the models calculate the recharge by difference between supplies (precipitation and irrigation) and the losses (evapotranspiration and runoff). These quantities are relatively large compared to the recharge, the accuracy of which is largely dependent on the precision of each term.

Values for evapotranspiration and runoff are usually not measured but estimated. In coarse textured soils (sandy and loamy sand) where infiltration is important, runoff is very limited and accurate estimates are not necessary. In other cases, runoff and corresponding residue transfer may be significant and should be estimated with sufficient accuracy.

In most models, problems can occur with the computing of potential evapotranspiration using generally average air temperature or pan evaporation with an adequate correction factor. Inaccuracies may result from both of the methods, so that the likelihood of estimates should always be checked in a simulation. For instance, prediction of residue movement with PRZM is modified according to the way evapotranspiration is estimated. Often, calculations using

average air temperature tend to underpredict evapotranspiration and therefore overpredicts residue movement compared to field measurements. However, the correction factor can also be a source of error, especially when crop coverage is low.

A frequent assumption in most of the models is that the role of soil macropores is not significant. Whereas macropores are frequent in fine textured soils and conditions conducive to residue movement are generally restricted to coarse textured soils, this assumption has minor consequences. Water fast flow allows the residues to move quicker than the model predictions. According to the placement of the product, overlooking the role of macropores may result in incorrect estimates of residue movement. If residues are present on the crop canopy or at soil surface, movement is induced by precipitation washoff and models underestimate real movement. Conversely, residues present in soil, particularly if the product is incorporated, are less likely to move in these conditions.

With regard to product behavior, several assumptions are current in all the models. A first order kinetics is assumed for residue degradation. As the degradation rate in not time dependent, the seasonal variations of soil temperature cannot be taken into account. Sorption of the product on soil particles is described using linear and reversible isotherms (identical for adsorption and desorption) and irreversible exchanges in successive adsorption and desorption cycles are not considered (hysteresis). A few models are able to simulate the behavior of metabolites produced according to various generation processes.

2 - Specification of Model Application

A model like PRZM is frequently used to help answer a few important questions on the behavior of a pesticide in soil. In a specific condition, can the residue reach the water table ? If yes, how long will it take and which part of the applied product will enter groundwater ?

Although more complex to perform, sensitivity studies are very useful to evaluate the influence of inputs on outputs in a model and to determine which parameters are critical. Pesticide degradation rates and sorption coefficients exhibit a relatively large statistical dispersion and, at the same time, are known to have a significant influence on leaching amplitude. A major benefit of modeling is to allow the user to represent the behavior of a product according to the variations of these parameters. Similarly, assessment of behavior at a regional scale is obtained by varying soil properties between limits representative of the area of interest.

3 - Selection of Model Input Parameters

3.1 - Data Availability

The most difficult parameter to determine for leaching models is probably the degradation rate of the pesticide in the unsaturated zone. It depends on temperature and soil properties, moisture, pH and microbial activity. Estimating the half-life of a product in specific conditions is not an easy task, particularly when data from the simulated site or from other sites are not available. Degradation rate below the root zone is generally slower than that observed in top

soil layers, notably when it mainly results from microbial activity, but is seldom known. Laboratory measurements are difficult to extrapolate. Therefore, if they are available, field measurements obtained on different sites should be preferred. This costly step is often necessary to produce relevant information regarding residue dissipation.

Although weather data are easily accessible in developed countries, gathering daily records of precipitation and air temperature may frequently pose a problem, particularly when long periods of continuous records are necessary for a sufficient climatic variability. On a specific site, the absence of continuous weather records for several years jeopardizes any modeling exercise. Similarly, except for a few cases in limited number, the use of averaged values (weeks or decades) to replace missing weather data must be avoided.

Soil data bases can provide useful information regarding soil properties and supported crops in a given area. Comprehensive and detailed information are available only in specific sites such as research farms which can usually provide relevant information regarding the simulated site (soil texture and organic matter profile). Complementary measurements are particularly useful for the calibration of a model or the verification of its correct operation (true evapotranspiration, etc.).

3.2 - Data Selection

3.2.1 - Pesticide Characteristics

The absence of information regarding the soil sorption and the degradation of a pesticide, and specific to the simulated site, is a typical problem. These parameters may be imported from other experimental sites, under the responsibility of the model user who has to determine which realistic variation the uncertain parameters will be allowed. Starting with an acceptable set of measurements for each parameter, the product behavior can be assessed correctly on the basis of simulations involving parameter values reasonably distributed around a central value. Simulations using extreme values, for instance particularly long half-lives or sorption coefficients measured on a different soil, may be useful to illustrate the behavior in conditions conducive to leaching. These results should be interpreted in this context of abnormal situation using, if possible, a statistical representation for an adequate comparison with normal situations.

Usually, the degradation rate of a pesticide in soil is accurately known in the top soil layer. The rate is uncertain or unknown in the lower horizons, particularly beneath the root zone. A few rules of thumb based on a good understanding of the product behavior may help overcame this hurdle.

For products which mostly undergo a microbial degradation, a relatively unfavorable degradation profile is obtained by dividing the degradation rate by a factor of two every twenty centimeters. Below one meter, a zero rate is assumed (residue do not degrade). Where a significant abiotic degradation has been demonstrated, the rate can be maintained constant below the root zone down to a greater depth.

3.2.2 - Soil Properties

Below the root zone or even below the top layer, soil properties, organic matter content in particular, are generally not accurately known. If necessary and to allow the user to simulate despite a poor soil description, several assumptions corresponding to worst case situations can be made on the basis of simple rules. For instance, the sorption coefficient is divided by a factor of two every twenty centimeters. Below one meter, no retention is assumed and the residues moving to that point can then leach freely.

Simulating the behavior of a product using one typical soil profile corresponds to a somewhat too restrictive set of conditions. Hence, predictions based on results of one single standard soil profile with a typical climatic scenario is extremely dangerous. Making available to users all relevant information regarding a set of sites representative of regional agricultural conditions, is certainly an excellent guarantee for the good use of modeling.

3.2.3 - Weather Data

From user experience, a correct assessment of residue movement in specific conditions requires simulations over a period of 15 to 25 years to allow a large climatic variability. Data from a representative weather station (local weather) choosen among a set of stations located close to the site should be used. Weather stations in agricultural areas are obviously preferred to stations in urban areas.

In countries where climatic variability is important and is particularly dependent on latitude, climatic scenarios should be established using regional climates, preferably to main climatic types. For instance, France can be divided into twenty regional climates representative of the major agricultural areas. For this purpose, it is recommended to use weather data recorded during the 30-year reference periods of the World Meteorological Organization (1961-1990).

Model predictions are not necessarily restricted to specific sites. A whole region or even larger areas can be concerned, providing the date used are representative of the area of interest.

4 - Validity and Acceptability of Simulation Results

4.1 - Examination of Simulation Results

The acceptability of simulation results is mainly based on the likelihood of the water balance and of the residue profile in soil.

4.1.1 - Water Balance

Examination of the monthly and yearly hydrologic balances during the simulation period is generally sufficient to verify if the results are acceptable. The fraction of water evapotranspirated compared to total precipitation should be in good agreement with reference

data collected on the simulated site or in the area (same order of magnitude for evapotranspiration and runoff). Evapotranspiration of well watered crops in various climatic conditions are known and should be used as a reference for comparison with simulated values.

Except for fine textured soils, runoff estimates must remain low (below 5 or 10 % of total precipitation). Unexpected runoff estimates, for instance in the monthly summaries, should be justified by weather records showing important precipitation at certain dates.

4.1.2 - Chemical Balance

Examination of the chemical balance allows the user to verify the relevance of input parameters regarding the properties of the chemical. Evidently, a simulation should be re-run over a longer period if the results show that residues are still present in the unsaturated zone at the end of the simulation.

Estimates regarding the chemical balance (amount of residues per hectare, residue concentrations in the solid and liquid phases of soil are often expressed with an excessive numerical precision with regard to the real performances of the model. Lower limits should be set for estimates of residue mass balance and concentrations to avoid the misuse of simulation results. The accuracy of concentration estimates cannot be greater than that given by the analytical methods available to forbid any prediction outside the validation domain of the application. By experience and as a general rule, leaching models are reasonably capable of predicting the behavior of pesticides in a range corresponding to two or, at the most, three orders of magnitude of the quantities applied. In absence of corresponding validation, estimates below this lower limit are merely conjectural and established at the user risks.

4.2 - Expression of Simulation Results

Preferably, simulation results should be expressed in terms of quantities or per cent of the product leached below a given depth because mass estimates are less sensitive to dispersion and to the shape of the residue concentration profile. Expressing the results in the form of concentration profiles can lead to misinterpretations inasmuch as the true residue concentration in a relatively homogeneous field is likely to vary within one or even two orders of magnitude [2].

Because of the extreme variability of soil properties and weather data, predictions should be represented statistically, for instance in a graphical way showing the distribution of cumulated probability of the predicted variable, for instance the amount of residues leaching below a given depth or likely to enter the aquifer.

If the simulation shows a significant mobility of the residues, or the possibility for the residues to enter groundwater, the results must be discussed not only in the light of quality of input data (frequency of residue occurrence in groundwater, amount of residues entering the aquifer, concentration in excess of a legal value, etc.) but also in relation to the model performances. In this case, expert judgement is required to evaluate the risk on the basis of modeling and experimental data.

5 - Bibliography

[1] FOCUS
Assessment of various Leaching Models
March 1994.

[2] R.L. Jones
Assessing Movement of Pesticides in Agricultural Environments - Hazardous Waste Containment and Treatment.
Encyclopaedia of Environmental Technology, Vol. 4, P.N. Cheremisinoff Ed., Gulf Publishing, 1990.

Appendix B

Runoff and Erosion Models
Concentrations in Surface Water

Contents

Runoff and Erosion Models
Concentrations in Surface Water

Runoff-erosion models simulate the transfer of pesticide residues to surface water. They predict both residue losses in solution or adsorbed on eroded soil particles. Developed more recently and in a lesser number than leaching models, they are also used in a lesser extent. None of them was specifically designed for purposes of pesticide registration.

As previously mentioned, the main error sources in mechanistic models result in the model assumptions, the way equations are solved and the selection of input parameters. The user is able to control these errors by choosing a model suitable for a specific application and by optimizing input parameters.

1 - Model Operation

In a way similar to leaching models, the model performances and hence the limits of possible applications strongly depend on the representation in the model of the various environmental processes. Runoff-erosion models usually include three sub-models, a specific function being assigned to each:

- runoff and infiltration production,
- sediment production and transport,
- residue transfer.

The corresponding transfer processes involved include:

- transfer in infiltration water,
- transfer in sub-superficial water,
- transfer in runoff water, dissolved or adsorbed on soil particles.

The vertical transfer component is generally less developed in runoff models than in leaching models. In most cases, runoff is calculated first with a production equation using the rainfall data (for instance the SCS curve number). Infiltration water is computed in the hydrologic balance. Consequently, runoff models have degraded performances with coarse textured soils where infiltration is important.

Modeling of residue transfer is based on a chemical balance in the top soil layer. The depth of this layer is variable according to the model and usually corresponds to the root zone. The fraction of the chemical likely to be transfered by runoff is supposed to be located in a small soil layer of about one centimeter depth. One assumes that the product is uniformly distributed in this layer. A conventional extraction coefficient is used to estimate the pesticide fraction transferred.

A very small number of models takes into account the foliar washoff of the chemicals. This process actually involves a fraction of the products likely to reach the soil surface, making them more available for runoff transfer or transferring them directly to water runoff [3].

Soil erosion, produced by impact of rain droplets and detachment of particles by runoff flow, is simulated in various ways by runoff models. Certain models include a sediment transfer component involving the deposition and suspension of particles in rills and gullies. In a few cases, the model uses the granulometric distribution of the particles during the transport. An enrichment ratio is computed for fine textured sediments in comparison to the soil remaining in place [11]. The value of this coefficient is critical when estimating the losses of a pesticide adsorbed for which the concentration is strongly dependent on the nature and the size of the soil particles.

Relevant pesticide physical and chemical properties are taken into account to simulate degradation, volatilization and adsorption. With some models, a first order kinetics, represented by one single equation, is assumed for dissipation which includes degradation and volatilization processes, e.g. CREAMS [11]. Metabolite movement can also be considered, e.g. in GLEAMS [4], in the new version of CREAMS, or in ARM, [6]. Most of the time, adsorption equilibrium is supposed to be reached instantaneously and is represented with a linear isotherm (Koc coefficient). In some cases, the Freundlich model is used with a non linearity parameter value different from one, e.g. in ARM.

Models may be used to simulate one single rainfall event, e.g. in ARM, or a scenario of continuous precipitation record over a period of several months, e.g. in GLEAMS. This second approach has a major interest inasmuch it involves pesticide persistence and it predicts the seasonal variation of residue losses.

The simulated processes are a function of the spatial scale considered:

The field scale is mostly suitable for studying the relationships between agricultural practices and land management with residue transfer [12]. Corresponding models scarcely include the contribution of sub-superficial flow to pesticide movement, e.g. in CREAMS and GLEAMS.

At the watershed scale, models are rather spatially distributed, e.g. in ACTMO [8], SWRRB [14] and ANSWERS [1, 2], in order to better handle spatial heterogeneity. They usually take into account the sub-superficial flow and include a runoff transfer function at the catchment outlet. These models are mainly suitable for the management of the water resource.

A few other models describe the transfer processes not only by runoff but also in the hydrographic network. For instance, HSPF [5, 7] includes the description of the watershed organized in smaller adjacent watersheds, and of the hydrographic network distributed in streams. One major drawback of this type of models is the huge number of parameters needed. Most of these parameters must be determined by calibration, which requires the acquisition of numerous time series of experimental data.

2 - Specification of Model Application

Before a model can be selected, the objectives of model application must be defined because they are critical in the choice of a suitable model. Typical model uses involve the assessment of runoff potential in a specific situation, the compared influence of various agricultural practices on the behavior of pesticides in different scenarios or the calculation of predicted environmental concentration in surface water (PEC_{SW}).

According to the type of model used, transfer by runoff can be simulated for one single rainfall event or using rainfall records. Objectives are different in each case. In the first one, the model is used to estimate a concentration profile in runoff water, eventually the maximum concentration, during the rainfall event. In the second, the objective is to estimate the seasonal variation of residue losses and the respective roles of rainfall succession and product application dates.

The time step corresponding to residue transfer by runoff is relatively short compared to that observed for leaching. The concentrations in surface water strongly depend on the period of time between the pesticide application and the rainfall. Therefore, one has to be fully aware of the considerable variation in time and space of the results when using runoff models. Hence the need to select a set of hydrologic events adapted to the objective of modeling.

In a way similar to leaching models, the success of model application strongly depends on the availability and the quality of input data. To alleviate the effects of uncertain or unknown parameters, applications based on determined situations (fixed scenarios, worst case conditions) are useful. They should be defined after a typology of pertinent cases is established.

Still in line with the general principles outlined for leaching models, valid applications of runoff models should be clearly specified, with the allowed variation limits for important variables, particularly the lower one when the model is used to asses the possibility for predictions to exceed a legal threshold.

Similarly, sensitivity analyses are particularly useful to determine the relative effects of inputs on outputs and to extract the critical parameters. They allow the user to set the variation limits of results in relation to the variability of important parameters such as the degradation rate and the sorption coefficient of the pesticide. This latter is known to vary over a larger range for runoff than for leaching.

3 - Selection of Model Input Parameters

Mechanistic models require a large number of input parameters, mainly data regarding climate, soil, crop, and pesticide properties and use. Input parameters are divided into two categories: those measured or estimated which correspond to physical or chemical properties, and those determined by model calibration. Selection of a few critical parameters used in runoff-erosion models is discussed below..

3.1 - Data Availability

The choice of the simulated site is a function of the selected application where the unavailability of certain parameter may be a limiting factor. One of the major problems encountered in the use of modeling is the availability of data representative of the specific situation studied. Once again, use of fixed scenarios may alleviate the effects of such constraints by restricting uncertainty to parameters regarding pesticide properties and use. Guidance provided in appendix A for parameter availability is applicable to leaching and runoff models as well.

3.2 - Data Selection

The selection of input parameters is a critical step, particularly for the following ones:

- pesticide characteristics (affinity for soil and sediments, degradation rate),
- soil properties affecting hydrologic behavior, erosion potential, and residue retention (texture, moisture, rugosity, organic matter content, extraction coefficient, enrichment coefficient),
- representative weather data.

For many other parameters of minor influence, a coarse calibration or the selection of model default values are adequate.

3.2.1 - Pesticide Characteristics

The absence of information specific to the simulated site is a typical problem and parameters may be imported from other sites in certain conditions and under user control. With runoff models, attention should particularly be drawn on the selection of sorption coefficients which exhibit a larger variability than for leaching. Sometimes, a clear distinction should be made between sorption on transported sediments and sorption on soil in place, the value of the former being seldom available [10].

Degradation rate should be determined in conditions as close to the real situation.

3.2.2 - Soil Properties

One of the major soil related parameter useful for runoff models is the pesticide extraction coefficient. This parameter corresponds to the fraction of soil which is likely to supply the flow of runoff water with residues [11]. Another critical one is the enrichment ratio in fine textured sediments which is frequently unknown [9]. Both parameters deserve the development of determination strategies and reference databases for modeling purposes.

3.2.3 - Weather Data

Guidance provided in appendix A for leaching is applicable to runoff-erosion, except that the time step required for rainfall might be shorter.

4 - Validity and Acceptability of Simulation Results

4.1 - Examination of Simulation Results

Caution should be exercised when using the results of runoff simulation. The areas of concern cover the knowledge of model operation, the assumptions made in the model itself, the application conditions, the selection of input data and the related assumptions (measurements, estimations and calibration).

Furthermore, validity of results is strongly dependent on the performances of the three sub-models and the corresponding predictions (hydrologic balance, erosion, chemical balance).

To make the interpretation of results easier, outputs data should be organised in synthetic tables or graphics. Criteria for estimating prediction errors should also be established and used.

Accurate predictions of residue losses in runoff water are mere illusion inasmuch as error may exceed 100 % [2, 10, 13]. Use of runoff models is nevertheless possible and acceptable in conditions where pesticide behavior and use scenarios may be compared.

Because of the considerable variability of soil properties, pesticide characteristics and weather data, a representation of the statistical distribution of predicted variables is probably the best way to make use of the outputs. Representative hydrologic time series should be used with extreme caution.

Once again, final decision falls upon experts whose judgement should be based on examination of experimental data and model predictions.

4.2 - Expression of Simulation Results

See corresponding paragraph in appendix 3.

5 - Bibliography

[1] D.B. Beasley, L.F. Huggins, E.J. Monke
ANSWERS: A Model of Water planning.
Trans. ASAE, 23 (4)938-944, 1980

[2] D.B. Beasley, G.Y. Platonova, T.A. Dillaha, V.Z. Kolpak, Y.M. Plis.
Adapting the ANSWERS Model for Water Quality Planning and Research on agricultural Watersheds in Chernozem Zone of the USSR. Work conducted as Part of Project 02.02.11 "River Water Quality Plannig and Management" of the joint US-USSR Agreement on Cooperation in the Field of environmental Protection. Tifton, Georgia, USA. 15 p, 1991.

[3] M.L. Cohen, W.D.Steinmetz
Foliar Washoff of Pesticides by Rainfall.
Environ. Sci. Technol. 20, 521-523, 1986.

[4] F.M. Davis, R.A. Leonard et W.G. Knisel
GLEAMS User Manual Version 1.8.55, March 1, 1990; USDA-ARS lab notr SEWRL-030190FMD, Southeast Watershed Research Laboratory, Tifton, Georgia. 62p, 1990.

[5] A.S. Donigian
Predicting Water Quality resulting from agricultural nonpoint Source Pollution via Simulation - HSPF.
In Agricultural Management and Water Quality, F.W. Schaller, G.W. Bailey Eds., Iowa State University Press, Ames, Iowa. 472 p., 1983.

[6] A.S. Donigian, N.H. Crawford
Agricultural Runoff Management (ARM) Model Version II: Refinement and Testing.
U.S. EPA, EPA-600/3-77-098, 294p, 1977.

[7] A.S. Donigian et al.1984
Application Guide for hydrological Simulation Program Fortran (HSPF).
Environmental Research Laboratory, U.S. EPA, Athens, Georgia, EPA-600/3-84-065, 177 p, 1984.

[8] M.H. Frere, C.A. Onstad, H.N. Holtan
ACTMO, an Agricultural Chemical Transport Model; ARS-H-3. USDA-ARS.
Washington DC. 54 p, 1975.

[9] H. Ghadiri, C.W. Rose
- a - Soil Processes and chemical Transport, sorbed chemical Transport in overland Flow: I. A Nutrient and Pesticide enrichment Mechanism. - b - Soil Processes and chemical Transport, sorbed chemical Transport in overland Flow : II. Enrichment Ratio Variation with Erosion Processes.
J. Environ. Qual. 20, 628-641, 1991.

[10] V. Gouy
Contribution de la modélisation à la simulation du transfert des produits phytosanitaires de la parcelle agricole vers les eaux superficielles.
Thèse de doctorat de l'Université Louis Pasteur, Strasbourg, 350 p, 1993.

[11] W.G. Knisel
CREAMS, a Field Scale Model for Chemicals, Runoff and Erosion from agricultural Management Systems.
Ed. US Department of Agriculture, Conservation Research Report 26, 643 p, 1980.

[12] J.F. Munoz
Méthodologie d'étude des produits phytosanitaires, étude d'un bassin versant viticole : l'Ardières (Beaujolais). Mise au point de méthodes analytiques de pesticides.
Thèse de doctorat de l'Université Claude Bernard, Lyon I. 175 p, 1992.

[13] Th.E.M. Ten Hulscher, W.A. Bruggeman, M.P.J.M. Kroot
A simple Model for evaluating the Fate of Micropolluants in aquatic Systems.
European Water Pollution Control, 6, 52-59, 1991.

[14] J.R. Williams, A.D. Nicks
SWRRB, a Simulator for Water Resources in rural Basins: an Overview.
In Proc. Natural Resources Modeling Symp., 1985.