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Leaching models and EU registration

The final report of the work of the Regulatory Modelling Work group of FOCUS (FOrum for the Co-ordination of pesticide fate models and their Use).

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INTRODUCTION

The Registration Directive, 91/414, concerning the placing of plant protection products was adopted by the Council of Ministers in 1991 and came into force in July 1993. This Directive laid the foundation for a harmonised system of registration of plant protection products. It became clear in the development of the Annexes which followed, which added flesh to the bones of the Directive, that mathematical modelling and Predicted Environmental Concentrations (PEC's) were going to play an important role in the decision-making process. It was also becoming clear at this time that there were many groups involved with the development of pesticide fate modelling, but that effective dialogue and exchange of ideas and experiences was not great.

An ad-hoc group met in November 1992 in Brussels to lay the foundations for the formation of FOCUS, the FOrum for the Co-ordination of pesticide fate models and their Use. FOCUS is an informal grouping of regulators, industry representatives, and experts from Government institutes - a combination of model developers, model users and people who review modelling results. The aims of this group are to promote dialogue and exchange of ideas on pesticide fate modelling issues. In particular there was an urgent need to provide guidance to the Member States, the European Commission, and Industry on the appropriate role of modelling in the rapidly developing EU registration process.

A work group was formed within FOCUS to address the issues of the role of *leaching* models in the registration process. The work group responded to the Steering Committee of FOCUS. Five one-day meetings were held between April 1993 and September 1994, funded variously by DGVI of the European Commission, the European Crop Protection Association, and COST Action 66. This report is the outcome of the work of the group. The report is intended to provide an expert opinion of the state of the art with regard to the use of leaching models in the EU regulatory process, and also to be a source of information and guidance on the key issues involved.

Taking a broader view, there is an important balance to be made between the roles of modelling and experimentation; these two disciplines are complementary to one another. However, this report unashamedly focuses on modelling alone, to provide guidance and information on this new discipline. One interface between modelling and experimentation is the selection of input parameters for modelling. There is a need for guidance on appropriate procedures for the selection of model input parameters; this is beyond the scope of this report, but will be an important area for the future.

OVERVIEW

The work of the group was split into specific tasks to address specific issues. Each of these tasks is represented in this document by a separate chapter. The overview presented here has the intention of guiding the reader through the various chapters, describing for each in turn what were the issues which the chapter sought to address. More detail can be found in the chapters themselves. Some overall conclusions are presented not here, but in the Executive Summary section which follows.

Before specific issues could be tackled, the basic ground rules have to be established, and the basic data on the state of the art has to be gathered. Three chapters cover these elements of the work. Chapter 1 is a list of definitions and terminology used in the modelling process; consensus on terminology is necessary in order to ensure a common understanding and is a pre-requisite for effective communication and debate. If you are to examine a range of models and assess their suitability and characteristics then you must first make a list of the elements which you need to look for. Chapter 2 is a consensus view of what should be included in such a checklist. Chapter 3 is a table which describes in detail the characteristics of the leaching models which were assessed by the group. This table was obtained by examining the models in conjunction with the checklist in Chapter 2; assistance in doing this was obtained from several of the authors of the models, whose help is acknowledged.

Having established the basics, some of the issues surrounding the use of leaching models are tackled in the subsequent chapters. The leaching models reviewed all suffer from some deficiencies and limitations in the way the processes affecting leaching are described. Some of these limitations are discussed in Chapter 4. If leaching models are to be used, then the user needs to have some weather, cropping and soils data to put into the models. For consistency it is important that there are some basic standard datasets, or "scenarios", available for weather, cropping and soils data. These scenarios need to cover the many different conditions which exist in the EU. The issue of how to define scenarios for the use of leaching models in the EU is covered in Chapter 5. Further work on crop, soil and weather scenarios is needed; the work on soil scenarios is continuing in the program of a new FOCUS workgroup examining modelling of soil issues (ie PEC_{soil}).

How can you validate a model? What data is needed to do this? What is the validation status of the leaching models assessed by the group? Chapters 6

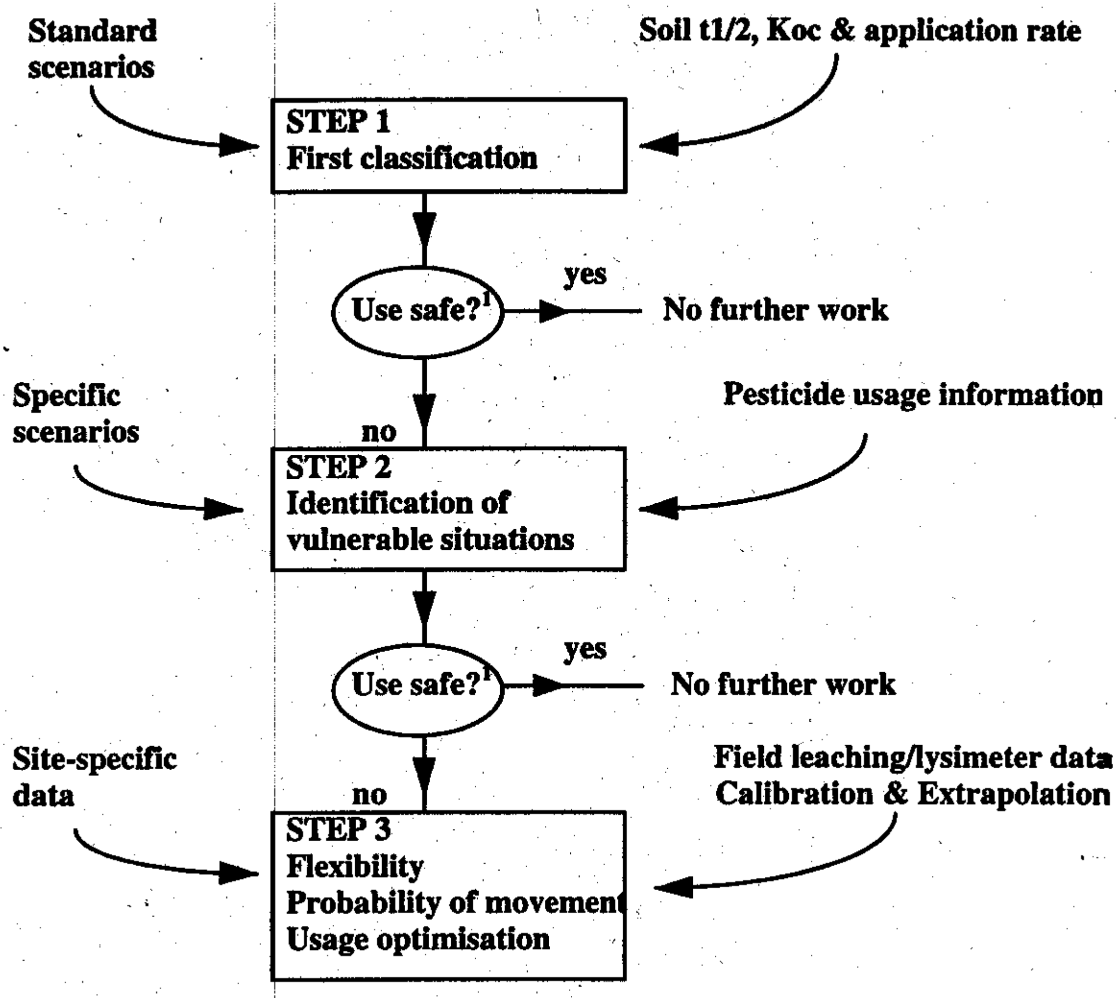
discusses the issue of what constitutes a good data set and Chapter 7 deals with model validation.

All agree that guidance is needed on how models can be used correctly in the regulatory process. In order for modelling to be used properly in this process there are certain guidelines which should be followed by model developers, maintainers and users, and these are developed in Chapter 8. This chapter covers the mechanics of modelling - what the model developer or model user has to do with the models. Chapter 9 discusses the broader issue of how models can fit into a tiered scheme for risk assessment, i.e. the proper role of leaching models in the regulatory decision-making process. The final chapter is a list of modelling tools available to researchers. It includes examples of run-off and persistence models as well as leaching models and, whilst it is not claimed to be comprehensive, serves as a catalogue for this and future work groups.

EXECUTIVE SUMMARY

What can we conclude about leaching models and their usefulness in environmental risk assessment and decision-making ***now***? What improvements are needed? Having made these improvements, what will be achievable with models ***in the future***? What will it take to get from where we are now to where we want to be? What is the alternative? The key messages of the group in each of these points are outlined in this section.

What can we conclude about leaching models and their usefulness in environmental risk assessment and decision-making *now*?



[1] As defined in Annexe 6 of the Registration Directive; decision-making criteria are beyond the scope of this document

Uses of leaching models at **Step 1**

- trigger for further work
- give a broad indication of leaching potential
- comparison with chemicals of known leaching behaviour
- enables uniform comparison and simple review

Uses of leaching models at **Step 2**

- identify vulnerable soils/crops/product uses
- but accuracy will be low at this Step, so Step 2 refines further investigation more often than resulting in a decision

Uses of leaching models at **Step 3**

- calibration at this Step increases the accuracy compared to Step 2, so that a decision can be made
- can say something about probabilities of leaching
- usage optimisation

Fully validated leaching model at the EU level does not exist

- but this does not mean that these models have no use in the regulatory process

Little relevant validation work has been done at residue levels which represent a very low fraction of the amount applied

The models are reliable for describing the movement of the bulk of the chemical

- when used correctly

Selection of a suitable model

- many factors to consider (Chapter 2)
- the key data in many models are displayed in Chapter 3
- none of the 9 models considered are ideal, but all are worthy of consideration
- many of the models are similar technically, so other factors such as ease of use and support become important

We need to use the models now

- they can be used now, in certain situations, including at a screening level
- their use can improve the quality of risk assessments

What improvements are needed?

Model maintenance; institutionalised models at the EU level

- version control, code quality etc.
- support
- manuals
- training
- register of users

Full set of <u>accessible</u> model scenarios for the whole EU

- crops
- weather
- soils

Procedures for the correct use and reporting of models (see Chapter 7)

Good leaching datasets (real measurements)

- high quality datasets (field and lysimeter)
- with the right measurements (see Chapter 6)

→ model validation

→ improve the models

Model validation

- requires high quality leaching datasets (see above)
- important for credibility and increasing confidence in decision-making

Better process description → better models

Basic science:

- preferential flow
- subsoil degradation
- chemical processes

Implementing established science:

- evapotranspiration

Having made these improvements, what will be achievable with models *in the future*?

Consistency of risk assessments (common basis for assessment)

because

- quality of and support for models
- common set of scenarios (crop, soil, climate)
- enable consistent use of models across
  - :companies
  - :countries where a.i. is used
  - :countries assessing data
  - :different a.i.s

Rapid assessment

Up-to-date modelling tools

taking into account

- new scientific developments
- new regulatory developments

Better appreciation by a wider audience of the causes of leaching, its assessment, and how to manage it

Better accuracy of model predictions, enabling more reliable decision-making at Tiers 1 and 2

What will it take to get from where we are now to where we want to be?

Willingness of all parties to work together towards a common understanding

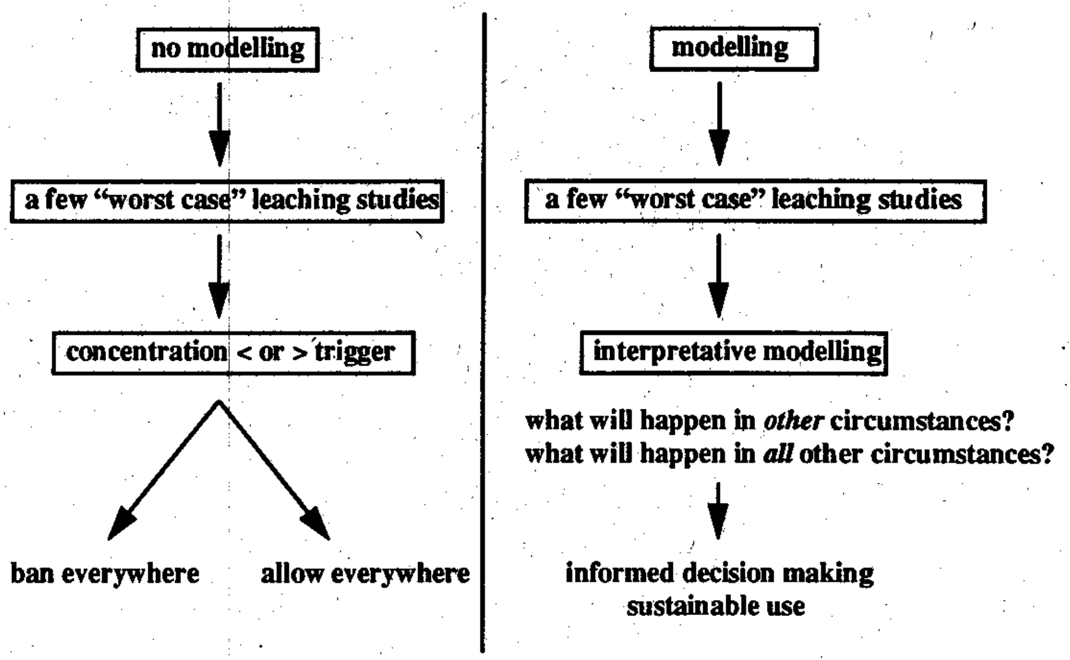
Funding (model institutionalisation, validation and improvement, scenario development and testing, research)

Dialogue between disparate modelling groups

What is the alternative?

Modelling is more generally applicable than monitoring because monitoring gives only information for the circumstances considered: any extrapolation in time and space of monitoring is based implicitly on some model, albeit non-mathematical. Another important advantage is that modelling can be done **before** the introduction of new compounds.

Modelling can give answers to important quantitative questions such as "Will this pesticide reach groundwater, if so then in what circumstances of use, region, crop, weather, soil, and at what concentration?". The following scheme shows how modelling leads to a higher quality and more flexibility of the risk assessment procedure.



Use of modelling alongside practical studies is the only route to a scientific risk assessment, the only way to ensure we share the benefits of pesticide use without unacceptable pesticide residues in groundwater. Alternative is decision-making on the basis of inadequate and non-comparable data, leading to unnecessary groundwater contamination and unnecessary restriction of safe products of benefit to agriculture. Also slower decisions and higher costs to all.

Chapter 1

Definitions to be used by the FOCUS Regulatory Modelling Work group

J. Boesten and K. Travis

model: simplified representation of a part of reality that contains mutually dependent elements

conceptual model: model in which the elements are described explicitly and in which their mutual dependencies are described; conceptual models are usually described in words or via a diagram

mathematical model: model that describes the conceptual model in terms of mathematical equations

computer model: model that describes the mathematical model in code that can be executed by a computer; this does not include the actual values of the input parameters

deterministic model: mathematical or computer model in which all parameters can have one unique value only and in which one parameter set results in one unique output

probabilistic model: mathematical or computer model which accounts for variability in one or more input parameters and expresses outputs as probability density functions; a probabilistic model is often just a deterministic model run many times

stochastic model: mathematical or computer model in which some or all parameters are handled explicitly as stochastic variables in the governing equations of the model, and which expresses outputs as probability density functions

verification: examination of the numerical technique in the computer model to ascertain that it truly represents the mathematical model and that there are no inherent numerical problems with obtaining a solution; this implies also a check on errors in the code (programming bugs)

calibration: adjusting one or more input parameters to improve the match between model output and experimental data

validation process: comparison of model output with data independently derived from experiments or observations of the environment; this implies that none of the input parameters is obtained via calibration; note that this definition does not specify any correspondence between model output and measured data

validated model: model which has gone successfully through a validation process for a specified range of validity; this implies that the number of data sets considered is sufficient for the intended use of the model

range of validity: that part of reality to which the validation of a model applies

validation status: the extent to which a model has successfully been validated within its range of validity

sensitivity analysis: analysis of the degree to which the model result is affected by changes in input parameters; often done by examining the % change in one output caused by the % change in an input parameter; the purpose is to obtain a better understanding of the behaviour of the model

uncertainty analysis: analysis of the degree to which the model result is affected by the uncertainty in input parameters; the purpose of uncertainty analysis is to examine the effects of lack of precise knowledge of input parameters caused e.g. by natural variation or variation resulting from measurement or analytical techniques

version control: the measures taken by the institute that delivers the software package to ensure that the specified number of the version identifies the package uniquely

software package: the computer code (both source and executables) that is provided to users; so the package includes all files on the diskette(s) which will usually include also one or more scenario's and standard data sets for checking

scenario: a representative combination of crop, soil, climate and agronomic parameters to be used in modelling; representative means in this context that the selected scenarios should represent physical sites known to exist, i.e. the combination of crop, soil, climate and agronomic conditions should be realistic

<u>distribution of scenarios</u>: a number of scenarios to be created which reasonably characterise the range of driving forces for the environmental fate mechanism being studied; driving forces are in this context the primary variables controlling the environmental fate mechanism

Part of the above definitions have been based ASTM Designation E 978 - 84 entitled "Standard practice for evaluating environmental fate models of chemicals" (p. 582-587 in 1990 Annual book of ASTM standards, Vol. 11.04, Section 11, Water and environmental technology).

Chapter 2

Elements for Assessing Models

H. Schäfer and R. Jones

1. General Information

- Name of model
- Name or number of most recent release
- Intended use of model
- Model developers
- Sponsoring institution
- Date of most recent release

2. Documentation and Systems Considerations

2.1. User manual

- Availability
- Language
- Clarity
- Defines model limitations
- Includes conceptual model description
- Includes mathematical model description
- Includes sensitivity analysis
- Provides assistance in determining model parameters
- Provides test examples
- Provides references

2.2. Other documentation considerations

- Tightness of version control
- Availability of source code

2.3. Systems considerations

- Hardware requirements
- Run time for standard scenario
- Reliability
- Clarity of error messages

2.4. Support

- Method of support (Existence of responsible institution?)
- Availability of information about bugs, corrections, and new versions
- Training for users

2.5. Input/Preprocessor
- User friendliness
- Help utility
- Data range checking
- Sample input files
- Database included
- Availability of needed data
- Flexibility

2.6. Output/Postprocessor
- Nature of output
- User friendliness
- Help utility
- Sample files
- Flexibility
- Documents input parameters
- Clarity of output reports

3. Model Science

3.1. Compartments considered

soil, soil water, soil air, plant, root zone, vadose zone, saturated zone

3.2 Numerical technique
- Adequacy of algorithm
- Definition of lower hydrologic boundary conditions
- Stability
- Numerical dispersion
- Time increments
- Space (depth) increments
- Verification of numerical technique

3.3. Soil model (horizontal and vertical heterogeneity)

3.4. Hydrology model
- Type (tipping bucket or water potential)

- Evapotranspiration model
- Capillary rise
- Runoff and erosion
- Preferential flow

3.5 Pesticide model

- Metabolites
- Adsorption
  Type of model (linear, non-linear, kinetic)
  Dependency on environmental parameters (i.e. temperature, moisture, soil
  depth)
- Degradation in soil
  Type of model (first order, power law, Menten)
  Dependency on environmental parameters (i.e. temperature, moisture, soil
  depth)
  Mechanisms considered (abiotic, biotic)
  Compartments considered (soil, soil water, soil air, plant)
- Dispersion in soil
- Volatility
- Plant uptake
- Degradation on plant surfaces
- Foliar washoff
- Runoff and erosion

3.6. Agronomy models

- Cultivation (i.e. ploughing, residues)
- Irrigation
- Application
  Frequency of application (single, multiple)
  Application technique (i.e. spray, soil incorporation)

3.7. Plant model

- Foliage
  - Purpose (use in computer program)
  - Description
  - Flexibility
- Rooting
  - Purpose (use in computer program)
  - Description
  - Flexibility

3.8. Heat model

- Purpose (use in computer program)
- Description

Chapter 3

Assessment of Various Leaching Models

R. Jones and H. Schäfer

This chapter tabulates the performance of 9 commonly used models against the criteria outlined in Chapter 2.

Assessment of Various Leaching Models
1. General Information

	PRZM-2	PRZM	PELMO
Name of model	Pesticide Root Zone Model - 2	Pesticide Root Zone Model	Pesticide Leaching MOdel
Name or number of most recent release	Release 1.02	Release 1.0	Release 1.0 (Release 1.5 beta test)
Intended use of model	Principal purpose is to calculate of pesticide movement in surface and subsoils. The model also considers volatility, runoff, and erosion losses from the soil surface.	Principal purpose is to calculate of pesticide movement in surface and subsoils. The model also considers runoff, and erosion losses from the soil surface.	Model is mainly intended to calculate leaching of pesticides in soil, but runoff and erosion are also included.
Model developers	R. F. Carsel et al.	R. F. Carsel et al.	M. Klein
Sponsoring institution	U.S. Environmental Protection Agency, USA	U.S. Environmental Protection Agency, USA	Fraunhofer Institut für Umweltchemie and Ökotoxikologie, Schmallenberg, Germany
Date of most recent release	1993	1984	1991 (Release 1.0) 1993 (Release 1.5 beta test)

Assessment of Various Leaching Models
1. General Information (continued)

	GLEAMS	PESTLA	VARLEACH
Name of model	Groundwater Loading of Agricultural Management System	PESTicide Leaching and Accumulation	VARLEACH (most recent version of the original CALF model)
Name or number of most recent release	Version 2.03	Version 2.3	Version 1.0
Intended use of model	Predict the effect of management decisions on water, sediment, and pesticide yields at the edge of a field and at the bottom of the root zone	Simulate pesticide leaching and persistence in soils	VARLEACH is a simple leaching model that incorporates subroutines to allow for the effects of temperature and soil moisture on degradation rates in soil.
Model developers	R. A. Leonard, W. G. Knisel, D. A. Still	J.J.T.I. Boesten et al.	A. Walker and P. H. Nicholls
Sponsoring institution	USDA/ARS Southeast Watershed Laboratory, USA	DLO Winand Staring Centre, The Netherlands	Horticulture Research International, U.K. Rothamsted Experimental Station, U.K.
Date of most recent release	January 1992	December 1993	August 1993

Assessment of Various Leaching Models
1. General Information (continued)

	LEACHM	MACRO	PLM
Name of model	Leaching Estimation And CHemistry Model	MACRO	Pesticide Leaching Model
Name or number of most recent release	Release 3.1	Release 3.0	Release 3.0
Intended use of model	Model ins intended to calculate leaching of pesticides in soil	Model simulates water movement and solute transport in macroporous systems	Simulates pesticide movement and degradation in soil, including preferential flow mechanisms
Model developers	J. L. Hutson, R. J. Wagenet	N. Jarvis	D. G. M. Hall, P. H. Nicholls
Sponsoring institution	Cornell University, Ithaca, NY, USA	Swedish Environmental Protection Agency; Swedish University of Agricultural Sciences, Uppsala, Sweden	Rothamsted Experimental Station, U.K.
Date of most recent release	1993	1993	August 1994

Assessment of Various Leaching Models
2. Documentation and Systems Considerations

	PRZM-2	PRZM	PELMO
2.1 User manual			
Availability	Included as a Word Perfect file with the source code	EPA Publication	Publication of Fraunhofer Institut
Language	English	English	German
Clarity	Good	Good	Good
Defines model limitations	Limitations of each module are specified in the user manual.	Limitations are specified in the user manual.	No
Includes conceptual model description	Lengthy description	Lengthy description	Short description
Includes mathematical model description	Yes	Yes	Description of differences with PRZM
Includes sensitivity analyses	Traditional sensitivity analyses are not in user manual; however, the model has a feature for simulating the effect of variability in input parameters.	Discussed in manual	No
Provides assistance in determining model parameters	The manual provides extensive assistance.	The manual provides extensive assistance.	Utility for estimation of diffusion coefficients
Provides test examples	Example input files listed in manual	Example input and output files listed in manual	Example output files listed in manual
Provides references	Extensive list	Extensive list	Yes
2.2 Other documentation considerations			
Tightness of version control	Version specified on output	Version specified on output	Tight version control
Availability of source code	Supplied on program diskette	Supplied on program diskette	Supplied on program diskette

Assessment of Various Leaching Models
2. Documentation and Systems Considerations (continued)

	GLEAMS	PESTLA	VARLEACH
2.1 User manual Availability	Included as a Word Perfect file with the source code	Report from DLO Winand Staring Centre supplied with program diskettes	Explanatory notes are available as README file with diskette, full annotation included in source code; no user manual available
Language	English	English	English
Clarity	Good	Good	(No user manual)
Defines model limitations	Limited discussion	Limited discussion	(No user manual)
Includes conceptual model description	A description of most of the submodels is included with the discussion on parameter estimation, but there is no overall discussion of the entire model	Yes	(No user manual)
Includes mathematical model description	A mathematical description of some of the submodels is included	Yes	(No user manual)
Includes sensitivity analyses	The manual does a very good job of discussing the sensitivity of the model parameters during the discussion of individual parameters. There is no overall discussion of parameter sensitivity	Yes	(No user manual)
Provides assistance in determining model parameters	The user manual provides extensive assistance	Yes	(No user manual)
Provides test examples	The user manual does not contain a test example	Yes	(No user manual)
Provides references	Extensive list	Yes	(No user manual)

2.2 Other documentation considerations

Tightness of version control	Tight version control	Tight version control	There is no strict version control for the original CALF model. The most recent version has been named VARLEACH 1.0 and any updates will be given new version numbers as appropriate
Availability of source code	Supplied on program diskette	Supplied on program diskette	Supplied with program

Assessment of Various Leaching Models
2. Documentation and Systems Considerations (continued)

	LEACHM	MACRO	PLM
2.1 User manual			
Availability	Publication of Cornell University	Publication of Swedish University of Agricultural Sciences, Uppsala	Published as MSc thesis (Nottingham University)
Language	English	English	English
Clarity	Good	Good	Good
Defines model limitations	Yes	Assumptions provided, but limitations not specifically discussed	Model assumptions are provided in discussion present in the user manual
Includes conceptual model description	Yes	Yes	Provides most information in the user manual, for some descriptions the user is referred to two articles in press
Includes mathematical model description	Yes	Yes	Provides information in the user manual, for some descriptions the user is referred to two articles in press
Includes sensitivity analyses	No	Yes	No
Provides assistance in determining model parameters	Utility for estimation of potential evapotranspiration. Utility for estimation of water retention data	Yes	Some guidance provided for a few parameters
Provides test examples	Input and output files in manual	No	Yes
Provides references	Yes	Yes	Yes
2.2 Other documentation considerations			
Tightness of version control	Tight version control	Tight version control	Tight version control
Availability of source code	Program is distributed as source code	Distributed upon request	Available

Assessment of Various Leaching Models
2. Documentation and Systems Considerations (continued)

	PRZM-2	PRZM	PELMO
2.3 Systems considerations			
Hardware requirements	386 or 486 compatible computer, MS or PC DOS 3.3 or higher, 640k base memory, 4 mb of extended memory, 4.5 mb hard disk storage	Original release was for a mainframe computer, later a version for PC was released	PC with math coprocessor, DOS
Run time for standard scenario	Depends on options selected	Depends on options selected	Medium (~1 CPU minute for 1 simulated year on a 486
Reliability	Program usually performs without problems if input parameters are correctly specified	Program usually performs without problems if input parameters are correctly specified	Program performs without problems if input data are correct
Clarity of error messages	List of error messages provided in the user manual	Sometimes difficult to understand	Difficult to understand

	PRZM-2	PRZM	PELMO
2.4 Support			
Method of support	Model is supported by the U.S. EPA Center for Environmental Modeling. Contact telephone and fax numbers are provided in the user manual.	More recent version now supported by U.S. EPA.	Staff at Fraunhofer are helpful in resolving problems (by phone or telefax)
Availability of information about bugs and corrections	No information about bugs is systematically distributed to users.	No information about bugs is systematically distributed to users.	No information about bugs is systematically distributed to users.
Training for users	Training sessions are held occasionally by the U.S. EPA	Training available only for more recent version	Training sessions possible upon request

Assessment of Various Leaching Models
2. Documentation and Systems Considerations (continued)

	GLEAMS	PESTLA	VARLEACH
2.3 Systems considerations			
Hardware requirements	IBM PC-AT or IBM-compatible systems having 512 or greater RAM. Program compilation requires at least 384K of RAM, more than 384K is preferable. Use of the 8-87 Arithmetic Coprocessor chip will execute programs much more rapidly	IBM compatible PC (386 or 486) with a math coprocessor	IBM compatible 80286 (or later)
Run time for standard scenario	Low (about 30 seconds per simulated year)	2-3 minutes per simulated year on a 486 PC using a maximum time step of 0.1 day	Low
Reliability	Programs performs without problems if input data are correct	Programs performs without problems if input data are correct	Program performs without problems if input data are correct
Clarity of error messages	Not very specific	Good messages for errors in input data, messages are limited for run time errors	No error messages generated by program
2.4 Support			
Method of support	Provided by Frank Davis, USDA and Walter Knisel, University of Georgia	Provided by J.J.T.I. Boesten of DLO Winand Staring Centre	Provided by A. Walker of Horticulture Research Institute and P.H. Nicholls of Rothamsted Experimental Station
Availability of information about bugs and corrections	No information about bugs is systematically distributed to users.	No information about bugs is systematically distributed. The user manual gives the anticipated date for release of the next version	No information about bugs is systematically distributed
Training for users	None	Training available upon request	None

Assessment of Various Leaching Models

2. Documentation and Systems Considerations (continued)

	LEACHM	MACRO	PLM
2.3 Systems considerations			
Hardware requirements	No special hardware specified, model is distributed as source code	PC with coprocessor, DOS	No special hardware specified. Model is distributed as an executable code for IBC compatible PCs
Run time for standard scenario	Depends on hardware, 486 is preferred	Depends on hardware, 486 is preferred	Fast with co-processor
Reliability	Program performs without problems if input data are correct	Program crashes sometimes without error message. Computer has to be rebooted	Object oriented for reliability
Clarity of error messages	Few error messages	Very few error messages	Error messages on data entry
2.4 Support			
Method of support	J. L. Hutson is helpful (phone or telefax)	N. Jarvis is helpful (phone or telefax)	P. Nicholls is helpful
Availability of information about bugs and corrections	No information about bugs is systematically distributed	No information about bugs is systematically distributed	No information about bugs is systematically distributed
Training for users	None	None	None

Assessment of Various Leaching Models
2. Documentation and Systems Considerations (continued)

	PRZM-2	PRZM	PELMO
2.5 Input/Preprocessor			
User friendliness	Minimal	Minimal	Low
Help utility	None	None	For Release 1.5
Data range checking	Some limited checking.	Some limited checking.	Some limited checking.
Sample input files	Included with source code	Included with source code	Yes
Databases included	Supplementary weather data base available. Much information on input parameters included in the user manual.	Supplementary weather data base available. Much information on input parameters included in the user manual.	No but weather and soil properties for standard scenarios included
Availability of needed data	All input parameters are readily obtainable from soil and weather data bases. Obtaining access to such information is difficult in some countries.	All input parameters are readily obtainable from soil and weather data bases. Obtaining access to such information is difficult in some countries.	All input parameters are readily obtainable from soil and weather data bases. Obtaining access to such information is difficult in some countries.
Flexibility	The wide range of options makes the program quite flexible but developing input data is somewhat daunting to occasional users.	PRZM is quite flexible, but simpler than PRZM-2. Therefore development of input data for PRZM is easier than for PRZM-2, especially for occasional users.	User can specify different options
2.6 Output/Postprocessor			
Nature of output	Tabular form only, program has the capability to produce files that are compatible with standard graphics packages.	Tabular form only, program has the capability to produce files which can be used with standard graphics packages	Tabular and graphical representation of concentration profile and leachate data
User friendliness	Minimal	Minimal	High
Help utility	None	None	None
Sample files	Included with source code	Included with source code	Yes
Flexibility	Ability to produce a wide range of reports. Snapshot feature is especially good for comparing predictions with field measurements.	Can produce daily, monthly, or annual reports	Daily, monthly, or annual reports
Documents input parameters	Yes	Yes	yes
Clarity of output reports	Good	Good	good

Assessment of Various Leaching Models
2. Documentation and Systems Considerations (continued)

	GLEAMS	PESTLA	VARLEACH
2.5 Input/Preprocessor			
User friendliness	Parameter editor files have been developed to assist in developing input parameter files	Minimal	Input parameters supplied by interactive input, help provided for location of parameters
Help utility	Generalised help tables provided	None	None
Data range checking	Yes, if editor is used	Yes	yes
Sample input files	Yes	Yes	Sample weather data file included
Databases included	Generalised help tables, including information on pesticide properties, are provided to assist in developing	No but weather and soil properties for standard scenario included	No
Availability of needed data	All input parameters are readily obtainable from soil and weather data bases. Obtaining access to such information is difficult in some countries.	Most data are readily available. Soil hydraulic properties are not readily available but can be estimated. Obtaining access to soil and weather data bases in difficult in some countries.	All input parameters are readily obtainable from soil and weather data bases. Obtaining access to such information is difficult in some countries.
Flexibility	The wide range of options makes the program quite flexible but developing input data is somewhat daunting to occasional users.	The wide range of options makes the program is quite flexible, but also difficult for the occasional user to use (except for simulations with the standard scenario).	Various options make simulations possible for a variety of situations
2.6 Output/Postprocessor			
Nature of output	Tabular	Tabular	Tabular but output provides summary data format suitable for direct input to FREELANCE graphics package
User friendliness	Minimal	Minimal	Reports automatically generated at user specified intervals
Help utility	Help table included for selecting output variables	None	None
Sample files	Yes	Yes	No

Flexibility	Output variables are selected individually. For a specific variable, frequency of reports can be daily, monthly, or annual	Produces fixed reports at specified intervals	Produces fixed reports at specified intervals
Documents input parameters	Some of the input parameters	Yes	Yes
Clarity of output reports	Good, but there is no explanation of output reports in the manual	Difficult to understand without carefully studying the explanation in the user manual	Good

Assessment of Various Leaching Models
2. Documentation and Systems Considerations (continued)

	LEACHM	MACRO	PLM
2.5 Input/Preprocessor			
User friendliness	Low	High	Editor screens developed for general simulation parameters, pesticide properties, and soil parameters. File containing weather data and crop activity must be developed outside the program.
Help utility	No	Yes	Yes
Data range checking	Yes	Yes, except weather data	Yes, except weather data and crop activity information. There is a utility to check the format of the weather file.
Sample input files	Yes	Yes	Yes
Databases included	No	No	No
Availability of needed data	Weather and soil data not readily obtainable, but can be estimated by utilities	Weather data obtainable. Soil parameters should be measured and calibrated against field data	Weather and soil properties are readily available, although obtaining access to this information may be difficult in some countries. Parameters describing macropores should be calibrated using field data.
Flexibility	User can specify different options	Low	Crop parameters inflexible; rest of input parameters relatively flexible.
2.6 Output/Postprocessor			
Nature of output	Only tabular form	Tabular and graphical form	Tabular and graphical forms
User friendliness	Low	High	High
Help utility	No	Yes	No
Sample files	Yes	No	Yes
Flexibility	User can specify kind and interval of output	High	Output very flexible
Documents input parameters	Yes	Yes	Yes
Clarity of output reports	Good	Good	Good

Assessment of Various Leaching Models
3. Model Science

	PRZM-2	PRZM	PELMO
3.1 Compartments considered	Plant (foliar washoff and degradation, plant uptake), soil surface (runoff, erosion, and volatilisation), and soil (soil, soil water, and soil air)	Plant (foliar washoff and degradation, plant uptake), soil surface (runoff and erosion), and soil (soil and soil water)	Plant (foliar washoff, degradation, plant uptake), soil surface (runoff, erosion), and soil (soil, soil water, in release 1.5 also soil air)
3.2 Numerical technique			
Adequacy of algorithm	User can choose one of two difference techniques: a backwards-difference implicit technique (which may be affected by numerical dispersion) and a method of characteristics algorithm, which takes more computational time, but is less affected by numerical dispersion.	Model uses a backwards-difference implicit technique (which is affected by numerical dispersion).	Model uses a backwards-difference implicit technique (which is affected by numerical dispersion).
Definition of lower boundary conditions	Automatically set by program to unsaturated flow	Automatically set by program to unsaturated flow	Automatically set by program to unsaturated flow
Stability	No problems reported.	No problems reported.	No problems reported
Numerical dispersion	Numerical dispersion can be significant with the backwards-difference implicit technique. Can be used to simulate physical dispersion. Use of the method of characteristics algorithm minimises numerical dispersion.	Numerical dispersion can be significant. Can be used to simulate physical dispersion.	Used to simulate physical dispersion
Time increments	1 day	1 day	1 day
Space (depth) increments	Set by user	Set by user	Set by user
Verification of numerical technique	Different techniques have been compared with analytical solutions and with each other	Predictions have been compared with analytical solutions.	Not reported

Assessment of Various Leaching Models
3. Model Science (continued)

	GLEAMS	PESTLA	VARLEACH
3.1 Compartments considered	Plant (foliar washoff and degradation, plant uptake), soil surface (runoff and erosion), and soil (soil and soil water)	Soil (soil and soil water)	Soil (soil and soil water)
3.2 Numerical technique Adequacy of algorithm	Not known	The water equation is solved via an implicit finite difference scheme, the heat equation is solved using an implicit finite difference technique, and the pesticide equation is solved using an explicit finite difference method.	The water equations is solved via step-wise integration.
Definition of boundary conditions	Automatically set by program to unsaturated flow	Seven options	Automatically set by program to unsaturated flow
Stability	Stable	Stable but additional compartments should be added at the bottom of the soil column to dampen numerical oscillations (as described in the user manual)	Excellent
Numerical dispersion	Not known	Minimal dispersion because a central difference approach is used in the pesticide algorithm	Program uses an automatic time and depth increment which determines the amount of numerical dispersion
Time increments	1 day	0.1 days, can be changed by the user	0.05 day
Space (depth) increments	Set by program	Set by user	1 cm
Verification of numerical technique	Not reported	Results of pesticide and heat algorithms have been checked against analytical solutions	Not reported

Assessment of Various Leaching Models
3. Model Science (continued)

	LEACHM	MACRO	PLM
3.1 Compartments considered	Plant (plant uptake), soil (soil, soil water, soil air)	Plant (plant uptake, processes on leaves) soil (soil, soil water, micropores, macropores)	Soil (soil, fast and slow mobile water, and immobile water)
3.2 Numerical technique			
Adequacy of algorithm	Model uses Crank-Nicholson implicit method	Explicit finite difference procedure for micropore region. Implicit scheme for macropore domain.	All of the pestidice is accounted for if the degradation rate is set to zero.
Definition of lower hydrologic boundary condition	Lower hydrologic boundary condition is set by user (constant hydraulic gradient, zero flux, unit hydraulic gradient, fluctuating water table, lysimeter tank)	Lower hydrologic boundary condition is set by user (constant hydraulic gradient, zero flux, constant potential with inflow and outflow, constant potential with no inflow)	Automatically set by program to unsaturated flow
Stability	No problems observed, evidently stability problems reported for earlier versions have been resolved	No problems observed	Good
Numerical dispersion	Numerical dispersion correction implemented	Numerical dispersion correction implemented	Not known.
Time increments	Set by program (<0.1 day)	Variable	1 day
Space (depth) increments	Set by user	Set by user (maximum of 15 increments)	5 cm
Verification of numerical technique	Comparison with analytical solution for uniform water content and flux density	Not known	Simulations have been checked against measured data and published.

Assessment of Various Leaching Models
3. Model Science (continued)

	PRZM-2	PRZM	PELMO
3.3 Soil model	Homogeneous soil (vertical and horizontal) within a specified soil layer, but properties in different soil layers may vary.	Homogeneous soil (vertical and horizontal) within a specified soil layer, but properties in different soil layers may vary.	Homogeneous soil within a specified soil horizon. Soil horizons with different soil properties can be specified
3.4 Hydrology model Type	In the root zone, a capacity model is used. Below the root zone, the user can choose either a capacity model or a Richard's equation routine.	Capacity model	Capacity model
Evapotranspiration model	Estimation of potential evaporation from pan evaporation data. Another option is to estimate potential evaporation from average temperature data.	Estimation of potential evaporation from pan evaporation data. Another option is to estimate potential evaporation from average temperature data.	Potential evaporation calculated using Haude (based on air temperature and humidity) or Hamon (based on air temperature) model
Capillary rise	Not considered.	Not considered	Not considered
Runoff and erosion	Soil Conservation Service curve number technique and the Universal Soil Loss Equation	Soil Conservation Service curve number technique and the Universal Soil Loss Equation	By Fraunhofer modified SCS curve number technique and MUSLE
Preferential flow	Not considered.	Not considered.	Not considered

Assessment of Various Leaching Models
3. Model Science (continued)

	GLEAMS	PESTLA	VARLEACH
3.3 Soil model	Homogeneous soil (vertical and horizontal) within a specified soil layer, but properties in different soil layers may vary.	Homogeneous soil, but most parameters can be varied with depth	Homogeneous soil but all parameters can be varied with depth in the profile
3.4 Hydrology model			
Type	Capacity model	Richards equation	Capacity model
Evapotranspiration model	Calculated from daily or monthly temperature data and monthly radiation data	Potential evaporation calculated using the Penman equation	Estimation of potential evaporation from pan evaporation data. Another option is to estimate potential evaporation from average temperature data.
Capillary rise	Not considered	Considered	Considered by water deficit equalisation routines
Runoff and erosion	Soil Conservation Service curve number technique and the Universal Soil Loss Equation. Sophisticated erosion routines including ability to simulate change flow and temporary impoundments.	If the amount of ponding water exceeds a value specified by the user, the excess water is assumed to disappear via runoff. Erosion is not considered.	Not considered
Preferential flow	Not considered	Not considered	Not considered

Assessment of Various Leaching Models
3. Model Science (continued)

	LEACHM	MACRO	PLM
3.3 Soil model	Soil column divided into homogeneous layers	Soil column divided into homogeneous layers	Soil column divided into homogeneous layers. Water is divided into fast and slow mobile water and immobile water.

	LEACHM	MACRO	PLM
3.4 Hydrology model Type	Richards equation	Richards equation plus macropore flow	Capacity model plus fast flow mechanism
Evapotranspiration model	Input of potential evaporation data or estimation using Linacres equation	Potential evaporation data required	Estimation of potential evaporation from measured or calculated pan evaporation data.
Capillary rise	Considered	Considered	Considered by water deficit equalization routines
Runoff and erosion	Not considered	Only runoff considered	Not considered
Preferential flow	Not considered	Two domain model with macropore flow	Considered when soil field capacity is exceeded

Assessment of Various Leaching Models
3. Model Science (continued)

	PRZM-2	PRZM	PELMO
3.5 Pesticide model Metabolites	The program can simulate up to 3 chemicals simultaneously (this permits simulation of parent and two metabolites).	The program can simulate one chemical.	One chemical considered
Sorption Type of model	Linear sorption	Linear sorption	Freundlich adsorption
Dependency on environmental parameters	Kd specified for each horizon or Koc specified along with organic carbon for each horizon. The program allows Kd to be reset to a new value at any time during the simulation so this feature can be used to approximate the effect of non-linear sorption.	Kd specified for each horizon or Koc specified along with organic carbon for each horizon	Kd specified for each horizon or Koc specified along with organic carbon for each horizon
Degradation in soil Type of model	First order kinetics	First order kinetics	Power law equation
Dependency on environmental parameters	No correction for temperature or soil moisture content. The decay rate can vary with depth. The program also allows the degradation rate to be reset to a new value at any time during the simulation.	No correction for temperature or soil moisture content. The decay rate can vary with depth.	Rate constants corrected for temperature (Q10-approach) and moisture influence (Walker model)
Mechanisms considered	Microbial degradation may be simulated separately from chemical degradation.	Only one degradation process considered (no distinction between biotic and abiotic mechanisms)	Only one degradation process considered (no distinction between biotic and abiotic mechanisms)
Compartments considered	May specify overall degradation rate or degradation rate in soil, soil water, or soil air.	Model uses overall degradation rate.	Lumped kinetics for pesticide in soil and soil water

Assessment of Various Leaching Models
3. Model Science (continued)

	GLEAMS	PESTLA	VARLEACH
3.5 Pesticide model Metabolites	Each pesticide may have up to two metabolites. Up to ten pesticides (including metabolites) may be simulated in a single simulation.	One chemical considered	One chemical considered
Sorption Type of model	Linear sorption	Freundlich adsorption	Linear sorption, with sorption increasing with time in upper soil layer
Dependency on environmental parameters	Koc specified along with organic carbon for each horizon	Koc specified along with organic carbon and bulk density as a function of depth	Kd can be specified as a function of depth
Degradation in soil Type of model	First order kinetics	First order kinetics	First order kinetics
Dependency on environmental parameters	No correction for temperature or soil moisture content. The decay rate can vary with depth.	Rate constants adjusted for effects of soil temperature, moisture, and depth.	Rate constants adjusted for effects of soil temperature and soil moisture
Mechanisms considered	Only one degradation process considered (no distinction between biotic and abiotic mechanisms).	Only one degradation process considered (no distinction between biotic and abiotic mechanisms).	Only one degradation process considered (no distinction between biotic and abiotic mechanisms).
Compartments considered	Model uses overall degradation rate	Model uses overall degradation rate.	Model uses overall degradation rate.

Assessment of Various Leaching Models
3. Model Science (continued)

	LEACHM	MACRO	PLM
3.5 Pesticide model			
Metabolites	Up to ten chemicals considered	One chemical considered	One chemical considered
Sorption Type of model	Freundlich adsorption or two-site adsorption kinetics	Linear adsorption	Linear adsorption, with sorption increasing with time in upper 5 cm of soil.
Dependency on environmental parameters	Kd calculated for each layer using specified Koc along with organic carbon of each horizon	Set for each layer by user	Sorption values can be set for each of three soil layers
Degradation in soil Type of model	First order kinetics	First order kinetics	First order kinetics
Dependency on environmental parameters	Rate constants corrected for temperature (Q10-approach) and moisture influence	Rate constants corrected for temperature and moisture influence	Rate constants adjusted for effects of soil temperature and soil moisture
Mechanisms considered	Only one degradation mechanism considered (no distinction between biotic and abiotic mechanisms).	Only one degradation mechanism considered (no distinction between biotic and abiotic mechanisms).	Only one degradation process considered (no distinction between biotic and abiotic mechanisms).
Compartments considered	Lumped kinetics for pesticide in soil and soil water or degradation in solute phase only	Different rates in soil surrounding micropores, soil surrounding macropores, water in micropores, and water in macropores	Model uses overall degradation rate.

Assessment of Various Leaching Models
3. Model Science (continued)

	PRZM-2	PRZM	PELMO
3.5 Pesticide model (continued)			
Dispersion in soil	Modelled by numerical dispersion or set by user	Modelled by numerical dispersion or set by user	Modelled by numerical dispersion or set by user
Volatility	Approach used is combination of previous research.	not considered	Only in release 1.5
Plant uptake	Simple model used.	Simple model used.	Proportional to water uptake by plant
Degradation on plant surfaces	First order kinetics.	First order kinetics.	First order kinetics
Foliar washoff	Simple model used	Simple model used	Proportional to daily rainfall and pesticide mass on foliage
Runoff and erosion	Mass balance approach based on results from hydrology model.	Mass balance approach based on results from hydrology model.	Mass balance approach based on results from hydrology model
3.6 Agronomy models			
Cultivation	Bulk density can be changed during the simulation.	Not considered	Not considered
Irrigation	The program has to ability to automatically trigger irrigation due to a drop in the soil water content. Calculations are performed for sprinkler, flood, or furrow irrigation.	Irrigation must be added to rainfall data.	Irrigation must be added to rainfall data.
Application Frequency of applications	Up to 50 applications can be simulated.	Model can be used to simulate multiple applications	Multiple applications (up to 50)
Application technique	Applications may be foliar sprays, applied to the soil surface, or incorporated into the soil.	Applications may be foliar sprays, applied to the soil surface, or incorporated into the soil.	Foliar application, applied to soil surface, incorporated into soil

Assessment of Various Leaching Models
3. Model Science (continued)

	GLEAMS	PESTLA	VARLEACH
3.5 Pesticide model (continued)			
Dispersion in soil	Dispersion set by program (modelled by numerical dispersion)	Set by user	Dispersion set by program (modelled by numerical dispersion)
Volatility	Not considered	Not considered	Not considered
Plant uptake	Simple model used.	Proportional to water uptake by plant	Not considered
Degradation on plant surfaces	First order kinetics.	Not considered	Not considered
Foliar washoff	All remaining dislodgeable residues are washed to soil when rainfall exceeds a threshold value	Not considered	Not considered
Runoff and erosion	Mass balance approach based on results from hydrology model.	Not considered	Not considered
3.6 Agronomy models			
Cultivation	Not considered for pesticide simulations	Not considered	Not considered
Irrigation	The program has to ability to automatically trigger irrigation due to a drop in the soil water content. The time window for irrigation is set by the user.	Irrigation must be added to rainfall data	Irrigation must be added to rainfall data
Application Frequency of applications	Multiple applications of up to 10 pesticides can be simulated. The program has an option which automatically allows the same crop to be grown each year with the same pesticide applications	Multiple applications (up to 20)	Single application
Application technique	Applications may be foliar sprays, applied to the soil surface, incorporated into the soil, or applied via chemigation.	Applied to soil surface or incorporated into the soil	Soil surface

Assessment of Various Leaching Models.
3. Model Science (continued)

	LEACHM	MACRO	PLM
3.5 Pesticide model (continued)			
Dispersion in soil	Set by user	Set by user	
Volatility	Volatility across soil surface	Estimated indirectly	Not considered
Plant uptake	Proportional to water uptake by plant	Proportional to water uptake by plant	Not considered
Degradation on plant surfaces	Not considered	Considered	Not considered
Foliar washoff	Not considered	Considered	Not considered
Runoff and erosion	Not considered	Only runoff considered	Not considered
3.6 Agronomy models			
Cultivation	Not considered	Not considered	Not considered
Irrigation	Not considered	Considered	Irrigation must be added to rainfall data
Application			
Frequency of applications	Multiple applications	Multiple applications	Single application
Application technique	Soil surface application	Applied to soil surface or incorporated into soil	Soil surface application

Assessment of Various Leaching Models
3. Model Science (continued)

	PRZM-2	PRZM	PELMO
3.7 Plant model			
Foliage — Purpose	Both areal extent and height of canopy are estimated for use in foliar application and volatilization calculations.	Areal extent of canopy is estimated for use in foliar application calculations.	Calculation of initial distribution of applied pesticide between soil and foliage
Description	Areal extent and height of crop canopy estimated by linear interpolation between emergence and maximum value reached at plant maturity.	Areal extent of crop canopy calculated by linear interpolation between emergence and maximum value reached at plant maturity.	Areal extent of crop canopy calculated by linear interpolation between emergence and maximum value reached at plant maturity.
Flexibility	Date of emergence, plant maturity, and harvest set by user (identical for root and foliage)	Date of emergence, plant maturity, and harvest set by user (identical for root and foliage)	Date of emergence, plant maturity, and harvest set by user (identical for root and foliage)
Rooting depth — Purpose	Used for hydrology and plant uptake model	Used for hydrology and plant uptake model	Used for hydrology and plant uptake model
Description	Rooting depth calculated by linear interpolation between emergence date and maximum value reached at plant maturity	Rooting depth calculated by linear interpolation between emergence date and maximum value reached at plant maturity	Rooting depth calculated by linear interpolation between emergence date and maximum value reached at plant maturity
Flexibility	Date of emergence, plant maturity, and harvest set by user (identical for root and foliage)	Date of emergence, plant maturity, and harvest set by user (identical for root and foliage)	Date of emergence, plant maturity, and harvest set by user (identical for root and foliage)
3.8 Heat Model			
Purpose	Used only to calculate surface and soil temperatures for use in the volatilization calculations.	Not considered	Used for correction of soil degradation rate
Description	Approach is based on previous work by a number of researchers including Van Bavel and Hillel, Thibodeaux, Hanks, Gupta, and Wagenet and Hutson.	Not applicable	Empirical model based on air temperature

Assessment of Various Leaching Models
3. Model Science (continued)

	GLEAMS	PESTLA	VARLEACH
3.7 Plant model			
Foliage			
Purpose	Partition of foliar applications between soil and foliage; partition of evapotranspiration between transpiration and evaporation	Partition of evapotranspiration between transpiration and evaporation	Not considered
Description	Partition of foliar applications set by user. Leaf area index data used for partitioning evapotranspiration	Soil cover data (specified by the user) is used for partitioning evapotranspiration	Not applicable
Flexibility	Parameters set by user.	Parameters set by user.	Not applicable
Rooting depth			
Purpose	Used for hydrology and plant uptake model	Used for hydrology and plant uptake model	Not used by model
Description	Constant throughout a cropping period	Linear interpolation in time between user-specified data	Not applicable
Flexibility	User specifies value for each cropping period	User specifies rooting depth as a function of time	Not applicable
3.8 Heat Model			
Purpose	Soil temperatures simulated but are not used for pesticide simulations	Used for adjustments to the soil degradation rate	Used for adjustments to the soil degradation rate
Description	Calculated from air temperature using a moving five-day daily average	Heat flux into soil based on air temperatures and a constant soil temperature at 10 m; heat flux in soil calculated with Fourier's law of heat conduction	Uses method of Walker and Barnes for temperatures greater than 7°C and the relationships of Nicholls, Briggs, and Evans for temperatures below 7°C

Assessment of Various Leaching Models
3. Model Science (continued)

	LEACHM	MACRO	PLM
3.7 Plant model			
Foliage			
Purpose	Partition between evaporation and transpiration	Calculation of evapotranspiration	Not considered
Description	Empirical sigmoidal curve	Leaf area index parameters specifying growth curve	Not applicable
Flexibility	One type of description	One type of description	Not applicable
Rooting depth			
Purpose	Used for hydrology and plant uptake model	Used for hydrology and plant uptake model	Used for hydrology; no plant uptake
Description	Rooting depth calculated by linear interpolation between emergence date and maximum value reached at plant maturity	Root volume is distributed logarithmically with depth	Root volume is distributed logarithmically with depth
Flexibility	Date of emergence, plant maturity, and harvest set by user	Date of emergence, plant maturity, harvest, and minimum and maximum rooting depth set by user	Date of emergence and plant maturity set by user
3.8 Heat Model			
Purpose	Used for correction of soil degradation rate	Used for correction of soil degradation rate	Used for correction of soil degradation rate
Description	Numerical solution of the heat flow equation	Calculates heat flux on the basis of air temperature and theoretical bottom boundary condition	Uses method of Walker and Barnes for temperatures greater than 7°C and the relationships of Nicholls, Briggs, and Evans for temperatures below 7°C

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Chapter 4

Model Limitations and Deficiencies

R. Jones

The mechanistic models described in the tables presented in chapter 3 can be useful tools in understanding the environmental fate of agricultural chemicals. However, knowledge of model assumptions and limitations is necessary for their proper application. This short discussion will cover only the most important assumptions regarding flow of water and agricultural chemicals in soil.

Probably the most important assumptions made by the models concern the flow of water. The simplest commonly used assumption is that water flow is governed by the water holding capacity of the soil with the kinetics of water movement assumed to be sufficiently fast as to be unimportant. With this assumption, water within a soil layer is considered to be stationary until field capacity is exceeded, with the amount in excess of field capacity moving instantaneously down to the next layer. This description of water flow is acceptable for relatively coarse textured soils, but tends to overpredict movement in finer-textured soils. A more complex approach is the Richards equation, which describes the kinetics of water movement based on relative permeability and pressure head as a function of water saturation. Although such a procedure is more computationally intensive, predictions for finer-textured soils are in better agreement with measurements compared to capacity models. Another limitation of the capacity model is they do not simulate upward flow of water due to capillary rise. This mechanism can be especially important in situations where the water table is above 1.5 to 2 m below the soil surface. Therefore if predictions are needed for movement on clay soils or in situations where upward movement of water is significant, then the modeler should choose a model based on the Richards equation. If the simulations are being performed for sand soils where water movement is predominantly downward, little differences would be expected between the predictions of models using the capacity approach or the Richards equation to describe water flow.

Preferential flow can be an important flow mechanism in some soils. Macropore flow is often important in fine-textured structured soils and funnel flow can be important in coarse-sand subsoils. None of the models consider funnel flow and most of the models do not consider macropore flow. Current models that consider macropore flow require that soil parameters be obtained by calibration.

More advances are needed before predictions of macropore flow can be made using soil parameters in existing data bases. Modelers must understand the limitations of the models when performing simulations in circumstances where preferential flow mechanisms are significant.

The shapes of predicted soil concentration profiles often do not precisely match measured soil concentration profiles. Predictions of the total amount moving past a specified depth and the maximum extent of movement are more accurate. Models are best at predicting the movement of the main portion of a residue plume. Estimates of behavior of the leading or trailing extremes of the plume are less accurate, probably due to the effects of preferential flow paths. In general, model predictions are not accurate below about 0.1 to 1 percent of the amount applied.

Most of the models use first order kinetics to describe degradation processes. Some models make corrections for temperature and soil moisture and most of the models allow for changes in degradation changes in depth. In laboratory studies, changes in degradation rates are often attributed to changes in the soil characteristics or soil microbes. However, even under field conditions, degradation rates may vary with time.. In many circumstances, observed dissipation rates slow with time perhaps due to movement deeper into the soil profile (elimination of photolysis or volatilization and lower microbial activity) or stronger adsorption to soil particles. In some cases degradation rates actually increase perhaps due to adaptation of soil organisms. The modeler should make certain that predictions of the amount of material remaining are consistent with available field and laboratory information.

Model simulations under circumstances where preferential flow is not important often show greater movement than actually occurs. This is true even for models using the Richards equation, which as mentioned earlier generally predicts slower movement than capacity models. One probable explanation for this is increasing sorption with time. Most modeling simulations use Koc values measured over a relatively short period of time, while research by Walker has shown that the sorption coefficient doubles after about 100 days and is about three times the original value at the end of a year. For some compounds, the effect of time is even more important. Inclusion of non-linear sorption can significantly affect simulation results. Although some models do have the ability to increase sorption as a function of time, more research including compound specific data would be useful in this area.

Another limitation associated with modeling is the ability to supply correct values of model input parameters. To perform detailed risk assessments, information on

climate, soil properties, and cropping patterns are needed. Such information, although existing for most areas of Europe, is not readily accessible to modelers. Even when data bases are available, defining model parameters may not be straightforward. Two areas where improvements are needed are estimation of evapotranspiration and degradation in subsoils. The amount of recharge water (and therefore movement of agricultural chemicals) is quite sensitive to the amount of evapotranspiration loss since recharge, approximately the difference between irrigation and rainfall minus evapotranspiration (assuming no change in storage), is usually a relatively small number obtained by the difference between two larger numbers. Potential evapotranspiration is commonly calculated from pan evaporation, average temperature, or radiation and other climatic data and these different methods sometimes give different estimates of evapotranspiration losses, resulting in considerably different estimates of recharge. Probably what is needed is not more basic research, but rather transfer of existing information to modelers to ensure that the most appropriate estimation procedure is chosen for the specific case of interest.

Describing degradation rates in subsoils is often an area of uncertainty affecting model predictions. For compounds degrading as a result of microbial activity, degradation usually decreases with increasing depth. However, because different microbes are responsible for degradation of different compounds, the decrease is not generally proportional to the general microbe population. Compounds that degrade by primarily chemical mechanisms may not be directly affected by the depth, but degradation rates may change due to physical changes in soil properties. Other compounds degrade by both chemical and microbial pathways, so describing degradation kinetics as a function of depth is even more complex.

Most of the available mechanistic models are deterministic in nature. That is, each input parameter has a single value and each simulation produces a single number at a specific time and depth. However, soil properties (such as organic matter, texture, and hydraulic properties) often have significant spatial variations, even within a single field. Concentrations of agricultural chemicals in individual soil samples from carefully controlled field studies usually have coefficients of variation in the range of 100 percent. The description of this variability is beyond the capability of current models.

Chapter 5

European Scenarios for Leaching models

M. Klein and H. Knoche

1 Scenarios already available in Europe

1.1 Introduction

At present fixed scenarios for leaching models are only used in the Netherlands and in Germany. The philosophy in these countries was to choose *realistic worse* (NL) or *realistic worst* (D) case situations with respect to leaching of pesticides to ground water.
"*Realistic*" means that the combination of model parameters should describe situations that could really happen in the field. For example, a combination of a soil from the dunes together with the climate of the Alps would **not** fulfil this condition.
Because of the different size of the Netherlands and Germany the spread of soil and meteorological parameters is different. This might be the reason for the different numbers of scenarios which are in use in both countries: In the Netherlands only one fixed scenario (one soil together with one climate scenario) is used, whereas in Germany a lot of combinations of four soil and nine climatic data sets are possible, which all lead to a specific scenario in the leaching model. But not all of these combinations fulfil the conditions of a *realistic worst case* scenario. Usually, the Umweltbundesamt uses the combination Borstel-soil together with the climatic condition of Hamburg (wet as well as normal) as "their" *realistic worst case*.
The data sets of the scenarios in the Netherlands and in Germany are different because they are related to different computer models: PESTLA (NL) and PELMO (D). Therefore it is not possible to transfer scenarios of PELMO directly into the format of PESTLA.

The following tables are performed to describe the differences between the scenarios. They do not contain the whole model input and (of course) cannot be used to create complete PELMO or PESTLA input files. Both models need meteorological data on a daily basis. The scenarios are summarised in table 1 using yearly data. A lot of parameters are strongly related to one of the computer models, PELMO or PESTLA; not all of them are listed in the tables.

1.2 Description of the climatic scenarios

Table 1: Climatic scenarios already available in Europe

Location	Condition	Annual Precipitation [mm]	Annual Average Air Temperature [°C]
Utrecht 1980	74 % wet year	862	9.3
Hamburg 1961	100 % wet	872	9.1
Hamburg 1971	100 % dry	542	9.1
Hamburg 1978	average	778	8.4
Schmallenberg 1964	100 % dry	753	6.7
Schmallenberg 1966	100 % wet	1501	6.7
Schmallenberg 1968	average	1082	8.9
Bad Kreuznach 1958	average	524	9.5
Bad Kreuznach 1965	100 % wet	757	8.9
Bad Kreuznach 1976	100 % dry	323	10.1

1) "100 % wet" year means, highest and "100 % dry" means lowest amount of annual precipitation which was observed (1951-1980).

2) 74 % wet year means, that 74 % of all years (1911-1984) are dryer than the precipitation of the year 1980

3) In the German Scenarios air temperatures are used to extrapolate to soil temperatures

1.3 Description of the soil scenarios

Table 2: Summary of soil scenarios already available Europe

Location	Soil type	No of Horizons	Soil depth [cm]
Landhorst (NL)	sand	4	100
Borstel (D)	sandy loam	5	110
Landau (D)	sandy loam	3	130
Hörstel (D)	sand	4	120
Jülich (D)	silty loam	5	120

The Dutch "Landhorst"-Scenario assumes groundwater at 100 cm and the German scenarios assume free drainage at 100 cm to 130 cm depth as the lower boundary condition.

Table 3: Data of the soil scenario "Landhorst"

Horizon [cm]	0-30	30-50	50-59	60-100
Sand [%][2]	92	96	95	-
Silt [%][2]	5	2	3	-
Clay [%][2]	3	2	2	-
OC [%]	2.73	0.46	0.11	0
Biodegradation factor[3]	1	1-0.9	0.7-0.9	0-0.7

2 no input parameters of the model PESTLA
3 linear interpolation

Table 4: Data of the soil scenario "Hörstel"

Horizon [cm]	0-20	20-40	40-70	70-120
Sand[%]	91.4	96.3	96.5	98.6
Silt [%]	6.8	1.5	2.08	0.83
Clay [%]	1.8	2.2	1.42	0.57
OC [%]	2.93	1.26	0.62	0.36
Biodegradation factor	1	0.38	0.24	0.36

Table 5: Data of the soil scenario "Borstel"

Horizon [cm]	0-30	30-57	57-73	73-90	90-110
Sand[%]	68.3	67.0	96.2	99.8	100.0
Silt [%]	24.5	26.3	2.9	0.2	0
Clay [%]	7.2	6.7	0.9	0	0
OC [%]	1.5	1.0	0.2	0	0
Biodegradation factor	1	0.16	0.09	0.13	0

Table 6: Data of the soil scenario "Landau"

Horizon [cm]	0-39	39-85	85-130
Sand [%]	54	47	92
Silt [%]	39	44	0
Clay [%]	7	9	8
OC [%]	1.57	0.48	0.34
Biodegradation factor	1	0.15	0.13

Table 7: Data of the soil scenario "Jülich"

Horizon [cm]	0-25	25-35	35-55	55-80	80-120
Sand [%]	10	5	4	3	2
Silt [%]	81	81	75	67	75
Clay [%]	9	14	21	30	23
OC [%]	1.7	0.57	0.45	0.25	0.22
Biodegradation factor	1	0.34	0.26	0.15	0.13

1.4Description of additional scenario information

Table 8: Summary of additional scenario information

	NL (PESTLA)	D (PELMO)
Calculation of Evapotranspiration	Penman	Haude
Cultivation	maize	maize[4]
Use of Soil Temperatures	experimental data	extrapolation based on air temperatures
Rate of Application	1 kg/ha[5]	according to the agricultural practice (dependent on the pesticide)
Frequency of Application	1 per year	according to the agricultural practice (dependent on the pesticide)
Date of Application	25 May/1 Nov (dependent on the pesticide)	according to the agricultural practice (dependent on the pesticide)

4 culture specific parameters for other crops under development.
5 in the risk assessments the actual rate is taken into account by assuming that the concentration in groundwater is directly proportional to the application rate.

2 Suggestion for new European Scenarios

2.1 Introduction

To simulate leaching to ground water on the European level climatic and soil scenarios are necessary that are representative for Europe. In this paper a suggestion of ten climatic zones together with 5 soil scenarios is made for Europe. Each climatic zone is represented by at least one typical climatic scenario. The idea was to cover (more or less) the whole area that is in agricultural use. Of course, the scenarios cannot correspond with the political borders of the different member states. They only depend on the climatic or soil conditions.
This suggestion includes a minimum of scenario data (i.e. monthly data on precipitation) and a map which shows the areas where the climatic scenarios should be used. Of course, for regional purposes the user may add more specific scenarios to this more common data set. In addition, the user a matrix is given showing the adequate combinations of soil and climatic scenarios.

2.2 Description of the European Climatic Scenarios

Ten zones for Europe are a relatively small number considering the variation of important climatic parameters that can be observed. The aim is to support regulators on the European level who want to use the pesticide leaching models.

Most of the scenarios can be used for more than one country. For each climatic zone a minimum of one scenario is given where monthly temperature and precipitation are available. Because of the size of all the climatic zones, there are, of course, some variations in temperature and precipitation within each zone. Therefore, the list of example locations (cities) should be enlarged dependent on the specific aim of a certain simulation (i.e. for national predictions).
The actual selection of example locations was determined by the data availability.

Apart these zones, we do not have to forget that in the Mediterranean countries also the irrigation water has to be considered. For example, for Italy the average irrigation water input used is of 500 mm/year, distributed in the summer months.

The geographic borders of the ten climatic zones are shown in Fig. 1. Figure 2 is a map showing potential evapotranspiration which can be used to check the model output (estimate of Lars Bergström and Mark Russell, pers. communication, 1994).

Table 9: Summary of European Climatic Zones

Zone	Climate description	Example areas	Scenario
1	Northern Europe, areas without maritime influence	southern part of Norway, Sweden, and Finland	Stockholm
2	North-Western Europe with strong maritime influence	UK (without Scotland and northern part of Ireland), south-western part of Norway, Atlantic coast (Normandy, Bretagne) North German low lands (western part) whole coast of the North Sea	Plymouth Amsterdam Hamburg Utrecht London
3	Northern part of Central Europe between maritime and continental climate	North German low lands (eastern part)	Berlin
4	Western part of Central Europe between maritime and continental climate	French low lands	Paris
5	Climate of the Central Europe low mountain range	German "Mittelgebirge" French "Massif Central" Foothills of the Alps	Nürnberg München Lyon
6	Climate of the Northern Alps		Salzburg
7	Climate of the southern European high mountain range	southern part of the Alps, the Pyrenees, northern part of the Apenines	Lugano
8	Coast areas of Western Europe and South-Western Europe	Atlantic coast from Gibraltar to Nantes	La Coruna
9	Southern European low mountain range	Iberian Peninsula, Corse, Sardinia, southern part of the Apennines, Sicily, Greece main land	Madrid
10	Southern European coast areas without maritime influence	coast of the Mediterranean Sea	Roma Athen

Table 10: Average Monthly precipitation of the European scenarios [mm]

Zone	City	Long.	Latitude	Jan	Feb.	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Year
1	**Stockholm**	59 21	17 57 E	43	30	26	31	34	45	61	76	60	48	53	48	555
2	**Plymouth**	50 21	04 07 W	105	77	73	55	65	58	71	80	82	94	115	115	990
2	**Utrecht***	52 06	05 10 E	68	54	45	49	51	58	77	88	71	72	70	63	767
2	**Hamburg**	53 38	10 00 E	57	48	39	52	53	64	84	83	63	59	59	59	720
3	**Berlin**	52 28	09 42 E	41	37	30	39	44	60	67	65	45	45	44	39	556
4	**Paris**	48 58	02 27 E	54	43	32	38	52	50	55	61	51	49	50	49	585
5	**Nürnberg**	49 30	11 05 E	43	39	35	40	55	71	90	75	46	46	41	42	623
5	**Lyon**	45 43	04 57 E	52	46	43	56	69	85	56	89	93	77	80	57	813
5	**München**	48 08	11 42 E	59	55	51	62	107	125	140	104	87	67	57	50	964
6	**Salzburg**	47 48	13 00 E	73	70	70	89	127	167	191	163	111	82	70	65	1278
7	**Lugano**	46 00	08 58 E	63	67	98	148	215	198	185	196	159	173	147	95	1744
8	**La Coruña**	43 22	08 25 W	121	80	95	70	60	46	29	47	71	92	125	139	975
9	**Madrid**	40 27	03 47 W	38	34	45	44	44	27	11	14	31	53	47	48	436
10	**Roma**	41 48	12 14 E	83	73	52	50	48	18	9	18	70	110	113	105	749
10	**Athen**	37 58	23 43 E	62	36	38	23	23	14	6	7	15	51	56	71	402

Ref: Climatological Normals (CLINO) for Climat and Climat Ship Stations for the Period 1931-1960. World Meteorological Organisation. Genf 1962, 1971.

* J. J.T.I. Boesten, DLO Winand Staring Centre, Wageningen, NL. pers. communication

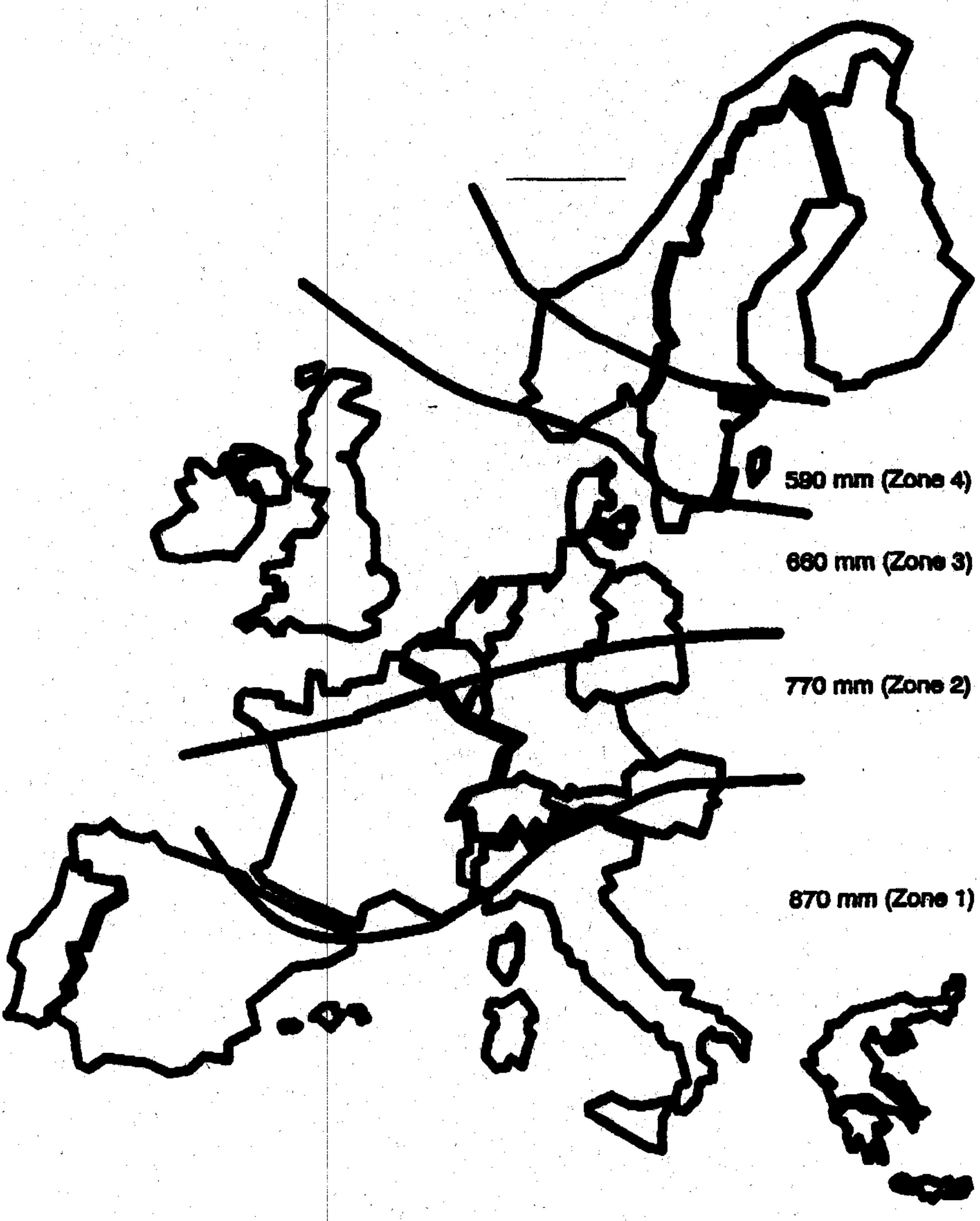
Table 11: Average Monthly air temperatures of the European scenarios [°C]

Zone	City	Long.	Latitude	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Okt	Nov	Dec	Year
1	Stockholm	59 21	17 57 E	2,9	-3,1	-0,7	4,4	10,1	14,9	17,8	16,6	12,2	7,1	2,8	0,1	6,6
2	Plymouth	50 21	04 07 W	6,2	5,8	7,3	9,2	11,7	14,5	15,9	16,2	14,7	11,9	8,9	7,2	10,8
2	Utrecht*			1,7	2,0	5,0	8,5	12,4	15,5	17,0	16,8	14,3	10,0	5,9	3,0	9,3
2	Hamburg	53 38	10 00 E	0,0	0,4	3,3	7,6	12,2	15,6	17,3	16,8	13,6	9,1	4,9	1,8	8,6
3	Berlin	52 28	09 42 E	-0,5	0,2	3,9	9,0	14,3	17,7	19,4	18,8	15,0	9,6	4,7	1,2	9,5
4	Paris	48 58	02 27 E	3,1	3,8	7,2	10,3	14,0	17,1	19,0	18,5	15,9	11,1	6,8	4,1	10,9
5	Nürnberg	49 30	11 05 E	-1,4	-0,4	3,7	8,2	13,0	16,6	18,2	17,4	13,7	8,3	3,8	0,1	8,4
5	Lyon	45 43	04 57 E	2,1	3,3	7,7	10,9	14,9	18,5	20,7	20,1	16,9	11,4	6,7	3,1	11,4
5	München	48 08	11 42 E	-2,2	-1,0	3,3	7,9	12,5	15,9	17,7	16,9	13,7	8,2	3,1	-0,7	7,9
6	Salzburg	47 48	13 00 E	-2,5	-1,1	3,7	8,3	13,2	16,0	17,8	17,1	14,0	8,4	3,3	-0,9	8,1
7	Lugano	46 00	08 58 E	1,9	3,6	7,5	11,7	15,4	19,3	21,4	20,5	17,4	12,1	6,9	3,1	11,7
8	La Coruña	43 22	08 25 W	9,9	9,8	11,5	12,4	14,0	16,5	18,2	18,9	17,8	15,3	12,4	10,2	13,9
9	Madrid	40 27	03 47 W	4,9	6,5	10,0	12,7	15,7	20,6	24,2	23,7	19,8	14,0	8,9	5,6	13,9
10	Roma	41 48	12 14 E	8,0	9,0	10,9	13,7	17,5	21,6	24,4	24,2	21,5	17,2	12,7	9,5	15,9
10	Athens	37 58	23 43 E	9,3	9,9	11,3	15,3	20,0	24,6	27,6	27,4	23,5	19,0	14,7	11,0	17,8

Ref: Climatological Normals (CLINO) for Climat and Climat Ship Stations for the Period 1931-1960. World Meteorological Organisation. Genf 1962, 1971.

* J. J.T.I. Boesten, DLO Winand Staring Centre, Wageningen, NL. pers. communication

Fig 1: Suggested Climatic Zone Map of Europe



Estimates made by Lars Bergstrom and Mark Russell, April 20, 1994

Fig 2: Potential Evapotranspiration in Europe

2.3 Description of the European Soil Scenarios

To simulate leaching to ground water on the European level also soil scenarios have to be made available. Up to now, no study has been performed on the selection of soil scenarios useful in leaching models. Therefore, scenarios have to be selected by using the results of projects that had similar objectives.
In this field some work has already been done by Brümmer et al. They have analysed the soil map of Europe by multivariate data processing (means of frequency and spatial statistics) to find the soils that are best suited for chemical testing within the European Union. On the basis of regionalization algorithms, the optimum location of sampling points was determined and the result corroborated on large-scale maps as well as be visual inspection in the field. Originally, the data compilation was aimed to support the OECD guideline on adsorption/desorption studies. The parameters chosen to describe the soil scenarios for adsorption studies are in large parts identical to the data used in soil scenarios for leaching models. Therefore, it makes sense to use this compilation also for leaching models
Brümmer and et al. found 55 soils in Europe (*see table 12*) representing the total area (not the agricultural area) of the EC. Considering the frequency of these soil types they made two suggestions for a selection of soil scenarios:

- Five representative soils for Europe
  (covering 36 % of the EC [1987], *see table 14*)
- Twenty representative soils for Europe
  (covering 65 % of the EC [1987], *see table 15*)

There are some scenario data available for the first suggestion (Five representative soils) which could be used in the leaching models. The pedological characterisation of these reference soils is listed in table 15 [Ref. Kuhnt, G. and H. Nuntau, 1992]. Additionally, in table 16 some information about the soil profile and the location of the soils is given.
When working with the leaching models on the European level the user has to find adequate combinations climatic and soil scenarios. A suggestion of possible combinations is shown in Table 17.

It should be clearly pointed out, that no study has directly been performed for the selection of European soil scenarios for leaching models. Though it is recommended in this paper to use the Eurosoils, there are big limitations on these scenarios, namely:

- The Eurosoils represent the total (not the agricultural) area of Europe. Consequently the five Eurosoils also contain forest soils.

- The pH and organic matter content of soil 5 (forest soil) is not typical for soils which have been in agricultural use
- Though the soil profile of the Eurosoils is roughly described (see table 16), no further information is given about the deeper horizons (which is essential for the leaching models).

Table 12: Distribution of soil types in the European Union [Ref. Brümmer, et al], 1987]

Soil Classification	Freq. (%)	Cum. freq(%)
•Gray-brown Podzolic Soils	12.8	12.8
*Gray-brown Podzolic Soils and Brown Forest Soils	7.7	20.5
Alluvial Soils	7.1	27.5
•Brown Mediterranean Soils	6.8	34.3
•Acid Brown Forest Soils	6.5	40.8
•Brown Forest Soils and Rendzinas	6.1	46.8
•Podzolized Soils	4.2	51.1
*Acid Brown Forest soils	4.1	55.2
*Gray-brown Podzolic Soils and Podzolized Soils	3.9	59.1
Reddish Brown Soils	3.8	62.9
*Rocky BA	3.6	66.5
Brown Forest Soils and Regosols	3.3	69.8
*Brown Mediterranean Soils/Lithosols	2.9	72.7
Reddish Brown Soils and Lithosols	2.4	75.2
*Organic Soils and Podzolized Soils	2.2	77.4
Lithosols, Rankers and Podzolized Soils	2.2	79.6
Red Mediterranean Soils/Lithosols	2	81.6
*Podzolized Soils and Organic Soils	1.8	83.4
Regosols and Rendzinas	1.8	85.2
Serozems	1.5	86.7
Lithosol and Rendzinas	1.5	88.2
Organic Soils	1.4	89.6
Regosols and Grumusols	1.2	90.8
Gray-brown Podzolic Soils and Pseudogley Soils	1.1	92
Chestnut Soils	1.1	93.1
Red Mediterranean Soils	1	94.2
Lithosols	0.7	94.8
*Hydromorphic P.	0.6	95.4
*Hydromorphic GB-P	0.5	95.9
*Hydromorphic GB	0.5	96.5
*Hydromorphic BF-RZ.	0.5	97
Grumusols	0.5	97.5
Lithosols and Podzlized Soils	0.5	98
Gray-brown Podzolic Soils/Lithosols	0.4	98.4
Hydromorphic A.	0.3	98.7
Rocky-SE	0.2	98.8
Regosols	0.2	99.1
Hydromorphic RE.	0.2	99.2
*Rocky BF-RZ.	0.2	99.4

Table 12 continued: Distribution of soil types in the European Union.

Soil Classification	Freq. (%)	Cum. freq(%)
Saline-Alkaline A.	0.2	99.6
Dunes A.	0.1	99.7
*Rocky P.	0.1	99.8
*Hydromorphic GB-BF.	0.1	99.9
*Hydromorphic BF-RE.	0	99.9
Chernozems and Brunizems	0	99.9
*Rocky P-O	0	100
*Hydromorphic BA.	0	100
Red Mediterranean Soils/Rubrozems	0	100
Hydromorphic LI-P.	0	100
Rocky A.	0	100
Hydromorphic RP-LI.	0	100

•Representative soils
*soils with implicit chronological representativity

Table 13: Distribution of five representative soil types in the European Union
[Ref. Brümmer, et al, 1987]

soil type No	soil scenario	EIRE	GB	NL	B	L	F	I	E	P	DK	D	GR	EG
1	Brown Mediterranean Soils						0,2	19,3	18,6	15,0				6,8
2	Brown Forest Soils and Rendzinas	3,3	5,8				4,7	5,8	7,1	1,1		5,8	23,3	6,1
3	Acid Brown Forest Soils	18,5	20,9				8,3	0,2	1,4	13,4		2,7		6,5
4	Gray-brown Podzolic Soils	11,8	20,8	3,9	29,1		22,7	5,2	0,9		46,9	14,6	2,2	12,8
5	Podzolized Soils		7,2	43,3	16,6		2,2			6,3	10,7	11,4		4,2
	Total	33,6	54,7	47,2	45,7	0,0	38,1	30,5	28,0	35,8	57,6	34,5	25,5	36,4

Table 14: Distribution [%] of twenty representative soil type in the European Union [Ref. Brümmer, et al, 1987]

Soil classification	EIRE	GB	NL	B	L	F	I	E	P	DK	D	GR	EG
Gray-brown Podzolic Soils	11,8	20,8	3,9	29,1		22,7	5,2	0,9		46,9	14,6	2,2	12,8
Gray-brown Podzolic Soils and Brown Forest Soils	16,9	11,6		14,0	52,8	17,3		1,6			7,6		7,7
Brown Mediterranean Soils						0,2	19,3	18,6	15,0				6,8
Acid Brown Forest Soils	18,5	20,9				8,3	0,2	1,4	13,4		2,7		6,5
Brown Forest Soils and Rendzinas	3,3	5,8				4,7	5,8	7,1	1,1		5,8	23,8	6,1
Podzolized Soils		7,2	43,3	16,6		2,2			6,3	10,7	11,4		4,2
Acid Brown Forest soils		0,0		5,1		3,0	6,1	5,1	28,9		4,2	1,4	4,1
Gray-brown Podzolic Soils and Podzolized Soils	6,0	0,8		9,4		6,3		4,0		28,4	3,9		3,9
Rocky BA				20,2	27,8	0,3	9,8				17,4		3,6
Brown Mediterranean Soils/Lithosols						2,1		6,5	6,6			14,4	2,9
Organic Soils and Podzolized Soils	24,6	7,3	7,8							0,2	0,1		2,2
Podzolized Soils and Organic Soils		9,0		0,5						4,5	4,6		1,8
Hydromorphic P.		4,2				0,2							0,6
Hydromorphic GB-P			1,5			1,0					2,4		0,5
Hydromorphic GB	7,0	2,4											0,5
Hydromorphic BF-RZ.											4,5		0,5
Rocky BF-RZ.	3,2										0,4		0,2
Rocky P.											0,7		0,1
Hydromorphic GB-BF.		0,3				0,2							0,1
Rocky P-O											0,2		0,0
TOTAL	91,3	90,3	56,5	94,9	80,6	68,5	46,4	45,2	71,3	90,7	80,5	41,3	

Table 15: Pedological Characterisation of the suggested soil scenarios
[Ref. Kuhnt, G. H. Muntau ,1992]

PEDOLOGICAL CHARACTERIZATION OF REFERENCE SOIL SAMPLES		SOIL TYPE N°1	SOIL TYPE N°2	SOIL TYPE N°3	SOIL TYPE N°4	SOIL TYPE N°5
Sand (total)		3.3	13.4	46.4	4.1	81.6
coarse + medium	%	2.0	4.4	23.1	1.1	64.8
fine	%	1.3	9.0	23.3	3.0	16.8
Silt (total)		21.9	64.1	36.8	75.7	12.7
coarse	%	4.0	21.3	19.4	52.2	7.4
medium	%	9.7	23.1	11.6	19.4	4.3
fine	%	8.2	19.7	5.8	4.1	1.0
Clay	%	75.0	22.6	17.0	20.3	6.0
pH Values						
water		5.9	8.0	5.8	7.0	4.6
calcium chloride		5.1	7.4	5.2	6.5	3.2
potassium chloride		5.1	7.5	5.2	6.5	3.4
total carbon	%	1.5	10.9	3.7	1.7	10.9
$CaCO_3$	%	0.0	60.45	0.0	0.0	0.0
organic carbon	%	1.30	3.70	3.45	1.55	9.23
organic matter	%	2.65	6.4*	6.44	2.86	15.92
N	%	0.17	0.20	0.26	0.16	0.30
C/N-Ratio	%	7.65	18.50	13.27	9.69	30.77
organic sulphur	%	0.054	0.028	0.055	0.034	0.078
total P	%	0.15	0.15	0.38	0.29	0.21
C E C mval/100 g		29.9	28.3	18.3	17.5	32.7
total Fe	ppm	37050.0	9850.0	14370.0	11500.0	1040.0
amorphous Fe	o/oo	3.22	0.18	4.75	1.93	0.56
HCl soluble Fe	o/oo	1,820	0.002	2.200	1.470	0.105
amorphous Al	o/oo	0.64	0.17	1.58	0.81	0.97
HCl soluble Al	o/oo	0.83	tr.	1.67	1.55	0.93
SiO_2	%	56.22	21.60	68.45	68.63	71.57
Al_2O_3	%	23.92	8.66	11.92	12.07	3.85
CaO	%	0.41	30.62	0.20	0.71	<0.02
K_2O	%	1.85	1.27	1.59	1.84	0.63
Fe_2O_3	%	10.76	1.66	4.14	2.71	<0.05
MgO	%	1.12	1.82	1.19	1.11	0.65
TiO_2	%	0.99	0.25	0.65	0.72	0.36

* = calculated from C org

Table 16: Eurosoils: Soil profile and location of sampling
[Ref. Kuhnt, G. H. Muntau ,1992]

Euro - Soil 1	
Soil association	: Brown mediterranean soils
Sampling site/State	: Sicily/Italy
Vegetation/Land use	: Grassland/Meadow
Soil horizons	: Ah (0-30 cm) coarse granular to subgranular blocky Bw (30-60 cm) angular blocky to prismatic Bc (60- cm) coherent
Euro - Soils 2	
Soil association	: Brown forest soils and Rendzinas
Sampling site/State	: Peloponnesos/Greece
Vegetation/Land use	: Brown-leaved trees
Soil horizons	: Ahk (0-30 cm) granular ACk (30-35 cm) granular to fine subgranular blocky Ck (35- cm) coherent
Euro - Soil 3	
Soil association	: Acid brown forest soil
Sampling site/State	: Wales/Great Britain
Vegetation/Land use	: Grassland/Pasture
Soil horizons	: Ap (0-30 cm) fine crumb to very fine subangular blocky Bw1 (30-60 cm) fine crumb...(as above) Bw2 (60-150 cm) polyhedral Bw3/C (>150 cm)
Euro - Soil 4	
Soil association	: Gray-brown podzolic soils
Sampling site/State	: Normandy/France
Vegetation/Land use	: Wheat/arable land
Soil horizons	: Ap (0-20 cm) fine crumb to subangular blocky E (20-55 cm) blocky to subpolyhedral Bt (55-90 cm) polyhedral Ck (> 90 cm)
Euro - Soils 5	
Soil association	: Podzolized soils
Sampling site/State	: Schleswig-Holstein/Germany
Vegetation/Land use	: Coniferous forest
Soil horizons	: O (-8-0 cm) poorly degraded, loose and spongy surface litter Ah (0-11 cm) single grain to fine granular E (11-25 cm) single grain Bhs (25-32 cm) loose subangular blocky Bs (32-48 cm) firmsubgranular blocky to coherent BC (48-65 cm) bridge C (65- cm) single grain

Table 17: Useful Combinations of European Climate and Soil Scenarios

Zone	Climate description	Soil 1	Soil 2	Soil 3	Soil 4	Soil 5
		Vertic Cambisol	Rendzina	Dystric Cambisol	Orthic Luvisol	Orthic Podzol
		Brown Mediterranean Soil	Brown Forest Soils and Rendzinas	Acid Brown Forest Soils	Gray-brown Podzolic Soils	Podzolized Soils
1	Northern Europe, areas without maritime influence			X		X
2	North-Western Europe with strong maritime influence			X	X	X
3	Northern part of Central Europe between maritime and continental climate			X	X	X
4	Western part of Central Europe between maritime and continental climate		X	X	X	X
5	Climate of the Central Europe low mountain range		X	X	X	X
6	Climate of the Northern Alps		X	X	X	X
7	Climate of the southern European high mountain range		X	X	X	X
8	Coast areas of Western Europe and South-Western Europe		X	X	X	
9	Southern European low mountain range	X	X			
10	Southern European coast areas without maritime influence	X	X			

3 Additional Information needed for the scenarios

The scenario data as presented in this paper are not sufficient for the direct use in the simulation models.

To operationalise the scenarios additional information must be made available concerning, both the climatic as well as the soil scenarios.

The computer models need daily weather data whereas the given scenarios are only characterised by monthly average values. To complete the scenarios the daily data should be made available at a central point in Europe.

Furthermore, detailed information is only available for the top horizons of the five Eurosoils. To use the Eurosoils in leaching models also data on the deeper soil layers have to be given. Though the Eurosoils can be principally used in leaching models, it is recommended that a special project should be started to select European soil scenarios for the use in leaching models. Furthermore, the results of such a project should be distributed like the climatic scenarios.

At least, no crop scenarios have been defined in this paper. At present, there are data available on different crops in some member states only (e.g. Germany, Ref. IVA 1994). Because some parameters of these national data sets vary within Europe (e.g. date of emergence and maturation), they should not be used without adaptation for the European scale. Therefore, activities should be started to develop a set of crop scenarios which can be used in the European Union.

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Chapter 6

Input and Output Data Needed for Validation of Pesticide Leaching Models

A. Helweg & R. Kloskowski

The purpose of this section is to define the input and output parameters, which are needed for validation of a model for pesticide transport in soil. Whether lysimeter experiments or field studies are used for the validation, essential data are of equal importance.

The basis for the selection of data requirements was a questionnaire filled in by members of the Focus-group. The following input and output parameters are considered urgent by most participants. Appendix 1 shows that from the point of 7 experienced scientists only few of the parameters mentioned are termed urgent by all. The reason is that the input requirements are not equal for all models. To ensure that the data set obtained will be useful also in the future, it is necessary to establish a data set which is adequate for as many models as possible.

Input data needed for modelling (driving variables and parameters)

Soil

Description of the soil horizon
Texture and organic C in all horizons in the profile
Depth of soil column or distance to ground water table
Bulk density of undisturbed soil
Retention curve in each horizon
Macropore flow - if possible
Hydraulic conductivity, saturated
Pesticide treatment history
Hydraulic conductivity, unsaturated - if possible

Crop

Crop development (description of growth development or leaf area index, LAI)
Time of planting
Time of harvest
Crop yield
Root depth - if possible

Weather

precipitation
intensity of precipitation / mean duration of precipitation event
air temperature (daily mean)
air temperature (minimum)
air temperature (maximum)
air temperature (measurement at 2 p.m.)
humidity (daily mean / measurement at 2 p.m.)
wind speed (daily mean; measured at 2 m height)
net radiation / global radiation (daily mean)
degree of cloud coverage (daily mean)

Application

Pesticide applied (kg/ a.i./ha)
Spray solution (l/ha)
Number of applications
Time of application
Incorporation depth

Pesticide

Persistence in plough layer (field concentration)
Adsorption (K_d) in plough layer
Adsorption isotherm in each horizon
Persistence in sub soil (field concentration) or lower - if possible
Persistence in each horizon - if possible
Adsorption (K_d) in subsoil - if possible
Volatilization

Output data needed for validation

Content of pesticide in leachate as a function of time. The first month leachate is determined weekly, later monthly or depending on amount leached.
Volume of water leached as a function of time
Residue of pesticide in the soil profile at the end of the experiment in 10 cm increments.
Soil temperature at 10 and 30 cm
Water content in soil at 10, 30 and 50 cm during experiment
Pesticide content in crop - if possible

Appendix 1

INFORMATION NEEDED FOR VALIDATION OF LEACHING MODELS

To run a satisfactory validation of a leaching model the following information is needed according to 7 participants in the FOCUS modelling group.

		Urgent	Needed	Not needed
Soil:	Texture (clay, sand, organic C):			
	0-30 cm	xxxxx	x	x[1)]
	30-60 cm	xxxx	xx	x[1)]
	60-90 cm	xxxx	xx	x[1)]
	others	___	___	___
	Cation exchange capacity	___	xx	xxxxx
	pH	xx	xxx	___
	Water content:			
	Field capacity	xxxxxxx	___	___
	Wilting point	xxxxxxx	___	___
	Water holding capacity	xx	xx	x
	Microbial activity	xx	x	xxxxx
	Pesticide treatment history (3 years)	xxx	___	xxxx
	Water content at pesticide application	xx	xxx	xx
	Depth of soil column (to water table)	xxxxxxx	___	___
	Hydraulic conductivity:			

Unsaturated	x	xx	xxx
Near saturated	—	x	xxxx
Saturated	xx	x	xxxx
Bulk density (undisturbed)	xxxxx	x	—
Infiltration capacity in situ	—	xxx(x)	xxx(x)
Diffusion coefficient	—	xx	xxx

1) May be estimated from water content and hydraulic conductivity.

		Urgent	Needed	Not needed
	Soil tillage history	xx	xxxxx	
Crop:	Root depth	xxx	xxx	
	Leaf area (maximum)	xx	xxx(x)x	(x)
	Time of planting	xxxxx	xx	
	Time of harvest	xxxxx	xx	
	Yield		x	xxxxx
	Information about growth	x	xxxx	x
	Pesticide uptake (leaf, root)		xxx	xxx
Weather:	Precipitation	xxxxxxx		
	Evaporation			
	Actual (difficult to measure)	x	x	xxxx
	Potential	xxxxxx	x	
	Temperature			
	Air (2 m)	xxxxx	x	x
	Soil 10 cm	x	xxxxx	x
	Soil 30 cm	x	xxxxx	x
	Hours of sunlight		xxxx	xxx
	Wind speed		xx	x
	Humidity		x	x

Pesticide:	Amount applied	xxxxxxx	___	___
	Spray solution (l/ha)	x___	xx___	xxxx___
	Number of applications	xxxxxxx	___	___
	Time of application	xxxxxxx	___	___
	Incorporation depth	xxxxxx	x___	___

		Urgent	Needed	Not needed
	Persistence:			
	Ploughlayer (field concentration)	xxxxxx	x	
	Sub soil field concentration	xxxxx	xx	
	1% of field concentration		x	xx
	Influence of temperature	xxx	xx(x)	
	Solubility	x	x	xxxxx
	Stable metabolites	x	xx	xxx
	Hydrolysis (T½)	x	xxx	xxx
	Volatilization	xxx	x	xx
	Residue in soil profile	xxxxxx	x	
Adsorption:	K_d and k_{oc} (OECD-method) Ploughlayer	xxxxxx		x
	Subsoil	xxxx	xx	x
	Freundlich constants	xx		
	K_d and K_{oc} for several soils	xx		
Leachate[2)]:	Content of pesticide	xxxx	x	
	Content of metabolites	x	xx	xx
	Content of tracer (Br^-)	xx	xxxx	
	Break through	x	xx	
	Volume of water	xxxxx	x	

pH	—	xxx	xxx
Nitrate	—	xx	xxxx
Conservation of water and analytical methods	x	x	—
Mass balance of pesticide	x	—	x
Mass balance of tracer	x	x	—
Mass balance of water	xx	—	—

2) Mainly for lysimeter experiments.

Chapter 7

Validation of Pesticide Leaching Models

M. Styczen

1. Theoretical framework

According to the mandate of the FOCUS group, 'models used for estimation of predicted environmental concentrations must be appropriate to the range of conditions in the Community and its various regions and be selected such that they are appropriate to the estimates to be made. All such models have to be validated against experimental data'.

The 'range of conditions' may be described through definition of the ranges of weather conditions, irrigation practices, soil types, positions of groundwater table, crop/tillage systems, and types of pesticides found within EU (Section 1.1). The final use of validated models for registration purposes will be to run a number of scenario's (for widely used pesticides probably in the order of 100), defined on the basis of the defined 'range of conditions' for each of the pesticides (and perhaps their metabolites) to be evaluated. The simulation results will form part of the basis for deciding whether a pesticide may be accepted for use within EU.

A number of computer models exist, which describe pesticide transport and which may be candidates to this particular model application. Each of these models have a claimed/ theoretical range of validity, defined as 'the part of reality to which the validation of a model applies'. This range may be less than the total range of conditions found within EU. It is, however, necessary to show that a computer model produces acceptable results within its range of validity. It should be noted that it is not possible to validate a computer model in general. However, through successful validation of a number of site specific models covering the 'range of validity' of the computer model in a representative way (Section 1.3), it may be made probable that a given computer model is valid also for similar sites on which it has not been tested. The validation status of a model is here defined as 'the extent to which a model has successfully been validated within its range of validity'.

As none of the proposed computer models have been tested on extensively (Section 2), it is necessary to define the experiments to be carried out (Section 3), the required measurement programme (Section 4) as well as the testing scheme the models have to pass through (Section 5). The experiments cover both lysimeter and field trials. Furthermore, success criteria must be defined, outlining when a model is performing satisfactorily. Some proposed success criteria are discussed in Section 6 and 7.

1.1 Range of conditions

The 'range of conditions' within EU covers a number of aspects:

- **weather/irrigation** (amounts of precipitation from 400-1500 mm, falling with different seasonality and different intensities, annual air temperatures from about 5-20^{o}C).
- **soils** (from sands to heavy clays and from soils low in organic matter to peaty soils,
- **position and variations of groundwater table** (from about .5 m to at least 10 m),
- **major crop/tillage systems**
- **types of pesticides** with different physico-chemical characteristics,
- pesticide concentration levels from about 100 µg/L to less than 0.1 µg/L.

1.2 Range of conditions for scenarios

In practice, models used for registration purposes will be used to simulate a number of specifically chosen scenario's which are expected to cover the range of conditions in a reasonable manner. It is necessary to validate the computer models for this particular purpose. This means, in principle that the computer model should be validated for each of these scenario's.

Presently, ten climatic scenario's are suggested, and it is expected that approximately ten soil types will be chosen as 'scenario soils'. However, not all of the ten are expected to be found within all climates. A probable estimate will be three to four within a climatic region. Taking into account different levels of the groundwater table or other lower boundary conditions, the number of scenario's lie in the order of 100 simulations. If, for validation purposes, different groups of pesticides have to be included in the validation, the number of validation

experiments would be at least in the order of 500. This is unrealistic, both with respect to funds required and workload involved, so a selection will have to be carried out. Some considerations concerning this selection are described in the following.

1.3 Range of conditions for validation purposes

1.3.1 Climate

While it may be relevant to run the 10 chosen climatic scenario's (M.Klein, handout to FOCUS meeting, April 1994) for registration purposes (depending on the use pattern of the pesticide), it may be possible to group the climates in broader groups for the validation exercise. It is critical whether the computer models are able to simulate a cold climate, a warm climate, and a climate with large variations in temperature. It is important that at least one of the scenarios include frost. This will test the ability of the models to simulate soil temperature, and the indirect effect of soil temperature on degradation of pesticides. These three groups may also have significantly different rain intensities, which will play a role for occurrence of surface runoff and macropore flow. Specifically for the validation exercise it is suggested to classify the climate in 'coastal climate' (2,3), 'Central European climate' (4,5), and 'Mediterranean climate' (8,9,10).

The climatic zones (1), (6) and (7) have been left out, (6) and (7) with the reason that these zones may be of limited interest with respect to agriculture, and (1) because it was hoped that it is possible to find a Central European site with (strong) frost during the winter. If this is not possible, and Norway, Sweden and Finland join EU, (1) may have to be included separately. (6) and (7) may be of interest for pesticides used for forestry.

1.3.2 Soils

Taking into account that the soils partly determine soil temperature, and to a large extent determine flow mechanisms, evaporation, and interactions with the pesticides, it is difficult to argue for less than three soils for each climatic zone. It is suggested to choose a sandy, a loamy and at least one clayey soil for each of the three climatic zones mentioned above. The sandy soils will differ between the regions due to different content and types of organic matter (temperature dependent), and there may be differences in parent material and pH. The clay

mineralogy also differs from north to south, with greater contents of illitic clay minerals in the northern region, and greater contents of kaolinite or montmorillonite in the southern region. The exact soils to choose will have to be determined when the scenario-soils have been decided upon.

The lower boundary condition for each of the soil classes will have to depend on what is relevant for the regions and soils in question. The two extremes whieh have to be included are 'groundwater at great depth' and 'a fluctuating groundwater table, which at least for part of the year is situated within the root zone'.

1.3.3 Crops

The exact choice of crops appears less important as long as both summer and winter crops are taken into account, in order to simulate both spring- and autumn applications. However, as it may be preferable to work with two or three pesticides only, the crop choice has to be standardised. Grain crops both cover a large area and are found in all of the zones wherefore they may be suitable candidates for the validation exercise. The final selection awaits the results of the crop mapping to be carried out.

1.3.4 Test substance

While ideally a large number of pesticides representing different chemical properties should be included in the validation, it may only be realistic to deal with 2-4 important pesticide groups. Test substances should have a Kom value in the range of 0-approx. 100 L/kg, and have a known metabolic pathway. Furthermore, analytical methods allowing detection at 0.05 µg/l and quantification in water of at least 0.1 µg/l must exist. In the lysimeter, preferably ^{14}C-labelled material should be applied.

1.3.5 Combinations

It must be ensured that all the important conditions are present in the validation experiments to be carried out. However, in order to limit the number of experiments, not all of the possible combinations of conditions may be included. This shortcut can be justified only by close monitoring of the experiments and

testing of the models, both with respect to process indicators (such as soil temperature, soil moisture) and leaching parameters.

An example of how conditions may be combined is shown in Table 1. The final number of combinations needed may be larger than shown in the example.

Table 1. An example of how a set of combinations of conditions to be included in the validation experiments could be organised.

	climate	soils	crops	pesticide	boundary cond.
1	1,2,3	'sandy'*	summer	test subst.1	gw. at ? m depth
2		'loamy'	winter	test subst.2	fluct. gw.table
3		'clayey'- illitic	summer	test subst.1	?
4	4,5	'sandy'*	winter	test subst.2	?
5		'loamy'	summer	test subst.?	?
6		'clayey'	winter	test subst.?	?
7	8,9,10	'sandy'*	summer	test subst.?	?
8		'loamy'	winter	test subst.?	?
9		'clayey'-kaolinitic	?	test subst.?	?
10		'clayey'-montmorillonitic ?	?	test subst.?	?

* The organic matter content should be considered as an important parameter. For podzolic types it is necessary to consider their possible uses.

2. Present level of model validation an applicability

A number of models have been reviewed with respect to general information, documentation, content, etc. in an earlier FOCUS-paper. These are PRZM, PRZM-2, PELMO, GLEAMS, PESTLA, VARLEACH, LEACHM, MACRO and PLM. Several of these models have been used extensively for a number of years.

A Dutch study has been carried out (Bosch, R. van den, 1994) with respect to the validation status of the pesticide leaching models PRZM, LEACHP, GLEAMS,

and PELMO. Model tests were only considered relevant if site specific sorption and transformation input data were available and if the field conditions were similar to conditions in Dutch agriculture and horticulture. For PRZM, one publication fully qualified, and three studies partly qualified with respect to independency of input data. For LEACHM, three studies were accepted, for GLEAMS one study qualified and on study was partly acceptable, and for PELMO, no studies qualified.

For PRZM, the studies showed that PRZM explains moderately well the movement of pesticides in a sandy, a sandy loam and a loam soil. However, all tests were carried out in a concentration range which was 10-100 times the level of most interest for registration purposes (<5 μg/l). LEACHP explained well the movement of pesticides in two sandy soils and a loam soil. The concentration levels were 2-50 times higher than the level of most interest. GLEAMS performed poorly in the one study which qualified.

The study concludes that the validation status is low to very low for the investigated models for the majority of conditions prevailing in Dutch agriculture and horticulture.

PESTLA has been successfully validated on lysimeter data from a Swedish sandy loam, where pesticide concentrations in the leaching water were all the time below the detection limit (Boesten, 1994). The hydrological part of the model had to be calibrated. Furthermore, PESTLA was tested on two Dutch sandy soils (Boekhold et al., 1993; Van den Bosch and Boesten, 1994). In both studies, the model explained the leaching of a mobile pesticide reasonably well (concentration levels about 10 times higher than the levels of most interest). In one of the studies the model overestimated leaching of a moderately sorbing pesticide: the measured concentration profile showed that 0.1 μg/L did not penetrate deeper than 15 cm whereas the model calculated a penetration depth of about 30 cm. So also the validation status of PESTLA is considered to be low for the majority of conditions prevailing in Dutch agriculture and horticulture.

MACRO has been tested on a Silt Loam soil (Neuenkirchen, Germany) (Jarvis,1994). Some calibration of the water phase was carried out, and the pesticide input was adjusted according to losses on leaves. The pesticide routines were successfully tested on pesticide concentrations in the soil in the range .1 - 5 mg/kg soil. Leaching did not occur within the study period.

Two studies of interest are awaiting publication. An intercomparison of models were carried out in Sweden, using lysimeter data representing five different soils. The models included were CALF, CMLS, GLEAMS, MACRO, PELMO, PESTLA and PRZM. The models were tested on data sets from five soils and two pesticides. However, not all of the models are tested on all cases. Conclusions were that laboratory data are not always reliable sources of input to simulation models which attempt to describe field conditions, and that process descriptions were not in all cases adequate. First order kinetics and lack of treatment of preferential flow processes were specifically mentioned (Bergström and Jarvis, 1994). It is presently not clear how many of the model tests were carried out successfully for each model.

Furthermore, a German study taking place at Fraunhofer Institute may shed light on the performance of PELMO.

The number of studies reviewing models with respect to applicability for specific field conditions is even lower. For Danish conditions, model requirements were discussed by Styczen and Villholth (1994), resulting in a selection of models able to simulate conditions in different parts of the country, as no single model contained all the necessary processes at the time of evaluation. However, data were not available for a proper validation of the selected models.

On the basis of the above studies it must be concluded that the validation status of the described models is low or very low at low leaching levels. However, the validation status at N 10% leaching level is generally high. A comparison of the theoretical range of validity for the computer models with the range of conditions within EU has not been carried out.

3. Experimental conditions

3.1 Type of experiments

When it comes to the choice of experimental frame for the validation experiments, requirements are conflicting.
Use of **lysimeters** are interesting from the point of view of easy control of the experiments, and the possibility of use of labelled pesticides. However, lysimeters

do not include a groundwater table as the lower boundary condition, they do not take into account horizontal flow patterns, variability and surface runoff. Furthermore, treatments of lysimeters (tillage methods, surroundings) may differ somewhat from actual field conditions.

Field trials, on the other hand, are more difficult to control, and the use of labelled pesticides may be impossible or impractical, but the flow patterns are more realistic. Very few combined lysimeter and field trials at the relevant level of concentrations have been carried out, and at least some of them (Smelt et al., 1981, 1983) indicate important differences in hydrology in the two types of systems.

It is therefore suggested that models must be validated on data from field trials as well as from lysimeters. Concerning future experiments it is recommended to carry out the experiments on the lysimeters, and in addition, to repeat all the sites with field trials. If this is not economically possible, field trials must be established for the majority of the sites, particularly where shallow groundwater or other critical factors are present. If the computer models are able to simulate the field sites 'blindly', it must then be assumed that a transfer is possible also for the rest of the conditions.

Taking into account that the cost of each experiment will be in the order of 0.5 to 1 million DM, a limitation in the number will be necessary. Use of results from already performed experiments may be possible.

3.2 Lysimeters

The lysimeters should have a surface area of at least 0.5 m^2, and a depth of at least 1 m. It must be equipped with facilities to remove the leachate. Each treatment requires two replications. The experiment must run for at least two years. The soil profile used for lysimeter studies must be undisturbed.

3.3 Field experiments

Must be designed to obtain a maximum of needed data without destroying the natural condition in the soil profile.

The surface area of the plot should be of the same order of magnitude as a normal agricultural field. Good results have been obtained with plots of about 1600 m^2.

Concentration profiles in soil and concentrations in groundwater (preferably at least 10 replicates in space) should be measured at e.g. five sampling times. The first sampling time should be immediately after application (on the same day) to check the dose and the analytical procedures. In general, soil cores collected to an adequate depth provide more reliable information than soil-suction lysimeters.

3.4 Application of the tests substance

Generally the substance must be applied to the soil. If applied to a field with plants growing, an estimate must be made on how much of the substance hit the plants. The application rate should follow the intended use as indicated in the application form for registration of a given plant protection product.

Together with the pesticide, a tracer is added to the soil and the break through of the tracer is described. If possible, it should be applied in the same tank mix as the pesticide.

3.5 Precipitation

Ideally, the precipitation is determined by the site chosen, in order to cover a particular climatic scenario. However, it is preferable to choose sites within the climatic scenario with a precipitation surplus for at least part of the year, and to add water to the level of a wet year or at least to the level of an average year. Irrigation intensities should be chosen such that they are realistic for the climatic scenario chosen.

It is important for the validation exercise that at least for some of the experiments, the pesticide is not allowed to break down undisturbed in the top layer as the obtained data will not be adequate for validation of other parts of the model than the degradation process.

A yearly precipitation of 800 mm could be chosen for the northern part of EU (climate 2 and 3).

4. Driving Variables and Parameters to be measured for each Experiment

The validation exercise will be carried out with driving variables and parameters measured or estimated on the basis of measured data. Please refer to separate chapter written by A. Helweg and R. Kloskowski.

5. Method of Validation using the established Data Sets

For each data set, the validation exercise may be carried out in four steps of which some require data from a lysimeter experiment (1a, 2a), some require data from a field (1b, 3) experiment, and some require data from both (2b, 4). For some soils, data may be available for some of the steps only. The data sets will, as described in Section 4, contain detailed information concerning flow, pesticide transport, and, in addition, data from a tracer experiment, eg. Bromide. In each of the four steps, simulations are carried out, and the relevant simulated data are stored. At the end of the test, the results will be evaluated according to specific success criteria (Section 6).

The model test will be carried out in the following steps:

1) **Blind tests**

a) **Lysimeter, blind test**

The computer model will simulate each of the lysimeter data sets 'blindly'. Results (moisture content, soil temperature, flow of water and pesticide, concentrations of pesticide) will be stored.

b) **Field experiment, blind test**

The field experiment will be simulated blindly. The results (moisture content, soil temperature, flow of water and pesticide, concentrations of pesticide) will be stored.

2) **Tests with calibration of flow and solute transport, but blind simulation of pesticide transformations and sorption.**

a) **Lysimeter with calibration of flow and solute transport**

The modeller will receive data for water flow and the bromide tracer, and carry out a calibration. Pesticide flow will be simulated, and the results stored.

b) **Field experiment, improvements based on lysimeter flow and solute transport data**

The model will be set up in accordance with the results of step 2a. The field experiment will then be simulated. The results (moisture content, soil temperature, flow of water and pesticide, concentrations of pesticide) will be stored.

3) **Field experiment with calibration of flow and solute transport**
The modeller will receive data for water flow and the tracer from the field experiment, and carry out a calibration. Pesticide flow will be simulated, and the results stored.

4) **Field experiment with calibration on lysimeter pesticide data**
The modeller will receive the pesticide data from the lysimeter experiment and set up the model for the field site in accordance with the calibrated lysimeter model. Pesticide flow will be simulated, and the results stored.

The purpose of the stepwise approach is to determine the level of information required to ensure adequate simulations. Step 1a/2a and 1b/3 show to which degree it is necessary to calibrate the hydrological part of the models. If the modellers do not fulfil the success criteria during step 1a and 1b, but only during step 2a/3, calibration is needed, also for the hydrological part of the scenario runs to be carried out at a later stage. It is therefore necessary also to define success criteria not only for the pesticide simulation but also for the hydrological part of the models.

It has been proposed to use both lysimeter experiments and model simulations in the registration process. It is therefore relevant to investigate whether lysimeter data may improve simulations of field conditions. Step 2b and 4 have been included with this purpose. If the transfer of data relating to hydrology and solute transport (step 2a) works well for the cases investigated, it will be assumed that it is possible to transfer the data obtained from lysimeters to field conditions. Step 4 shows whether pesticide parameters derived from lysimeter trials may be scaled up to field scale.

A very likely result of the exercise is that none of the models are able produce reasonable results for all experiments without some calibration of the water phase. It should be noted that it is also not necessary to be able to carry out step 1a and 1b successfully - the most important step is step three. It is so because the

intended use of the models imply that all pesticide/soil properties should be derived from independent laboratory experiments. Difficulties in applying laboratory estimates for pesticide parameters in both lysimeter and field trials may lead to the conclusion that the laboratory methods of determination are not adequate for the purpose and must be changed. However, if the problem arises only for particular conditions, step 4 may show whether lysimeter data provides an adequate base.

6. Criteria for Evaluation of Simulation Results

The outputs specified for evaluation of simulation results are:

Primary

i. Pesticide concentrations in lysimeter leachate and in groundwater (collected via direct sampling or from drainage pipes).

ii. Residual pesticide content in the soil as a function of time and depth during and at the end of the experiment. For lysimeter experiments, only pesticide content in the soil at the end of the experiment can be determined.

Secondary

iii. Flow recordings in the form of continuous or at least daily measurements of flow at the bottom of lysimeters, in drainage pipes or water table recordings (timing and nature of measurements depends on site characteristics).

iv. Soil moisture content as a function of time and depth.

v. Soil temperature as a function of time and depth.

For all of the four steps of the test it is necessary to evaluate (i). and (ii). It is suggested to carry out the following tests:

I Visual comparison of measured and simulated concentrations,

II Comparison of
- peak concentrations (daily values) and
- weekly averaged concentrations,

III Comparison of accumulated pesticide leaching,

IV Comparison of residual pesticide content.

For step 1 and 2, it is necessary also to evaluate (iii), (iv) and (v). It is suggested to carry out the following tests in relation to (iii):

V Visual comparison of measured and simulated discharges,

VI Comparison of the total water balance,

VII Comparison of weekly (or daily) discharges

VIII Comparison of measured and simulated moisture contents and soil temperatures. For the specific data sets it may, however, be of interest to specify certain periods which are most critical to the simulations and compare moisture and temperature calculations with measurements specifically for these periods.

For each of the tests performance criteria must be specified to decide when a certain test has been passed. These criteria has to be decided upon taking into account prediction uncertainty based on spatial variability (several of the parameter measurements are point measurements which are chosen to represent a certain area). Boekhold et al. (1993) suggests to log-transform the measured data and estimate a confidence interval about the estimated mean of the log transformed data. The mean ± one or two standard variations is then compared with an interval around the simulated values defined as P/f-P*f:

$$[10^{(Mav - n*\sigma)}, 10^{(Mav + n*\sigma)}] \quad \text{compared to} \quad [P/f, P*f]$$

where

- M_{av} is the mean of the log transformed measured data
- σ is the standard deviation of the log transformed data
- n equals 1 or 2
- P is the predicted value
- f is usually in the order of 2-5

The described approach is possible for data which are based on several measurements. In addition to this, a number of standard methods of analyses are available. Some suggested success criteria are given in Appendix 2, and the details of the suggested analyses of residual errors are listed in Appendix 1. The exact statistical criteria to use must be defined before the simulations are carried out.

It may be advantageous also to establish how many criteria have to be successfully fulfilled to be able to talk about a successful validation of the computer model for the given site.

It may be necessary to review the criteria after a number (eg. five or so) of the sites have been simulated to see whether the suggested success criteria are scientifically adequate to describe the model performances.

7. Criteria for Assessment of Validation Status and Model Applicability

As mentioned in section 2, it is necessary to distinguish between that a computer model has been proven valid for a number of cases within its range of validity, and that a computer model may be applied for the total range of conditions within EU. For this reason it may be necessary to operate with two different assessments.

1. The validation status may be assessed from the probability of a sufficiently accurate model estimation of the pesticide concentration in groundwater within the range of validity of the computer code. This probability is called P. To estimate P, a number of model tests are required, drawn from the range of validity. To achieve a moderate validation status, a comparatively large number of model tests covering the whole range of validity is needed. The following nomenclature is proposed:

   $P < 25\ \%$ very low
   $25\ \% < P < 50\ \%$ low
   $50\ \% < P < 75\ \%$ moderate
   $75\ \% < P$ high

   A first guess of P could be obtained from testing the model on the data sets obtained section 4 and 5, which are within the range of theoretical validity for the computer code in question.

   It may be relevant to investigate why a model in some cases fails to perform well. Failures may be related to specific soil types, groups of

pesticides, particular boundary conditions, specific climatic conditions, etc. which the model is not able to handle adequately. If the number of experimental data sets allow, a scheme for testing this can be derived. The cases with the given characteristic (e.g. heavy clays, or frozen soils, or high intensity rainfall) may then be removed from the population of tests and P may be redetermined. This means, in practice, that the theoretical range of validity is reduced to a proven range of validity. For data sets where all models fail, it may be relevant to recheck the data quality and to consider the need for further model development.

2. In order to assess the applicability of the computer model for registration purposes within the EU, however, it is necessary also to assess the coverage of the model compared to the range of conditions described in section 1. This could be done in a manner similar to the estimation of validation status, but taking into account all the established data sets. If a more sophisticated approach is needed, each of the data sets weighted by an area-fraction, indicating their extent within the EU.

The two assessment approaches will indicate to regulators whether a particular computer model is performing well within in range of validity, and how this range of validity compares to the range of conditions within EU. Finally, it may be necessary to choose two or three models, each of which have a high validation status, and which together cover the range of conditions within EU.

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Appendix 1

Measures suggested for Analysis of residual Errors

Root mean square error

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_1-O_i)^2}\cdot\frac{100}{0}$$

Coefficient of residual mass

$$CRM = \frac{\sum_{i=1}^{n} O_i - \sum_{i=1}^{n} P_i}{\sum_{i=1}^{n} O_i}$$

P_i	=	predicted valves
O_i	=	observed values
_	=	mean of observed data
n	=	number of samples

Nash-Sutcliffe coefficient (R^2):

$$R^2 = 1 - \sum_{i=1}^{n}(Q_{obs}-Q)^2 / \sum_{i=1}^{n}(Qobs-Q_{av})^2,$$

Q_{obs} is the daily/weekly flows for the whole period
- Q_{sim} is the daily/weekly flows simulated for the period, and
- Q_{av} is the average daily/weekly flows for the whole period,

Appendix 2

Suggested Success Criteria

The Roman figures relate to the tests specified in Chapter 6.

II a If peak concentrations (daily values) are based on single measurements, the suggested success criteria for percent deviation is [50-200%] (equal to an f-factor of 2). If based on several determinations, the described factor f-method can be used.

II b For a time series of weekly averaged concentrations, Root Mean Square Error can be used for evaluation of fit. Suggested criteria: RMSE < 30 %.

III For comparison of accumulated pesticide leaching, the Coefficient of Residual Mass may be used. Due to increased uncertainty with decreasing concentrations, it may be reasonable to specify a scale as a function leached amount. For small concentrations (below 1 µg/L) and small total amounts (below 100 µg), an f-factor of 4-5 may be acceptable to registration authorities: [25 % - 400 %] or [20 % - 500 %], but initially it is proposed to use an f-factor of 2.

IV For comparison of residual pesticide in the soil, the f-factor approach is suggested. As in (III), the acceptable error may be a function of concentration levels. It is suggested to use a factor of 1.2 for concentrations after application, increasing to a factor of 2 as concentration levels decrease.

VI For comparison of the total water balance, % deviation of each component can be used as a measure. Suggested success criteria: +/- 8 %. This criteria is very strict, but taking into account the precision needed for solute transport, it is necessary that the errors related to the hydrological simulation are minimised.

VII For comparison of weekly (or daily) discharges, a scatter diagram and a Nash-Sutcliffe coefficient (R^2) or alternatively the Root Mean Square Error may be used. It must be noted that the Nash-Sutcliffe coefficient (Nash and Sutcliffe, 1970) can only be compared for different computer models used on the same test case. As it is a function of variation within the observed time series, the level of determination is also a function of the records used. R2 must therefore be defined according to test cases. RMSE also depends on records, but to a lesser degree. For RMSE, the suggested success criteria is: RMSE < 10 %

VIII Depending on the number of measurements at a given time and depth, different approaches may be used. In general, the Root Mean Square Error approach is recommended, with the suggested success criteria: RMSE < 10 %. If more measurements are available, an approach similar to the f-factor approach could be considered, taking into account the deviation on the measurements and comparing this to an interval around the predicted value ($[P-\sigma_p, P+\sigma_p]$), where σ_p is an estimated/acceptable error for the predicted value.

Chapter 8

Recommendations for the Correct Use of Models and Reporting of Modelling Results

K.Z. Travis

Introduction

Models of the fate of pesticides in the environment have an important and increasing role in the risk assessment, and in the pesticide registration process. This is particularly true in the case of the EC Registration Directive (Anon., 1991), where the derivation of Predicted Environmental Concentrations (PEC) is required. There is a recognised need for guidance on correct procedures for the use of models and the reporting of modelling results. This need is addressed in this document, which has been produced by the Regulatory Modelling Work group of FOCUS.

A natural question to consider first is whether modelling is in some way covered by the requirements of Good Laboratory Practice (GLP). The document then turns to the concept of Good Modelling Practice, and its implications for the authors, maintainers and users of models.

Modelling and GLP

It makes sense to examine closely the scope of Good Laboratory Practice, to see if it applies to the development or use of models of pesticide fate.

The majority of work performed on pesticides in order to achieve a registration is performed to the principles of Good Laboratory Practice. This is certainly the case for dossiers submitted under the EC Registration Directive, which refers to another EC directive on GLP (Anon., 1987). This latter EC Directive in turn relies primarily on recognising the OECD principles of GLP (latest version: OECD, 1992), in which the following definitions of *GLP* and of a *study* are to be found:

"Good Laboratory Practice (GLP) is concerned with the organisational process and the conditions under which laboratory studies are planned, performed, monitored, recorded, and reported."

"*Study* means an experiment or set of experiments in which a test substance is examined to obtain data on its properties and/or safety with respect to human health and the environment."

It is clear from the definitions that *GLP* is concerned only with *studies*, and *studies* involve the application of a test substance, i.e. a sample of a chemical. Using computer models of the fate of pesticides does not involve the application of a test substance. Therefore modelling work cannot be a *study*, in the GLP sense, so modelling is not covered by the provisions of GLP.

Good Modelling Practice

Experience with using models in a regulatory framework has clearly indicated to all parties involved that there would be benefit to having clear guidance of the correct use of models and reporting of modelling results. The benefit obtained would be in terms of quality, consistency and integrity of the modelling effort, enabling meaningful communication of model results and implications between regulator and registrant. The term Good Modelling Practice has been coined for this idea (note that abbreviation to GMP is not advised due to possible confusion with the established principles of Good Manufacturing Practice). Good Modelling Practice has recently been defined as "The development, maintenance, distribution and use of computer simulation models whereby the integrity of the model, its various improvements and utilisation is assured" (Estes & Coody, 1993).

Responsibility for following Good Modelling Practice lies with those responsible for the development, maintenance and use of models, and each has a particular role in this process. These responsibilities are outlined in Figures 1 and 2, for which credit is due to the authors of the 'German codex' (Görlitz, 1993) and to the FIFRA-Environmental Fate Modelling Group (Estes & Coody, 1993).

Often the roles of model developer and model maintainer are combined - their joint responsibilities are listed in Figure 1. These common-sense procedural requirements say nothing about the quality of the model algorithms or the level of validation of the model. The scientific suitability of a model is an entirely different and very important issue, which has to be considered in addition to the documentation and user support requirements of Good Modelling Practice.

The designation of a particular institution to provide support such as error logging and reporting, training, a register of users and version control is extremely important for the integrity of the modelling process. Specification of which versions of each model are approved for regulatory use (officialisation) is necessary since the models used are developing and changing rapidly, and sometime many versions exist (for example it is important to prevent outdated, flawed or uncompleted versions of models from being used in the regulatory process).

Model users included anyone who uses a model to generate predictive results for assessing the fate of pesticides in the environment, and their responsibilities are given in Figure 2. A fundamental principle guiding the model user in reporting modelling work is that enough information should be provided so that it is potentially possible for an independent person to reproduce the results. All the reporting responsibilities of the model user are a simple consequence of applying this principle.

FIGURE 1: Responsibilities of the model developer and maintainer

DOCUMENTATION

- Version control and information on changes in code
- Availability of source code
- Installation and use information
- Description of all model inputs and outputs
- Advice on input value selection
- Precise definition of input file formats
- Description of the governing equations
- Supply of test input datasets and their expected output files
- Code verification results (i.e. bug checking)
- Summary of significant model assumptions and limitations
- Description of model validation work done
- Conclusions from the validation concerning validation status and range of validity

SUPPORT

- Defined institution should provide support
- Maintain error log and communicate appropriately
- Maintain a register of users
- Version control and supply, tracking version changes
- Training and technical support
- Notification of upgrades

OFFICIALISATION

- Specific version numbers should be authorised for regulatory use

FIGURE 2: Responsibilities of the model user

A fundamental principle guiding the model user in reporting modelling work is that enough information should be provided so that it is potentially possible for an independent person to reproduce the results.

SUITABILITY OF MODEL USED

- Use a version officially approved for regulatory use
- Have a good knowledge of the chemical and a good understanding of the model
- Does it include all relevant processes, and represent them in a reasonable way?
- Use a scenario within the range of intended use and validity of the model
- Confirm system integrity by using test input files provided

INPUT DATA

- Choice, quality and justification of inputs to suit the chemical and scenario modelled
- Theory used in the interpretation of experimental data should be consistent with that used in the model[1]

DOCUMENTATION AND REPORTING

- Confirm results are reasonable
- Document program version and date
- Detail any modifications made to the software
- Give any essential hardware/software specification
- Give all inputs used
- Where model output has been processed, give method for evaluating outputs
- Give results

[1] For example, an adsorption coefficient derived from data using a Freundlich isotherm is not appropriate for use in a model with a linear isotherm

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Chapter 9

Recommendations for Using Soil Leaching Models in Regulatory Environmental Risk Assessments

R. Jones.

Modeling can be a useful tool in assessing the environmental behavior of agricultural chemicals. Potential uses of such assessments in the registration process include preliminary assessments, triggers for additional studies or more comprehensive modeling, detailed modeling simulations, and development of management practices. In the registration process model simulations can also be helpful in understanding or interpreting the results of lysimeter or field experiments, but this discussion will be limited to the use of modeling in performing regulatory environmental risk assessments.

Separating modeling into different phases or Steps is somewhat arbitrary since there are no clear divisions between modeling for simple and more complex assessments. Often the same model is used, but more care is given to the definition of input parameters and probably the number of simulations increases as the assessment becomes more comprehensive. For the purposes of this discussion, Step 1 modeling consists of simple assessments using prescribed models with standard scenarios which may or may not reflect actual use of the agricultural chemical, Step 2 modeling consists of simple assessments using standard models and scenarios which are representative of the actual use of the compound, and Step 3 modeling consists of assessments using models that may have been modified to reflect the behavior of a specific chemical and input parameters developed specifically for the assessment.

Modelling in Step 1 should be sensitive enough to identify chemicals with potential problems, but clear most chemicals without problems with a minimum of work. Most simulations performed in Step 1 will focus on realistic, worst case situations (for example, heavy rainfall and sandy soils). Modeling simulations performed in Step 1 should be quite routine and require little judgement by the modeler. Regulatory review of simulations as well as the conduct of modeling in Step 1 is greatly facilitated by having specified input parameter data sets, with perhaps only the specific properties of the agricultural chemical being supplied. Examples of such systems include the PELMO scenarios for Germany or the standard Dutch scenario used with PESTLA. A similar system of scenarios should be developed for EU registrations. From a logistics point of view, use of a

single model for Step 1 is highly desirable. However, since different models (but equivalent for Step 1 modeling) are currently used in different EU countries, the selection of a single model may be difficult especially since there is no clear scientific justification for choosing one over another. Any model recommended for regulatory applications must have an official sponsor responsible for distribution, version control, upgrades, and maintenance.

Step 1 simulations should never be considered as independent cutoff criteria. However, such simulations could trigger additional modeling or field studies, and should only be used as the basis for adverse regulatory decisions in the absence of such studies. Results of appropriately conducted more comprehensive simulations (such as Step 2 or 3) should be considered as adequate replacements for Step 1 simulations (assuming agreement between regulators and registrants about the appropriateness of input parameters used in the simulations). Degradation estimates should be the best information available (for example, field study results, when available, should usually be preferred to laboratory measurements). Results of field studies should also be considered more definitive than modeling predictions.

A second Step of modeling is needed because simulations under the standard scenarios prescribed in the Step 1 may not be realistic for the specific chemical being assessed. For example, a cold climate is not realistic for a compound applied only to a warm climate crop such as citrus. Sometimes, a product cannot be used on certain soil types, or specific crops are not grown on certain soils. In these circumstances, the standard scenarios may need to be adapted, especially if potential problems are identified under unrealistic scenarios in Step 1.

Model simulations in the Step 3 need to be tailored to the specific objectives of the modeling study. Simulations may be performed over a number of years with a variety of soil types to estimate the probability and magnitude of residue movement. Simulations may be used in the development of management practices, such as optimisation of application timing or use restrictions in certain soil types. Although the use of existing models is preferable, sometimes modifying model subroutines may be necessary to account for compound-specific behavior, such as degradation or sorption processes. After any modifications, the modeler must demonstrate that the modified model is working properly. Procedures for conducting Step 3 simulations should not be fixed; it is the job of the modeler to technically justify the work and document the results according to good modeling practices. Often procedures and input parameters in such simulations will be the subject of discussions between modelers and regulators.

Although existing models such as PELMO and PESTLA have been used to estimate average concentrations below 0.1 μg/L, model users and regulators should realise that the model predictions are not accurate for concentrations below about 1.0-0.1 percent of the amount applied. This is because the equations in these models focus on the movement of all of the material present via classical leaching. When the amount of material remaining drops below about 1.0-0.1 percent of the amount applied, the concentration profile of the remaining material has often been significantly affected by preferential flow processes not included in these models. Although predictions to 0.1 μg/L may be necessary for regulatory purposes, such predictions will not agree with actual behavior in the environment, especially for applications greater than about 100 g/ha. Similarly, model predictions using deterministic models will only represent the mean behavior of chemicals in the environment, and do not consider spatial variability. In field studies, coefficients of variation in individual soil samples are in the range of 100 percent. Even in well-controlled studies such as large-diameter lysimeter studies with sandy soils, variations by factors of 4-20 at low concentration levels (~0.1 μg/L) are not uncommon in leachate from replicate lysimeters.

One common deficiency among currently existing soil leaching models is the inability to accurately account for preferential flow processes such as funnel flow in coarse sands or bypass flow through cracks or wormholes in more structured soils. Progress continues to be made in understanding these processes and recently models have been introduced which include preferential flow processes; however, soil parameters in these models must be obtained by calibration. The models can be used to assess behavior of agricultural chemicals in soils in standard scenarios where these soil parameters have been experimentally determined. Further advancements are needed before such models can be routinely used for predictions without performing calibration experiments.

The use of models in regulatory applications raises a number of questions about the standards by which the results of such simulations should be interpreted. Such standards encompass the severity of the standard scenario (type of soil, depth of soil, severity of weather, etc.), the inclusion of macropore flow, the concentration deemed to be of relevance (for example, peak concentrations or time-averaged values), and the concentration used as the regulatory guideline (for example, the EU drinking water limit of 0.1 μg/L drinking water; however it should be emphasised that soil water or ground water concentrations predicted by leaching models are usually significantly higher than drinking water concentrations due to continuing degradation in subsoils and ground water, dispersion, dilution, and other processes). In general, the aim is to devise a reasonable combination of standards by which simulation results are to be interpreted so that compounds that pose unacceptable risk are not granted

registrations and compounds that are environmentally acceptable receive registrations. Such standards need to be regarded in the context of the total set. For example, peak concentrations are always higher than average concentrations. However, a set of standards based on average concentrations may be more stringent than another set of standards based on peak concentrations if, for example, the standard scenario used with the average concentration criterion is more favourable to leaching. Sets of apparently reasonable standards can be developed with the result that essentially all compounds will fail ranging to essentially all compounds passing. Although proposing a set of standards is beyond the scope of this document, the following comments are made on macropore flow and time averaging of concentrations.

Whether or not to include preferential flow in the evaluation process depends on the objective for the simulations. If the purpose of the simulations is to evaluate leaching potential relative to other compounds, then preferential flow probably does not need to be included, since for moderately and weakly sorbed compounds preferential flow may depend more on soil structure and timing and magnitude of rainfall events than on specific chemical properties. If the objective of the simulation is to assess movement under a specific standard scenario in which preferential flow paths are important, then preferential flow mechanisms cannot be excluded for a result that will compare favourably with actual behavior. However, careful consideration must be paid to the appropriateness of the other standards. Very few agricultural chemicals would have less than 0.1 μg/L in leachate from a lysimeter study conducted with cracking clay soils in which a heavy rainfall occurred within a few hours after application.

Simulation results should be interpreted on the basis of time averaged-concentrations rather than peak concentrations. Peak values are more sensitive to the shape of the concentration profile than time-averaged values. For example, differences in dispersion may result in quite different peak concentrations while the total amount of material moving below a specified point may be identical. Therefore, peak concentrations are sensitive to the choice of model or factors related to the numerical solution such as number of depth increments or the length of the time step. Time-averaged concentrations may also be more representative of ground water concentrations that occur as the soil water is dispersed into ground water, although such concentrations may also be sensitive to dispersion, especially when only small portion of the applied material moves below this depth. Choice of the appropriate length of time for averaging in leaching simulations is not straightforward but probably averages should be over at least a month and no longer than a year. For ecological evaluations involving surface water, values averaged over the time relevant for toxicological effects are usually used. Averaging over the time relevant for toxicological effects is not possible

for leaching evaluations in the EU since ground water concentrations are not necessarily representative of potential concentrations in drinking water and since the EU drinking water limit has no toxicological basis. Two different criteria for time averaging of concentrations are currently used in Europe. The German authorities use average concentrations over a year when evaluating PELMO simulations. The Dutch authorities use peak concentrations in ground water present between 1 and 2 meters below the soil surface. This approach actually provides a time-averaged concentration since the amount of water present in this layer is about equivalent to the amount of yearly recharge.

Chapter 10

Model Types and Modelling Philosophy

D. Yon and A. Walker

One of the aims of the FOCUS Regulatory Modelling Work group is to define/develop the role of environmental fate modelling required for EU harmonised registration. This document reports the work done to achieve this aim. It highlights philosophical considerations on the use of models in the registration process, identifies different categories of models and finally provides an inventory of modelling tools currently available.

Within the framework of the EC directive there are requirements for a number of different types of mathematical models to fulfil a number of different functions. These may be summarised as follows:

1. Models for behaviour in soil to calculate: (a) concentrations in soil (PEC's) taking into account the number of applications, (b) equilibrium levels in soil where accumulation occurs, (c) total and bioavailable concentrations in the plough layer, (d) leaching to groundwater, (e) behaviour in the saturated zone and (f) concentrations at the water table.

2. Models for behaviour in surface waters considering both concentrations in water (PECsw) and sediment.

3. Models for calculating exposure to operators, bystanders etc.

4. Models for calculating theoretical lifetime in the top layers of aqueous systems from quantum yield data.

5. Models for predicting volatility and entry into air and subsequent degradation and dispersion in air.

6. Models for extrapolating the degradation rate at 10 and 30 degrees Celsius from experimental data produced at between 15 and 25 degrees Celsius.

Having identified areas in which modelling would be beneficial, some key questions as to the nature of the use should also be addressed. The most rational use of models in all of these applications is by a systematic tiered approach with

calculations of increasing complexity and input data requirements resulting ultimately in an assessment of the relative impact of a number of key environmental parameters. Correct modelling applications should account for relevant governing processes at an appropriate level of detail (time step and scale) and accuracy relative to achieving the objectives of the study. The level of sophistication required in a modelling study reflects constraints such as : (1) accuracy required, (2) time frames, (3) available technology to describe environmental fate behaviour and (4) availability of data. These constraints dictate model selection , whether modelling is an appropriate tool for achieving the objectives and the limitations in interpreting modelling results.

Models are often divided into three groups - Screening, Primary and Secondary. These categories more accurately describe the use of the models, since some models can be ascribed to more than one category.

Screening Models

Screening models should be used to provide rapid prediction of the potential environmental fate of a compound. Screening models should come with "potted" environmental scenarios which can be used to quickly assess the effects of different soil types and climatic conditions on pesticide behaviour. These models can also be used to compare the environmental fate of a new compound with other compounds in a simple bench marking process. Examples of models in this category include Jury's Behaviour Assessment model (BAM), and some versions of the Mackay FUGACITY model. However, more complex models such as PESTLA and PELMO can also be used for screening purposes.

Primary Models

These models should provide a standardised approach, where possible, to characterise pesticide behaviour and, hence, should permit rapid review of modelling submissions by regulators and help to ensure consistent regulatory decision making. Specific models should be selected based on acceptance by regulatory officials and the ability of the models to accurately describe environmental fate processes for many typical pesticide conditions. Examples of models falling in this category would include CALF, PRZM2, GLEAMS, LEACHM-P, PESTLA, PELMO and EXAMS.

Secondary Models

Secondary models are appropriate for chemical and site-specific predictions. Most of the primary models can be used in this way, but the group also includes

MACRO, PLM, and CRACK (or any other macropore flow model) which all offer added sophistication and increased data requirements compared with most of the primary models listed above.

All of the models cited above are given as examples only; a list of models covering all of the categories is presented in the Appendix.

APPENDIX
List of modelling tools.

Annex II

2.3.2 Henry's Law

DTEST (Part of E4CHEM, Projektgruppe Umweltegefährdungs-potentiale von Chemikalien, Gesellschaft für Strahlen und Unweltforschung mbH, München))

2.9.3 Calculations to estimate lifetime in aqueous systems

GC Solar (Zepp & Cline, 1977, Environ. Sci. Technol. **11**, 359)

Frank & Klopffer program (UBA research report no. 10602046, 1985)

2.10.1Estimation of Gas phase degradation

Atmospheric oxidation programme (Meylan & Howard, 1991, Syracuse Research Corp, Syracuse, NY)

7.1.1.2 Route of degradation

PAVAR (Programm Zur Auswertung Von AbbauReihen, Timme and Frehse, 1993, Bayer AG, Monhein, Germany)

Annex III

9. Predicted Environmental Concentrations

PEC_s

BAM (Jury *et al*, 1983, J. Environ. Qual, **12** ,558 - 564)
FUGACITY (Mackay & Stiver, 1991, Environmental chemistry of Herbicides, **2**, CRC press, 281 - 297)
PERSIST (Walker & Barnes, 1981, Pest. Sci. , **12**, 123 - 132)
PELMO (1.0) (Klein. M, Fraunhofer Gesellschaft, 1991, Schmallenberg, Germany)
CALF (Nicholls *et al.*, 1982 Pest. Sci., **13**, 484 - 494)
VARLEACH (Walker *et al.*, 1989, Weed Res., **29**, 375 - 383)
PESTLA (2.3) (Boesten & Van der Linden, 1991, J. Environ Qual., **20**, 425 - 435)

PEC_{sw}

Dutch Drift calculations (EPPO/OEPP Bulletin, 1993, **23**, Blackwell Scientific Publications.)
German Drift calculations (Ganzelmeier *et al.* 1993, Pflanzenschutz-Praxis, March issue, pp14 - 15.)
TOXSWA (Adriaanse. P, DLO Winand Staring Centre, 1994, Wageningen, Netherlands.)

PEC_{gw}

PELMO (1.0) (Klein. M, Fraunhofer Gesellschaft, 1991, Schmallenberg, Germany)
CALF (Nicholls *et al.*, 1982 Pest. Sci., **13**, 484 - 494)
VARLEACH (Walker *et al.*, 1989, Weed Res., **29**, 375 - 383)
SESOIL (Bonazountos & Wagner, 1984, A D Little & Co. , Cambridge , Mass.)
PESTLA (2.3) (Boesten & Van der Linden, 1991, J. Environ Qual., **20**, 425 - 435)
CMLS (Nofziger & Hornsby, 1987, Univ. of Florida , circular no. 780)

PEC_a

EPPO PEC_a calculation (EPPO/OEPP Bulletin, 1993, **23**, Blackwell Scientific Publications.)

10.2.5.1 Effects on Earthworms

EPPO recommendations (EPPO/OEPP Bulletin, 1993, **23**, Blackwell Scientific Publications.)

Annex VI

2.5.1.2 Groundwater

EPPO PECgw (EPPO/OEPP Bulletin, 1993, **23**, Blackwell Scientific Publications.)

PELMO (1.0) (Klein. M, Fraunhofer Gesellschaft, 1991, Schmallenberg, Germany)

PESTLA (2.3) (Boesten & Van der Linden, 1991, J. Environ Qual., **20**, 425 - 435)

CALF (VARLEACH) (Nicholls *et al.*, 1982 Pest. Sci., **13**, 484 - 494; Walker *et al.*, 1989, Weed Res., **29**, 375 - 383)
PRZM-1 (1.0) (Carsels *etal*, 1984, EPA, Athens, GA)

PRZM-2 (1.02) (Carsels *etal*, 1993, EPA, Athens, GA)

GLEAMS (2.03) (Leonard *etal*, 1993, USDA, Tifton, GA)

LEACHM (3.1) (Hutson & Wagenet, 1992, Research Report no. 92-3, Cornell Univ., Ithaca, NY)

SESOIL (Bonazountos & Wagner, 1984, A D Little & Co. , Cambridge , Mass.)

2.5.1.3 Surface water

EPPO PECsw (EPPO/OEPP Bulletin, 1993, **23**, Blackwell Scientific Publications.)

PELMO (1.0) (Klein. M, Fraunhofer Gesellschaft, 1991, Schmallenberg, Germany)

PRZM-1 (1.0) (Carsels *etal*, 1984, EPA, Athens, GA)

PRZM-2 (1.02) (Carsels *etal*, 1993, EPA, Athens, GA)

GLEAMS (2.03) (Leonard *etal*, 1993, USDA, Tifton, GA)

EXAMS (Burns *et al*, 1982, User Manual and System Documantation. EPA-600/3-82-023, US Environmental Protection Agency, Washington D.C.)

SWRRB (Arnold *et al.*, 1990, SWRRB: A basin Scale Simulation Model for Soil and Water Resource Management. Texas A&M Press. 255 pp.)

EPIC-WQ (Sharpley and Williams, 1990, US Department of Agriculture Technical Bulletin no. 1768. 127 pp.)

TOXSWA (Adriaanse. P, DLO Winand Staring Centre, 1994, Wageningen, Netherlands.)

2.5.1.4 Air

EPPO PEC_a calculation (EPPO/OEPP Bulletin, 1993, **23**, Blackwell Scientific Publications.)

AGDISP (5.3) (Curbishley, 1990, Continuum Dynamics, Princeton, USA)

FSCBG (3.05) (Curbishley, 1990, Continuum Dynamics, Princeton, USA)

2.5.2.3 Bees

EPPO proposal (EPPO/OEPP Bulletin, 1993, **23**, Blackwell Scientific Publications.)

2.5.2.4 Beneficial Arthropods

EPPO proposal (EPPO/OEPP Bulletin, 1993, **23**, Blackwell Scientific Publications.)

2.5.2.5 Earthworms

Use PEC_s