24.2.97

SURFACE WATER MODELS
AND EU REGISTRATION
OF PLANT PROTECTION PRODUCTS

Final report of the work of the Regulatory Modelling Working Group on Surface Water Models of FOCUS (FOrum for the Co-ordination of pesticide fate models and their USe).

Contributors: P. Adriaanse, R. Allen, V. Gouy, J. Hollis,
J. Hosang, N. Jarvis, T.Jarvis, M. Klein, R. Layton,
J.Linders, H. Schäfer, L. Smeets, D. Yon.

Working Group Membership

P. Adriaanse	DLO Winand Staring Centre, NL
R. Allen	AgrEvo, UK
V. Gouy	CEMAGREF, F
J. Hollis	Soil Survey and Land Research Centre, UK, secretariat
J. Hosang	Ciba Geigy Ltd, CH
N. Jarvis	Department of Soil Sciences, S
T. Jarvis	Pesticide Safety Directorate, UK
M. Klein	Fraunhofer Institute, D
R. Layton	Dupont Agricultural Products, USA
J. Linders	RIVM, NL, chairman
H. Schäfer	Bayer AG, D
L. Smeets	European Commission, B
D. Yon	DowElanco, UK

CONTENTS

1. SUMMARY

The Steering Committee on FOCUS has installed a working group on the applicability of mathematical models in the environmental compartment surface water and the role these models can have in the registration process, taking into account the validation status of the models identified. With respect to terminology and approach the working group has built on the earlier work of the FOCUS-leaching group. Initially, the group made an inventory of possible entry routes into surface water: spray-drift, drainage, run-off and atmospheric deposition. The latter is, however, considered of minor importance for the contamination of surface waters. For each item the selected and currently used mathematical models were then analysed and judged on their merits. The same has been done for models describing the fate of pesticides in surface water. Several models appear to be promising in their possibilities for use in the registration process, e.g. in order to estimate spray-drift, tables have been derived from scientific research based on distances of > 5m. These tables have been adjusted for shorter distances. For drainage the models PESTLA, MACRO and CRACK_P can be recommended by the group because their validation status is reasonably well advanced compared to other models. The models GLEAMS, PRZM and PELMO appear to be the most suitable models to be used in providing 'edge-of-field' concentrations of pesticides in run-off water and eroded sediment. Models on atmospheric deposition along with associated evaluation tools are considered to be at too early a stage of development to enable them to be used on a regular registration basis. Finally, for estimating the concentrations of pesticides in surface water, the models SLOOT.BOX and ABIWAS provide reasonable screening estimate whereas EXAMS, WASP and TOXSWA are more sophisticated tools for determining possible surface water concentrations. However, even on the local scale these models are not considered validated. It should be stressed that none of the models currently studied fulfil the requirements for the label of "validated on a community level". Generally, it was concluded that the accuracy of the models reviewed was such that the peak concentrations could be predicted within one order of magnitude.

Mathematical models have been developed for a wide variety of situations even for the description of pesticide behaviour in the environment. The FOCUS Surface Water Group has limited itself to the scale of the field where plant protection products are applied. Therefore, regional models or models for catchment areas are not considered.

For the evaluation of the possible contamination of plant protection products entering surface waters the group recommends to use a tiered approach, which means starting with a simple estimation of the PEC's in surface waters and if toxicity-exposure-ratios (TER) are expected to be exceeded a more sophisticated modelling tool using realistic worst case assumptions can be applied. If still TER's are exceeded a third level of modelling, e.g. using a local realistic scenario simulating a situation as close to reality has to be applied.

The FOCUS Working Group recommends further research on harmonisation of model use, development of a community model for surface water with full and recognised scientific validation. In addition it is recommended to develop standard scenarios for the European Union.

2. INTRODUCTION

2.1 Background

Council Directive 91/414/EEC of 15th July 1991 concerning the placing of plant protection products on the market, describes the requirements which have to be fulfilled in order to obtain an authorisation for a plant protection product.

Detailed evaluation and decision making criteria to be applied by Member States when granting an authorization are provided in the Uniform Principles, Annex VI of the Directive. The data to be submitted by the companies when applying for the authorization of a plant protection product are contained in the Annexes II (for the active substance) and Annex III (for the plant protection product).

In addition to the required experimental data, results from different model calculations should be considered in the registration procedure. The Directive, while referring in general to the use of suitable calculation models validated at community level, does not recommend any specific models.

At present, no model has been validated at Community level but there are many models, which are already in use for the assessment of the environmental behaviour of chemicals. In order to "organise the use of models" within the EU countries and to help the user/regulator in using models a "Forum for the co-ordination of pesticide fate models and their use" (FOCUS) was established.

Guidance on the use of leaching models has been provided in document 4952/VI/95. The present report deals with input to and fate in surface water, detailing the possibilities, status and validation of mathematical modelling. It should be stressed that the report does not pretend to be complete in the description of all existing models.

Performing measurements of environmental concentrations that are representative of all conditions under which plant protection products could be used in the EU is very expensive. Therefore both results of model calculations and of field studies should be used as optimally and economically as possible. This is best achieved by treating measurements and model calculations as complementary activities. Generally PEC's are mostly dealt with in a two step process, starting with very simple calculations based either on empirical equations and tables (e.g. spray drift tables) or on common sense (e.g. calculation of initial concentrations in the upper soil layer from the application rate). Since these simple calculations are mostly based on worst case assumptions, they may be sufficient for risk estimations. However, in many cases more sophisticated approaches are needed because either the simple approaches are not satisfactorily estimating the concentrations in surface water or the environmental concentration has to be calculated also for chronic exposure scenario. In these cases more complex simulation models can be applied in a second step.

In July 1994 the FOCUS Steering Committee installed the Working Group on Surface Water to analyse the role of mathematical models applied to surface waters and their role in the registration process The Group met 5 times in one-day meetings in the period between

November 1994 and February 1996. and were partly funded by the Directorate General for Agriculture of the European Commission. The result of the Group’s meetings is the present report, which is intended to provide experts’ opinion on the use of surface water models in the EU-registration process.

2.2 Remit of the group

The remit of the Surface Water Modelling Working Group was established as follows:

> The issues are run-off, drift, drainage and fate of pesticides within surface waters.

- What models exist which might be used in a regulatory context?
- Assess the relevance of these models for estimating Predicted Environmental Concentrations in surface water (PEC_{sw}).
- What are relevant scenarios, especially at a screening level?
- How can fate within surface waters be considered e.g. to take into account chronic toxicity and multiple applications
- Aquatic sediment toxicity testing protocols and guidelines are under development in the EU. For interpretation, PEC-values in aquatic sediment will be required. More detailed aquatic fate models include consideration of the concentration in the aquatic sediment. At the screening level in particular, methods for deriving PEC-values for aquatic sediment need to be discussed.

The group should be mindful that the need is for models to be used in a regulatory context, and that validation, model availability, model quality and usability will need to be considered.

2.3 Working procedure

The work of the group could be enhanced by that already completed by the leaching group (DOC. 4952/VI/95), because several items count for surface water as well as ground water.

The working group established for each item to be addressed, spray-drift, drainage, run-off and fate, a subgroup consisting of 2 to 4 members. The task of each subgroup was to prepare a chapter on its assigned subject. In preparing these chapters the principles established by the leaching group with respect to terminology definition, the tiered approach (see paragraph 2.4) to models (model hierarchy) and validation strategy were adopted. In addition, where appropriate, reference was made to the report of the leaching group.

In addition, also the list of Elements for Assessing Models was also adopted. The surface water models described in this report are following the same outline. The easiness for making comparisons is therefore increasing, also in relation to the leaching models.

As the remit of the group indicated the estimation of Predicted Environmental Concentrations after application of plant protection products to specific agricultural fields was primarily aimed for. Therefore, the group decided to limit itself to the field scale, which means the field where a plant protection product is applied and from there has the possibility to be distributed into the environment and then entering surface water. Thus, catchment areas and regional scales are not taken into account by the group.

2.4 Regulatory risk assessment of surface water contamination

Application of mathematical models and pesticide registration in the past has been undertaken solely via national legislation which has led to various different methods and assumptions being used in the calculation of the concentrations likely to reach surface waters. Before examining in detail the available methods for determining PEC under common European legislation (91/414/EEC) it is worth to give briefly some examples of procedures which have been used by some national bodies to date. An inquiry carried out among Member States revealed the following information.

One of the simplest procedures occurs in the UK where a first tier assessment of surface water exposure is made by a simple calculation of the concentration obtained after overspray of a 1m deep water body (currently under review). This is considered to be the worst case for entry routes into surface waters. If the PEC from overspray leads to an unacceptably high toxicity/exposure ratio for aquatic flora and fauna, as defined in the Uniform Principles, a buffer zone is imposed. Since buffer zones do not protect water bodies from drain flow a further crude assessment of drainage loss has been made on occasions when buffer zones have been imposed. A similar scenario of overspray of a 1m deep pond has been used in Sweden and a worst case approach is also in use in Finland.

In Germany, the PEC is determined mainly on the basis of spray drift to a 0.3m deep water body. (These drift values have been experimentally obtained on a generic basis, see later sections). Other routes of entry may be considered if particular data is available. The Belgian authorities also use spray drift values but to a 1m deep static water body. In the Dutch registration procedure spray drift values into a 0.25m deep ditch are used feeding the generic model SLOOT.BOX to calculate an initial PEC, a short and a long term PEC. In addition, the PESTLA simulation model is used with a standard scenario to determine the PEC in groundwater and a standard value of 60% of this output is used as the contribution of drainage to the PEC_{sw}.

2.5 Tiered approach

Mathematical models used in decision making may vary in complexity and this group recommends a tiered approach to the calculation of the behaviour of a substance in surface waters as was advocated by the leaching group.

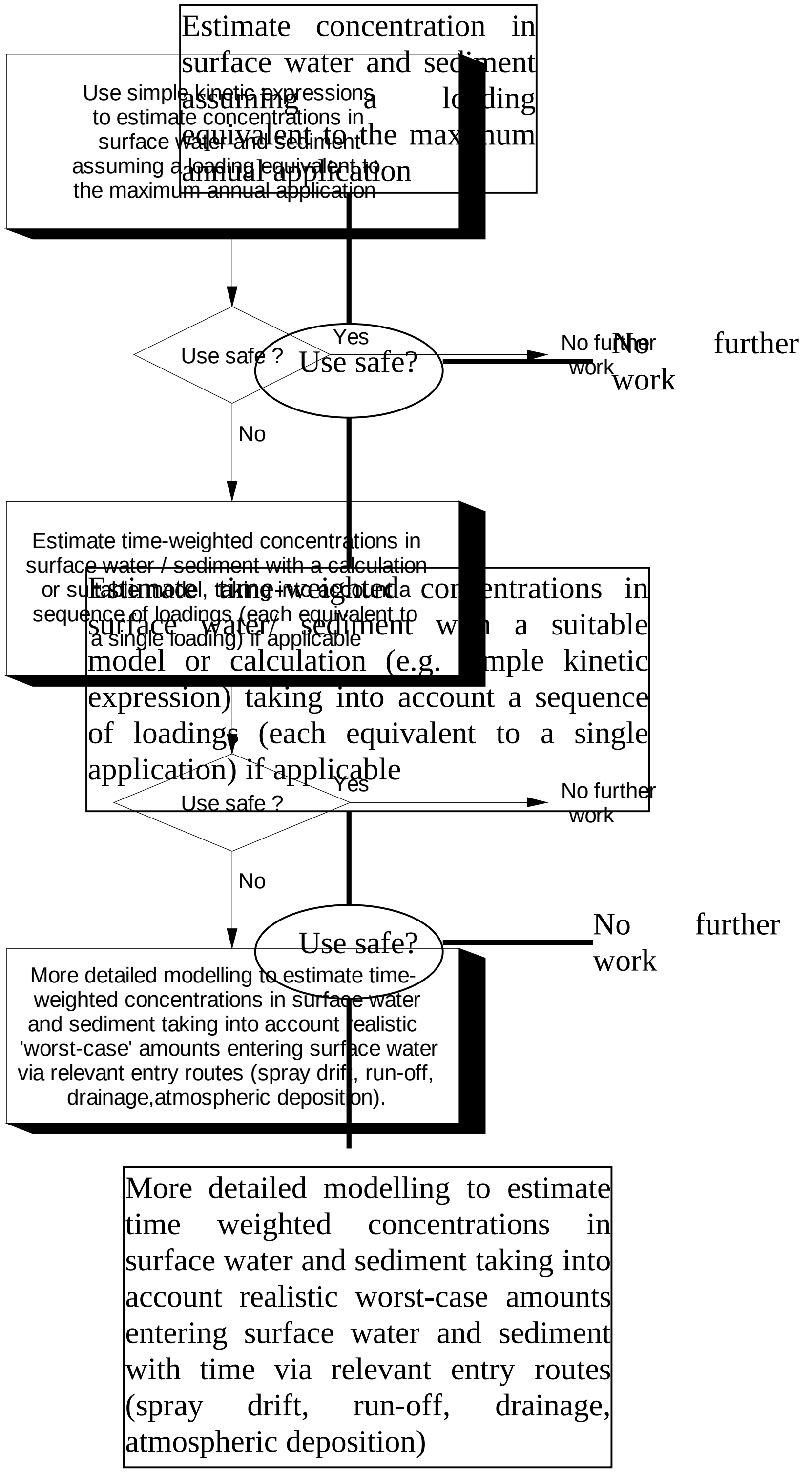
In many cases the earliest tier could be a simple calculation using overspray of a maximum annual application rate. This is not a realistic scenario but, being the worst possible case, may preclude the need for more complex modelling of more realistic situations.

Higher tiers of decision making require models, but these themselves vary and not all are suitable for all levels of complexity. Screening models on the one hand have a basic simplicity, whereas other models, for example those developed as scientific research tools, may be very complex. In general, a model needs to be suited to its proposed use, which in turn, depends on whether the questions to be answered require a rough estimate or as accurate as possible calculation of the behaviour of the substance based on state-of-art modelling. Each type of model, simple or complex, has its own limitations and these themselves are directly related to the complexity of the model: a simple model is easy to use but may be quite inaccurate, whereas a more complex model may give quite accurate results but requires a large amount of input data that may not be directly available. If estimated input data are to be used, these may directly influence the accuracy of the complex model.

A simple scheme for a stepwise (tiered) procedure is shown in figure 1.

This document largely provides information on the most detailed, highest tier models for exposure to, and fate of, pesticides in surface water, since it is these models that are the most complex to understand and use. Some screening models are also described.

Figure 1. Stepwise procedure for predicting environmental concentrations in surface water and sediment.



2.6 Report outline

Concerning the report itself, Chapter 3 builds on the terminology definitions of the leaching group in adding surface water related terms and appropriate definitions. It should be noted that other definitions may be used elsewhere. As far as possible internationally accepted phrasing was adopted, but sometimes more specificity was needed.

Chapter 4 gives an overview of the several input route models that are available and used, along with a similar overview of the surface water fate models. At the end of each section, subsections address model validation status and give some overall conclusions and recommendation. In Chapter 5 the model limitations and deficiencies are outlined. Possible solutions to the problems are mentioned if appropriate.

The group thought it useful to start the discussion on European scenarios. It is aware of the wide variety of possible scenarios and in Chapter 6, an introductory section discusses this problem and presents some potential solutions. In order to illustrate the complexity of the problem, the group felt it important to include an example scenario calculation. This example is described in the final section of Chapter 6.

An important item in the EU-registration process is the validation status of the mathematical model used. Preferably a model validated at the Community level is to be used. Therefore, a separate Chapter 7 on validation is included in the report. In Chapter 8 the Conclusions and Recommendations of the Working Group are presented. Finally, the more detailed descriptions and comparisons of each model considered are given in a set of annexes following the adopted list of elements for assessing models.

3. DEFINITIONS

This chapter elaborates on the corresponding chapter of the leaching group’s report. Where necessary additional definitions have been formulated, specifically relating to surface water. The definitions below have been developed specifically for use with respect to modelling the fate of pesticides in surface water. Care should be taken if the definitions are extrapolated to other topic areas where other interpretations may be necessary.

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

compartments -A specific matrix in the system that is being modelled, for example soil, water, air, etc. Compartments may be subdivided into segments, sections, layers or other discrete units.

distribution of scenarios - 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.

drainage - the removal of surplus water from land, via within-field drains, to surface waters.

entry routes - pathways via which chemicals can enter surface water after or during their use.

erosion - Lateral transport of soil particles at the soil surface induced by run-off.

interflow - transient saturated lateral movement of water within the generally unsaturated soil profile (not via drains) to edge of field watercourses.

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

model, computer - 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.

model, conceptual - 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.

model, deterministic - 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.

model input- all data for which the user has to set values before the model can give calculation results.

model, mathematical - model that describes the conceptual model in terms of mathematical equations.

model, probabilistic - 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.

model, stochastic - 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.

quantitative methods - systematic procedures, techniques or sets of rules to determine definite amounts or numbers.

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

run-off - Lateral flow of water at the soil surface triggered by precipitation, snow melt or irrigation events to surface waters.

scenario -a unique combination of agronomic and environmental conditions***** that realistically represents significant areas within which conditions are relatively homogeneous with respect to modelling input parameters.

*****These conditions include climate, hydrogeology, surface water characteristics, soil and topography.

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.

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 scenarios and standard data sets for checking.

space increments - continuous horizontal or vertical segments whose dimensions are used for numerical purposes.

surface water - natural water located at the earth surface; it includes lakes, ponds, rivers, canals, streams, canals and ditches; (in the framework of FOCUS) brackish estuaries or saltwater seas and oceans are not included.

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.

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.

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.

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

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).

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.

4. ASSESSMENT OF VARIOUS MODELS

4.1 Simulation Models and Methods Describing Spray drift During Application

4.1.1 Introduction

Over the last few years the drift of pesticides caused by spraying during application has been known to be a problem for the environment. High fractions of pesticides can be transported through the air and deposited in neighbouring ecosystems (surface water). One important parameter influencing the drift of pesticide is the spraying system itself: It has been known for a long time that the problem of spray drift only occurs if nozzles are used producing very small droplets, because the rate of deposition depends on the diameter of droplets. If the drop diameter decreases, the velocity of descent will also decrease. On the other hand it must be considered that an optimum interaction between plant and pesticide is only possible when spraying fine droplets resulting in high coverage of the area to be sprayed (usually the plant surface but also the soil itself).

In addition to the spraying equipment, local meteorological conditions such as the wind speed, relative humidity and temperature also influence the amount of spray drift. To minimise transportation of pesticides via the atmosphere, wind velocity should be as small as possible to get more deposition within the sprayed area.

In order to quantify the amounts of pesticides transported by spray drift, many studies have been performed in the last few years. The latest of these was the German Task Force on spray drift, initiated in 1991 and finished in 1993. In The Netherlands, a field study on drift has also been carried out recently. The study was aimed at the quantification of spray drift from field sprayers under different circumstances (Holterman, 1994) and was finished in 1994. Its results are currently being developed into decision making tools.

Building on these spray drift studies, most EU countries now use tables describing fixed scenarios for their assessment. However, some computer models of spray drift have also been developed. A brief comparison of models and tables is presented in Table 1 and a more detailed description of the various drift tables considered can be found at the end of this section.

Detailed assessments of the spray drift models are given in Annex 9.1.

4.1.2 Spray drift tables

At present in most countries, tables are used to assess spray drift during application. These tables describe the spray drift of pesticides based on fixed scenarios. Due to present expert knowledge the dominant processes responsible for drift of pesticides do not depend on pesticide properties but on climatic situations (wind speed, relative humidity in air, air

Table 1 Overview of Methods

	Name	Developer	Intended Use	User Manual	Hardware required	Standard data set or databases included	Validation	Use for Pesticide Registration
IDEFICS	IDEFICS	H.J. Holterman	Model to quantify spray drift from field sprayers	For internal use only	80286/ 80287 Coproc., MSDOS		Compared with experimental data	Will be used
MOPED	Model for pesticide drift	M. Klein	Screening model to predict the spray drift during application dependent on meteorological, crop, and nozzle parameters	UBA-report in German language available	80286/ 80287 Coproc., MSDOS	Yes	Calibrated using experimental data	No
PEDRIMO	Pesticide Drift Model	P. Kaul, S. Gebauer, R. Neukampf	Screening model (sediment and loss to the air) for field sprayers and aircraft	Not necessary, the program explains itself (English.)	PC 386 Co processor	?	Validation in comparison with field experiments	No
PSMDRIFT	Linear Interpolation of German Drift tables		To estimate input into aquatic ecosystems	User manual available in German language, publication of tables in prep.	80286/ 80287 Coproc., MSDOS	Yes	Tables are based on spray drift experiments	Pesticide Registration in Germany
	Drift table of The Netherlands		To estimate input into aquatic ecosystems	RIVM-Report (in English)		Yes	Tables in part based on measurements	Pesticide Registration in The Netherlands
	UK Drift table		To estimate input into aquatic ecosystems			Assumption: 100 % drift		Pesticide Registration in the UK

temperature), the crop (leaf stage, crop height), and the spraying equipment (nozzle type, nozzle pressure, droplet spectrum). Consequently, none of these tables consider pesticide properties such as water solubility or vapour pressure.

In The Netherlands and in Germany tables have been developed that take into account specific situations (different crops and leaf stages, distance dependency, types of applications). In other countries however, the assessment is performed using a single standard situation**.**

The German table is the most detailed one: spray drift can be estimated dependent on the crop, the leaf stage, and the distance to the agricultural field. The table is based on experimental data that have been carried out by German authorities involved in pesticide registration, German industry and research institutes. A worst-case situation has been chosen for the evaluation of the data (95th percentile of the individual values). As in the Netherlands no buffer zone is taken into account and the drift is considered to take place at the edge of the field

When using tables for estimating the input of pesticides into surface water the drift deposits may vary within the width of the ditch because of the strong distance dependency of the drift values. It is, therefore, recommended to use the width weighted average of the drift deposits as input for the surface water fate models (see also the example calculation in chapter 6.2.2).

4.1.3 Computer models

Computer models may also help to quantify the extent of drift, but more important, identify areas of poor understanding which cause important errors in the assessments. As the user can modify all input parameters models can be used in a more flexible way than the static drift tables. If combined with Monte Carlo routines the frequency at exceeding various thresholds can also be calculated. Three computer models are described in this paper. Though the algorithms built into these models are different (IDEFICS: random walk, PEDRIMO, MOPED: box type models), they all combine a typical weather situation (usually expressed by the wind speed) with properties of the spraying equipment (drop size spectrum, velocity of droplets) and the geometry of the agricultural field. The result is not dependent on the pesticide used.

Of course, it is not possible to build the models without a number of simplifications. In reality all climatic parameters vary with space and time, but spray drift models usually consider only single values for wind speed or humidity. Additional assumptions have to be made for the spraying equipment itself: the droplet spectrum which is produced by the nozzles, and the velocity of droplets are only simplifications of the real spray drift situation. Finally, influence of the crop on drift is based on assuming fixed values for its height and density. All these assumptions will lead to errors in the calculations.

4.1.4 Validation status

The models described in this section have either been calibrated (MOPED using the German drift tables) or validated with a limited number of experiments (PEDRIMO, IDEFICS). But as they are all recently developed these comparisons have been made to only a limited extent.

4.1.5 Conclusions and Recommendations

Each of the models is able to estimate spray drift of pesticide during applications. However, they do not simulate all the same spectrum of applications: PEDRIMO calculates spray drift caused by field sprayers as well as aeroplanes whereas MOPED only considers spraying in tall growing crops (air-blast sprayers). The third model, IDEFICS, which has an interesting concept (2D random walk), was developed only to predict spray drift from a conventional boom sprayer to a crop field. In addition to these differences none of the three models depend on the properties of the pesticides and will thus give the same result for any pesticide, given the same environmental input parameters.

As all models are at an early stage of development and have hardly been validated it is strongly recommended to use tables instead of computer models for estimating spray drift. Spray drift tables have been developed in The Netherlands and in Germany. In these tables the drift is expressed dependent on a limited number of scenarios. As the German table is currently the most detailed and fully based on experimental data performed with commonly used spraying equipment, it is recommended to use this data for regulatory assessment. However, when using tables it is important to take into account the experimental conditions the tables are based on: the German spray drift tables were all based on weather conditions typical for Central Europe (air temperature below 25 °C, wind speed below 5 m/s, maximum deviation from the main wind direction not more than 30°). There is presently no table available in Europe which considers the weather condition in a southern European country. To estimate spray drift for the southern European countries new tables may have to be developed, which should also be based on experimental studies. Alternatively, models that allow extrapolation from the available data to other climatic conditions should be developed and validated.

Detailed Description of Tables

PSMDRIFT

1.0 Overview

Purpose:

PSMDRIFT is a small computer program used in the German registration of pesticides to assess the spray drift during application. It is based on the German drift tables (Ganzelmeier et al 1995)
and interpolates linearly between the columns of the table.

Current Version No.: 2.00

Author and Affiliation:
M. Klein
Fraunhofer-Institut für Umweltchemie und Ökotoxikologie

2.0 Model Algorithms

PSMDRIFT is based on the German Drift tables which are summarised in the following table: The given percentiles are related to individual value.

	vineyard		orchards		hop	vegetable etc.		field
distance [m]	deposition [% of applied dose, 95th] early	late	deposition [% of applied dose, 95th] early	late	deposition [% of applied dose, 95th]	deposition [% of applied dose, 95th] H < 50cm	H > 50 cm	deposition [% of applied dose, 95th]
5	1.6	5.0	20	10	12.5	0.6	5	0.6
10	0.4	1.5	11	4.5	9.0	0.4	1.5	0.4
15	0.2	0.8	6	2.5	5.0	0.2	0.8	0.2
20	0.1	0.4	4	1.5	4.0	0.1	0.4	0.1
30	0.1	0.2	2	0.6	2	0.1	0.2	0.1
40	0.1	0.2	0.4	0.4	-	-	0.2	-
50	0.1	0.2	0.2	0.2	0.3	-	0.2	-

In addition to the above table with basic drift values which are officially used by the three German authorities involved in pesticide registration (BBA, UBA and BGA) PSMDRIFT will use the following table for distances smaller than 5 m, which has also been determined in the same task force (Ganzelmeier et al 1995)

When using PSMDRIFT, the user can select the distance of the ecosystem to the agricultural area and the percentile (usually 95th).

	vineyards		orchards		hops	vegetables etc.		field
distance [m]	deposition [% of applied dose, 95th] early	late	deposition [% of applied dose, 95th] early	late	deposition [% of applied dose, 95th]	deposition [% of applied dose, 95th] H < 50cm	H > 50 cm	deposition [% of applied dose, 95th]
1						4.0		4.0
2						1.6		1.6
3	4.9	7.5	29.6	15.5		1.0	7.5	1.0
4						0.9		0.9

3.0 Software features

The programme runs on any personal computer (640k RAM) with an MS-DOS operating system.

4.0 Availability & support

Documentation and User’s manual:
yes (German language)

Contact:

M. Klein
Fraunhofer-Institut für Umweltchemie und Ökotoxikologie
D-57392 Schmallenberg

Phone: +49-2972-302 317
Fax: +49-2972-302 319

Drift Estimation of the UK

1.0 Overview

Purpose:
In the UK the assumption of direct overspray, at the maximum application rate (100 %), to a static water body of 1 m depth is made. (under review within UK)

Contact:

Dr T. Jarvis
Pesticides Safety Directorate
Ministry of Agriculture Fisheries and Food
Mallard House, Kings Pool
3 Peasholme Green
York Y01 2PX

Phone: +44 1904 455916
Fax: +44 1904 455711

Drift Table of The Netherlands

1.0 Overview

Purpose:
The Drift table is used in The Netherlands registration of pesticides to access the spray drift during application. The amount of drift was estimated as a function of the way and the place of treatment. In the evaluation system the non-target area is a ditch with a mean depth of 0.25 m. The value is valid for edge of field, no buffer zone, therefore.
Remark: the table is currently under review in The Netherlands.

Current Version No.: not applicable

Author and Affiliation:
J.B.H.J. Linders, National Institute for Public Health and the Environment

2.0 Model Algorithms

Percentage drift related to place and way of application. The table is mostly based on expert judgement

Location and way of application		Pdrift (%)
1. Indoor applications [1]		
(excl.greenhouse	- storage cells, etc.	0
	- shower rooms, etc.	0
2. Protected applications		
a. Specific applications	- overhead irrigation	0
	- manual pouring	0
	- soil treatment	0
	- granule application	0
	- trickling	0
	- chicory for silage	0
b. Non-specific applications	- remaining ways of application in greenhouse(spraying, mist blowing, fogging, smoke generating, etc.: mainly through condensation on glass roof) [2]	0.1

Location and way of application		Pdrift (%)
3. Field applications:		
a. Specific applications:	- manual pouring	0
	- dipping	0
	- granule application [3]	0
	- baiting	0
	- injecting soil/plant	0
	- treating plant base	0
	- smearing	0
	- brushing	0
	- spraying with direct incorporation into soil [4]	0
	- seed treatment	0
b. Spot applications:	- waste dump	0.5
	- row spraying [5]	0.5
	- knapsack spraying	0.5
	- road signs	0.5
c. Non-specific applications:	1. crop height < = 25 cm:	
	- soil treatment	1
	- bare soil	1
	- herbicide in fruit culture	1
	- under-leaves spraying	1
	- plant bed	1
	- before germination	1
	- paved terrain	1
	2. crop height > 25 cm	
	- downward spraying	2 [6]
	- treatment field border	5 [6]
	- edge along ditch slope	5 [6]
	- sideways or upward directed spraying in arbori- and fruit culture	10 [6]
	3. ditch slope application	10 [6]
d. Specific applications:	- spraying by aircraft	100
	- willow-coppice	100
	- dry ditch bottom	100

1 Whenever no direct exposure of surface water by drift is to be expected by the way of applying, the load through this route is determined to be 0 %.
2 From research into condensate discharge, it was derived that approximately 0.1 % of the plant protection products dosage on the glass roof can load the surface water via condensate. Up to now, it has been impossible to explicate per way of application.
3 With special synthesis granule broadcasting device.
4 Spraying with direct incorporation into the soil during a sole run of labour.
5 This figure is based on the assumption that, during row spraying, less drift will occur than during field application, as the distance from nozzle to soil is substantially less during row spraying than during whole field treatments.
6 Based on experimental results

4.0 Availability & Support

Contact:

Dr. J.B.H.J. Linders
RIVM -ACT
P.O. Box 1
NL-3720 BA Bilthoven
The Netherlands

Phone: +31-30-274 3164
Fax: +31-30-274 4401

References

Emans, H.J.B., M.A. Beek, and J.B.H.J. Linders (1992), Evaluation system for pesticides (ESPE) - 1. Agricultural pesticides, RIVM-Report, 679101004, Bilthoven, NL, 80 pp.

Ganzelmeier H. et al (1995), Studies on the spray drift of plant protection products, Mitteilungen aus der Biologischen Bundestanstalt für Land-. und Forstwirtschaft, Berlin, Heft 305.

Holterman, H.J. , H.A.J. Porskamp, J.F.M. Huijsmans (1994), Modelling spray drift from boom sprayers, Institute of Agricultural and Environmental Engineering (IMAG-DLO), Wageningen, The Netherlands.

Jarvis, T. (1995), Personal communication. , Pesticides Safety Directorate, York, UK.

Kaul, P., S. Gebauer, and R. Neukampf: Direkte Abtrift von Pflanzenschutzmitteln - Pflanzenschutzgeräte für den Feldbau (Direct Drift of Plant Protection Products - Field Sprayer) *in preparation.*

Kaul, P., E. Meyer und S. Gebauer (1995): Direkte Abtrift von Pflanzenschutzmitteln - Flugzeug (Direct Drift of Plant Protection Products - Airplane), Nachrichtenbl. Deut. Pflanzenschutzd. **47**, 36-44.

Klein, M. MOPED Model for Pesticide Drift, User’s manual (German language), Environmental Protection Agency Berlin, Report 126 05 080.

4.2 A critical summary of simulation models accounting for pesticide inputs to surface waters via drainage systems

4.2.1 Introduction

In this report, pesticide fate and mobility models which explicitly deal with coupled unsaturated/saturated flow are described and compared. These models, which dynamically predict the transient position of the groundwater table, are potentially useful tools to assess pesticide losses to surface waters via drainage systems.

Firstly, it should be noted that by making some simple assumptions, any of the existing pesticide leaching models which deal only with the unsaturated zone (e.g. PRZM, PELMO, see the FOCUS leaching group report) could, in principle, be used to calculate losses to drainage systems. For example, it can be assumed that a given fraction of the pesticide reaching the bottom of the profile is lost to drains. Such an approach is equivalent to assuming that the water table position is fixed and equal to drain depth (say, at 1 m depth). In reality, the water table position can and will vary throughout the year, often by up to 1 to 2 m. Such fluctuations in the water table position will have great impact on pesticide losses to surface waters via drains, particularly if the water table rises into shallow surface layers (where pesticide concentrations are largest) at critical times of the year (e.g. in spring, following spraying). Thus, the use of simple partitioning of flows at the base of the soil profile in unsaturated leaching models may seriously underestimate the importance of the drainage loss pathway, and is therefore not to be recommended.

In the remainder of this report, we discuss those models which explicitly account for the dynamics of the saturated zone, concentrating our attention on differences and similarities in model treatments of water flow, drainage fluxes, sorption and degradation and on the scope and limitations of the various approaches.

Table 2 presents a summary of the six models included in this comparison. The names and addresses of authors/contact persons for each model are listed in the Appendix. Annex 9.2A presents detailed information on each model, including important management aspects, such as the user-interface for both inputs and outputs. Brief descriptions of three other models (WAVE, SoilFug and SWAT) are given in Annex 9.2B. WAVE is a coupled unsaturated-saturated zone model of water flow and solute transport. Examples of its use for nitrate leaching have been published, but the pesticide version has not yet been generally released (M. Vanclooster, pers. comm.). SoilFug and SWAT do not explicitly consider a dynamic water balance, and may be considered as essentially screening models rather than as comprehensive simulation models.

4.2.2 Treatment of pesticide fluxes in the saturated zone

OPUS use the Hooghoudt equation to calculate water flow to field drains of known depth and spacing. Although it is not stated in the manual, the treatment of pesticide loss in OPUS is essentially one-dimensional, since the model assumes that the concentration of pesticide in water entering the drains is simply equal to the resident concentration of pesticide at drain depth (R. Smith pers. comm.). Therefore, the use of OPUS to calculate pesticide inputs to surface waters via drainage systems may not represent any significant advance on the use of simple unsaturated leaching models.

Table 2 Comparison of model treatments of saturated flow/transport.

Model	Process/Feature				
	Treatment of pesticide fluxes in saturated zone		Field drains	Multiple drainage systems	Preferential flow
	Quasi-2D	Fully 2D			
PESTLA 3.0	√		√	√	
PESTRAS 2.1	√				
OPUS 1.63	(√)		√		
CHAIN_2D 1.1		√	√	√	
MACRO 3.2	√		√	√	√
CRACK_P 1.0	√		√		√

Four models (PESTLA, PESTRAS, MACRO, CRACK_P) employ quasi two-dimensional approaches to calculating (lateral) pesticide fluxes in the saturated zone. In PESTLA, the Ernst equation is used to predict total drainflow, knowing the water table height and drain depth and spacing. The total water flow is partitioned between individual soil layers in the saturated zone by simply assuming a constant lateral water flux with depth in the soil, implying an exponential travel time distribution in the saturated zone. Pesticide concentrations reaching drains are calculated by adjusting for the residence time of water in different layers.

In PESTRAS, lateral drainage fluxes in the saturated zone are calculated as a function of the saturated conductivity in each layer, and two empirical parameters describing `base flow' and `quick flow' components. Pesticide loss in the drainflow is calculated by simply multiplying the drainage flow rate from each layer by the solution concentration in each layer and then summing. There is one significant disadvantage of the approximate, empirical, treatment used in PESTRAS to partition lateral water and pesticide fluxes in different layers of the saturated zone. Without calibration, empirical modelling approaches cannot easily account for widely varying site and soil characteristics (e.g. depth and spacing of drainage systems, the vertical distribution of hydraulic conductivity).

MACRO and CRACK_P both employ the same mechanistic treatment (i.e. seepage potential theory) to calculate lateral drainage fluxes from each layer as a function of the water table height, saturated conductivity in each layer, and drain depth and spacing. In MACRO, the pesticide loss to drains is calculated accounting for the flow contribution and concentrations in two pore systems (i.e. macropores and micropores, see `Preferential flow'). In CRACK_P, all the drain flow is assumed to be derived from the crack system, so that losses to drains are calculated using the pesticide concentration in `crack water'.

In the quasi two-dimensional approaches described above, complete mixing of solute in the horizontal dimensions is assumed. Only one of the seven listed models, CHAIN_2D, employs a fully two-dimensional approach (based on a finite element numerical scheme) to calculating fluxes of water and pesticide to drainage systems (Table 2). One of the main advantages of such a two-dimensional model is that the (potentially) significant effects of lateral transit times in the saturated zone on sorption and degradation are automatically accounted for in a mechanistic way.

4.2.3 Field drains

In PESTRAS, the depth and spacing of field drains are not explicitly specified. Thus, PESTRAS is perhaps best suited to predicting pesticide losses to regional groundwater flow, rather than to predicting potential inputs to surface waters at `edge-of-field', from field drainage systems. Indeed, PESTRAS appears to be primarily designed for such regional applications, being incorporated into a GIS framework.

4.2.4 Multiple drainage systems

Three of the models (PESTLA, MACRO and CHAIN_2D) can be used to simulate pesticide losses to surface waters via two or more drainage systems of different order. PESTLA is the most developed model in this respect, since losses may be calculated for four drainage systems, from field trenches to large canals and rivers. Two drainage systems can be simulated with MACRO (within-field drains, field boundary ditches or catchment area). In theory, any number of drainage systems can be simulated with CHAIN_2D, but for practical reasons, this would probably be limited to 2 orders of drains.

4.2.5 Preferential flow

Fine-textured heavy clay soils of poor subsoil conductivity constitute a large proportion of the under-drained agricultural land in Europe. Rapid preferential flow and transport in soil structural features (e.g. cracks, worm channels, root holes) is known to dominate the hydrology in such soils. Thus, two of the models listed in Table 2 attempt to account for such processes. The CRACK_P model deals specifically with processes operating in cracking heavy clay soils, and its use is restricted to such soils, since the soil matrix is assumed to comprise aggregates containing immobile water. MACRO is a dual-porosity model which can simulate preferential flow and transport of both water and pesticide in a wide range of soil types.

4.2.6 Degradation

In PESTRAS, the pesticide degradation and sorption routines have been taken from version 2.3 of the PESTLA model (see FOCUS leaching group report) and have evolved only to a limited extent. Similarly, the sorption and degradation routines developed in the CALF/VARLEACH model have been used in CRACK_P, without any changes.

PESTLA, PESTRAS, OPUS, MACRO and CRACK_P all use exclusively first order degradation. CHAIN_2D is more complicated in that it allows for zero order reactions in addition to first order. The moderating effects of temperature and moisture content on the degradation rate can be very important, although consideration of these factors is not always addressed by models. For all the models discussed here, the effect of temperature on the degradation rate is modelled based on the Arrhenius equation (generally the most common method). The effect of the soil moisture content is considered by empirical relationships for PESTLA, PESTRAS, OPUS, MACRO and CRACK_P, but is not accounted for in CHAIN_2D.

Table 3 Comparison of model treatments of sorption and degradation.

Model	Process/Feature					
	Degradation model		Soil water and temperature effects on degradation	Metabolites	Sorption model	
	First-order	Others			Linear or Freundlich	Instantaneous or kinetic
PESTLA 3.0	√		√	√	Freundlich	Kinetic[b]
PESTRAS 2.1	√		√	√	Freundlich	Instantaneous
OPUS 1.63	√		√		Linear	Kinetic[b]
CHAIN_2D 1.1	√	√	√	√	Freundlich	Kinetic[b]
MACRO 3.2	√		√		Linear	Instantaneous
CRACK_P 1.0	√		√		Linear	Kinetic[c]

[a] temperature effect only
[b] Two-site model
[c] Sorption constant increases with time

Changes of degradation rate with depth are perhaps less important for models dealing with drainage compared to those addressing groundwater contamination, since the depth of the soil profile is often less. Nonetheless, changes in the degradation rate below the plough layer will occur and these are considered in various ways. PESTRAS includes inputs for reduction factors at specified depths. CRACK incorporates reduction factors for specified soil horizon depths (or at least CALF does), while degradation rate coefficients are specified by the user for each layer (or compartment) in MACRO, PESTLA and CHAIN_2D. The OPUS manual acknowledges that degradation below the microbially active zone (c. 20 cm) will be much slower, but there doesn't seem to be an input for defining this or a stated default value.

The majority of the models require a single overall degradation rate, which is the easiest to obtain experimentally. As an option, PESTLA treats degradation in the sorbed and solution phases separately, whilst MACRO specifies degradation rates in the solid and liquid phases for both the macro- and micropores. A more extreme situation occurs with CHAIN_2D which allows for up to nine different rate constants, including volatilization rates. Providing a number of rate constants for different compartments/transformations can potentially give a more accurate result if all the component rate constants are measurable. However, in the absence of such measurements, there is no advantage over a single lumped rate constant. PESTLA, PESTRAS and CHAIN_2D can be used to examine the first-order degradation of metabolites linked to that of the parent. This requires the appropriate rate constants for the transformation of the metabolites, but is potentially useful for assessing the relative amounts present at various times.

4.2.7 Sorption

PESTLA, PESTRAS and CHAIN_2D provide the option of non-linear (Freundlich) sorption. MACRO, OPUS and CRACK_P assume simple linear sorption. PESTRAS and MACRO assume instantaneous sorption, while two-site (i.e. equilibrium/kinetic) sorption can be modelled in both PESTLA and CHAIN_2D. The OPUS model allows the option of either equilibrium or kinetic sorption. The phenomenon of increasing sorption with time is addressed empirically by CRACK_P, where the sorption coefficient increases with the square root of time. MACRO divides the sorption sites between macropores and micropores.

4.2.8 Validation status

Most of the models accounting for drainage flows described in this section are only recently developed and have been compared to field data to only a limited extent, if at all. Therefore, the validation status of all of the models must be considered low. As far as the authors are aware, predictions of PESTRAS, OPUS and CHAIN_2D have not, as yet, been compared with measurements of pesticide losses in drainage water.

Dijkstra et al. (1995) compared PESTLA 3.0 predictions with measured concentrations of metamitron and hydroxychlorothalonil in drain pipe outflow on two sandy soils with shallow groundwater tables. Measured and predicted concentrations agreed reasonably well, in that both were nearly always below the detection limits (which ranged from 0.02 to 1.0 ug l^{-1}). Drainflow concentrations were overestimated when the groundwater level reached the plough layer. This was attributed to the concept of lateral solute flow as formulated in the model.

Styczen and Villholth (1995) compared MACRO model predictions (version 3.0) with measurements of MCPA, dichlorprop and 2,4-D concentrations in tile drainage outflow from a loamy soil in Denmark. The simulations were considered successful, given the lack of directly-measured soil and pesticide parameter data, together with the limited amount of measured data points (concentrations were only occasionally above the detection limit). In a second test, MACRO failed to match observed water table fluctuations in a sandy soil due to an inappropriate description of the bottom boundary condition (Styczen and Villholth, 1995). However, this problem with the model has been rectified in later versions of MACRO.

MACRO is currently being applied to predict isoproturon losses from a drained clay loam soil at Cockle Park, Northumberland, U.K. (Colin Brown, pers. comm.). Preliminary results suggest that isoproturon concentrations were accurately predicted, without any model calibration, for autumn storm events soon after application, but were overestimated by c. one order of magnitude later in the winter. MACRO has also been used to predict losses of a spring-applied herbicide to tile drains on two soils (sandy loam and clay loam) near Birmingham, U.K. (unpubl. report, N.J. Jarvis). With some calibration of soil hydrology (root water uptake parameters), the model generally predicted concentrations in drainflow to within one order of magnitude, and mostly to within a factor of two.

A comparison of measurements of isoproturon concentrations in mole drain outflow from a heavy cracking clay soil in the U.K. with CRACK_P predictions was reported by Armstrong et al. (1995). CRACK_P successfully matched the observed concentrations for a one-week period in mid-winter, following autumn application to winter cereals.

Current experience with the macropore flow models MACRO and CRACK_P suggests that water table response and thus, pesticide leaching to drains, is sensitive to model parameters related to the macropore volume and conductivity. Thus, the inherent accuracy of these models may be low, although validation tests performed to date have given surprisingly good results. For many drained soils of low matrix conductivity, they will certainly perform better than those models which do not account for macropore flow.

4.2.9 Conclusions and Recommendations

Prior to selecting a model, the user should be aware of the limitations of each of the models discussed in this report. OPUS does have the advantage of dealing with both surface runoff and drainage inputs in one and the same model. However, it suffers from an essentially one-dimensional treatment of pesticide flux in the saturated zone and rather incomplete documentation, and otherwise offers no significant advantages compared to the use of say, PESTLA 3.0. CHAIN_2D has the potential to be one of the most useful models in the context of modelling drainage system inputs to surface waters, since it is fully two-dimensional. However, the current version of the model is complicated and difficult to use. The Windows-based version 2.0 currently under development (released in March 1996) should certainly remove this limitation for the use of the model for management purposes.

PESTRAS is designed for use at the regional scale, and does not explicitly treat `within-field' drainage systems. Empirical parameters are used to calculate lateral saturated flow, rather than any physically-based approach, and this may limit, to some extent, the general applicability of the model. PESTRAS and PESTLA both contain advanced, flexible, descriptions of chemical and biological processes (i.e. Freundlich sorption, metabolites).

However, use of PESTLA and PESTRAS should be restricted to non-structured sandy soils. MACRO and CRACK_P both account for preferential flow processes, and also represent the soil saturated zone in a physically realistic manner, whilst the pesticide degradation routines include all relevant moderating factors (soil water content, temperature, depth). CRACK_P is specifically designed for use in clay soils, but cannot be applied to lighter-textured permeable soils. MACRO is the most generally applicable model with respect to physical transport processes.

Model users should be aware of the low validation status of all the available models when used for predicting drainflow concentrations, and that the predictive accuracy of the models may not be better than one order of magnitude for predicting peak concentrations (i.e. acute exposure) and perhaps a factor of two for predicting long-term loads (i.e. chronic exposure).

References

Armstrong, A.C., Portwood, A.M., Harris, G.L., Catt, J.A., Howse, K.R., Leeds-Harrison, P.B., Mason, D.J. 1995. Mechanistic modelling of pesticide leaching from cracking clay soils. *In BCPC Monograph no. 62: Pesticide movement to water* (eds. A. Walker, R. Allen, S.W. Bailey, A.M. Blair, C.D. Brown, P. Günther, C.R. Leake, P.H. Nicholls), 181-186.

Dijkstra, J.P., Groenendijk, P., Boesten, J.J.T.I & Roelsma, J. 1995. Emissions of pesticides and nutrients in flower bulb culture. Modelling of leaching of pesticides and nutrients. (In Dutch) Report 387.5, DLO Winand Staring Centre, Wageningen, Netherlands, in press.

Styczen, M. & Villholth, K. 1995. Pesticide modelling and models. *Bekæmpelsesmiddelforskning fra Miljøstyrelsen, nr. 9,* Danish EPA, pp. 149.

4.3 A critical summary of simulation models accounting for pesticide inputs to surface waters via surface runoff

4.3.1 Introduction

Measurement of environmental concentrations of pesticides due to surface water runoff is difficult, expensive, and time consuming. In most cases Predicted Environmental Concentrations for surface water (PECsw) can be calculated using appropriate simulation models. This chapter summarises and compares the major simulation models that are used to estimate surface runoff of pesticides from agricultural fields. These values can then be used as inputs to appropriate surface water transport models to calculate the PECsw.

Model Name	Runoff Method	Erosion Method	Simulates Non-Uniform Slopes?	Sorption Algorithm	Volatility Supported	Degradation
EPIC	USDA Curve Number or Rational Equation	USLE, MUSLE or Onstad - Foster	Yes	Simple linear	No	First order kinetic
GLEAMS	USDA Curve Number	MUSLE	Yes	Simple linear	No	First order kinetic
OPUS	USDA Curve Number or Dist. Dynamic Simul.	MUSLE	Yes	Simple linear	No	First order kinetic
PELMO	USDA Curve Number	MUSLE	No	Freundlich	Yes	First order kinetic
PRZM2	USDA Curve Number	MUSLE	No	Simple linear	Yes	First order kinetic
SWRRBWQ	USDA Curve Number	MUSLE	No	Simple linear	No	First order kinetic

A brief comparison of model treatments of selected parameters important in estimating agrochemical runoff is presented above. A more complete summary of the models can be found in the tables in Annex 9.3. The underlying assumption of each of these models is that soluble and adsorbed pesticide loss from a field can be predicted based on water runoff and soil erosion. Runoff and erosion prediction models have been used for many years to design best management techniques to reduce flooding and field soil loss. In general, the models were designed to be used to compare erosion and runoff results from various scenarios, rather than to predict absolute values. Algorithms to predict nutrient loss were added to the runoff and erosion models to predict water quality problems. Pesticide loss algorithms were added later to predict loss of other agricultural products.

4.3.2 Runoff

The surface water runoff component of each of these models is generally based on the "runoff curve number" method. This method was developed to estimate runoff volumes (USDA 1972, Haith and Loehr 1979) and is based on daily rainfall and a retention parameter. The retention parameter is based on a "curve number" obtained generally from a table based on mainly empirical data for runoff from studies with various soils, land uses, and management.

The curve method is used because:

- it has been shown to be reasonable reliable,
- it is computationally efficient,
- the required inputs are generally available, and
- it takes into account the effects of soil type, land uses, and management.

Limitations of the method include:

- it is based on average conditions and does not contain an expression of time and therefore does not account for rainfall duration or intensity,
- it does not reflect any runoff from interflow or areas with high ground water levels, and
- since it is based on US conditions and storm events, curve numbers may need to be adjusted to accurately reflect conditions in other areas of the world.

Various modifications of the curve number technique have been made to address method limitations. All of the models incorporate some modification to account for snow and frozen conditions. PRZM continually modifies curve numbers on a daily basis as a function of soil water status in the upper soil layers. EPIC uses a modification of the rational equation in an attempt to better simulate peak runoff. OPUS allows the user to choose between randomly selected peak runoff estimates or use the rational equation to simulate peak flows. OPUS also has an option to use a distributed dynamic simulation process to vary flow across the field surface over time and space.

Other factors that may affect hydrologic response include surface layer conditions, cracking soils, and subsurface flow. Several of the models attempt to account for these effects. OPUS modifies infiltration rates based on the development of soil crusts. EPIC considers tillage operations, including actual equipment type. Cracking soils are not considered in most of the models, but SWRRBWQ and EPIC modify infiltration rates based on soil moisture and soil clay content to account for possible crack flows. SWRRBWQ considers both subsurface flow and can simulate flows from many fields within a basin.

4.3.3 Erosion

Erosion is generally calculated using some modification of the Universal Soil Loss Equation (USLE, Wischmeier and Smith 1978). USLE depends only on rainfall as an indicator of energy of erosion. The Modified Universal Soil Loss Equation (MUSLE, Williams 1975) utilises runoff parameters to estimate sediment yield. MUSLE also allows estimation of erosion from single storm events - and so this equation is used in most of the models. The Onstad-Foster (Onstad and Foster, 1975) equation combines both the USLE and MUSLE equations and accounts for erosion energy from both precipitation and runoff.

Of the models listed above, PRZM, PELMO, and SWRRBWQ use MUSLE without further modification. In essence they simulate a simple homogeneous field with a given slope, soil, and management condition. EPIC allows the user to chose among USLE, MUSLE and Onstad-Foster which gives some flexibility in terms of calculating PEC’s. OPUS uses MUSLE but also offers several options for calculation of sediment transport and concentrated flow erosion. OPUS and GLEAMS provide options to divide the simulated field into several segments to simulate areas of the field with different slopes, soil condition, or crop management. For example, a simulated field could have sufficient slope to erode one part of the field, but the area near a stream could be flat and planted as a buffer strip which could reduce runoff and erosion.

4.3.4 Agronomics and Soils

Each of the models has methods for simulating agricultural management and soil characteristics. In most of the models, agricultural management is reflected in the user’s choice of curve numbers and parameters for MUSLE. Different curve numbers reflect the pre-planting, cropping, and post-harvest periods. A “soil erodibility factor” based on texture class and organic matter content is a soil specific factor developed by USDA to describe erodibility of various soils. In addition to the MUSLE parameters, EPIC and OPUS modify soil conditions during the simulation based in the soil layers closest to the surface based on tillage operations.

4.3.5 Relevant Processes

For the most part, the pesticide loss component of the models tends to be a simplistic representation of what actually occurs. All of the models permit multiple applications of a pesticide to soil or plants. Plant interception is usually assumed to increase linearly between plant emergence to some user specified maximum value (although most models offer optional functions to describe interception). Degradation on plant surfaces is modelled as a first-order process. Plant washoff is specified by the user and is related to rainfall amount. Soil sorption is based on a simple linear relationship using Koc, except in PELMO which uses the Freundlich adsorption isotherm. Soil degradation is first-order kinetic with no correction for moisture or temperature except for PELMO and OPUS. In each of the models soil degradation rates can be specified for various depths. In addition in PRZM2 degradation rates (as well as other parameters) can be changed during the simulation to reflect changes due to temperature or to simulate a non-linear degradation. PRZM2 and PELMO are the only models of the six reviewed that simulate volatilisation of the material.

4.3.6 Usability

User manuals are available for each of the models. Because most of the models were written in the United States, the common language is English. Some of the manuals, for example for PRZM2, are quite comprehensive and contain numerous tables, graphs, and references to help the user design appropriate scenarios. Unfortunately, since the models were originally written in the United States, little data is available in the manuals for non-US scenarios. Example datasets, where included, are also for US applications. The exception to this is the PELMO model. This does not preclude use of the models within the EU, but makes it slightly more difficult.

None of the models can be considered “user friendly.” PELMO is the probably the easiest model to operate because it contains a relatively easy to use interface. The user interface gives on-line help and replaces much of the functionality of a paper manual. PELMO also has a useful output post-processor that allows the user a quick visual picture of the results. EPIC, SWRRBWQ, and GLEAMS all use a version of UTIL, a relatively easy to use pre-processor that performs some data checking although with limited help capabilities. These models have tabular output with no post-processor. OPUS and PRZM have no pre- or post-processor. Input files for these models are “fixed-format” (values must be located in specific row and column locations within the input file or errors will result) with relatively obscure error messages when errors do occur.

Each of the models except EPIC can be configured to provide daily estimates of pesticide transport by way of erosion and runoff. While current versions of EPIC provide only monthly summary data, the model developers indicate that future versions will provide daily data. In most cases, the daily runoff and erosion data must be extracted and summarised from large tables of model output before they can be used as input to a surface water fate and transport model. The only exception to this is that PRZM can produce a file that can be loaded directly into the EXAMS surface water model.

4.3.7 Validation Status

While all of the models have been widely used, specific studies to validate the models across a wide range of conditions have not been done. Most validation type studies have involved only the hydrology and erosion algorithms and have not included definitive validation of pesticide transport. Attempts have been made to validate the MUSLE and USLE equations with varying degrees of success. Several versions of runoff curve numbers are available and can be used. For most conditions within the United States the curve number concept appears reasonably valid. The validity of the curve numbers to accurately represent conditions within the EU is uncertain.

GLEAMS and PRZM are the most widely used of the models world-wide and in general it is felt that in most cases the models predict runoff losses within one order of magnitude. Some work has been done to attempt to validate PELMO for leaching but no formal work has been done for runoff. Each of these three models, GLEAMS, PRZM, and PELMO has been used for regulatory purposes (although PELMO has not been used for runoff). As deficiencies have become apparent in the models, they have been updated. For example, PRZM2 was found to significantly overestimate runoff of compounds such as atrazine that had low sorption. A new non-uniform mixing algorithm was developed and has been incorporated into the code and now model results more closely predict what has been seen in field studies (PRZM2.3 is expected to be released in early 1996). The hydrology algorithms in GLEAMS are being updated to be more similar to those used in EPIC which are more accurate in predicting runoff events. EPIC, OPUS, and SWRRBWQ have been used less widely and have not been utilised for regulatory purposes to any great extent.

Currently PRZM and GLEAMS are being validated for both runoff and leaching by the FIFRA Environmental Modelling Validation Task Force. This is a group sponsored by twelve agricultural product companies with advisors USEPA and various academic and government institutions. The intent of this group is to take the models and compare them to data from derived from field studies. Results are expected to be available as early as 1997.

4.3.8 Conclusions and Recommendations

Each of the models can be used to predict edge of field pesticide losses in runoff waters and eroded sediment. Because of the common foundation (curve number runoff and MUSLE) for all of the models, predictions for simple scenarios should be similar. With complex and more realistic scenarios the appropriate model selection becomes more important. For example, if volatilisation is a significant factor then PRZM2 or PELMO might be selected. Simulation of actual field scenarios with vegetative buffers or level areas near the edge of the field would require use of models such as OPUS or GLEAMS that allow simulation of non-homogeneous slopes. While EPIC would appear useful to represent various specialised agronomic scenarios, the lack of daily output of pesticide runoff and erosion values makes it not very useful in helping calculate PECsw.

On the basis of history and breadth of usage, GLEAMS, PRZM, and PELMO appear to be the most suitable models to be used in providing edge of field loading values to help calculate PECsw. If significant differences in tillage practices need to be considered, then a model such as OPUS should be used that can simulate these conditions. All of these models appear able to simulate a wide range of climatic and agronomic conditions, however, since the runoff curve numbers were originally based on studies conducted in North America, they may need to be re-evaluated for EU conditions.

References

Haith, D.A. and R.C. Loehr, eds. 1979. Effectiveness of Soil and Water Conservation Practices for Pollution Control. U.S. Environmental Protection Agency, Athens, Georgia. EPA-600/3-79-106.

Onstad, C.A. and G.R. Foster, 1975. Erosion modelling on a watershed. Trans. ASAE 18(2):288-292.

U.S. Department of Agriculture, Soil Conservation Service. 1972. National Engineering Handbook, Hydrology Section 4, Chapters 4-10.

Williams, J.R. 1975. Sediment yield prediction with universal equation using runoff energy factor. U.S. Department of Agriculture, Agricultural Research Service., ARS-S-40.

Wischmeier, W.H. and D.D. Smith. 1978. Predicting rainfall erosion losses, a guide to conservation planning. U.S. Department of Agriculture, Agricultural Handbook No. 537, 58 pp.

4.4 Atmospheric Deposition

Although atmospheric deposition has been identified as an input route into surface waters it is thought to be too early to propose a specific modelling approach. There are several research tools available for the determination of long range transport of particles in air but none has been used in the evaluation of pesticides behaviour in the environment.

However, the EPPO/CoE-panel on Environmental Risk Assessment, which has developed several risk assessment schemes for the application of pesticides, has now installed a working group on Air. This working group is developing a decision-making scheme for estimating the risk to and through the compartment ‘air’. Some drafts have already been discussed and it is hoped that the activity will be completed during 1996. It is therefore recommended to await the report of EPPO/CoE, before attempting any assessment of modelling and numerical methods for atmospheric deposition of pesticides to surface waters.
The FOCUS working group estimates that atmospheric deposition will be of minor importance for establishing a PEC in surface waters.

4.5 A critical summary of simulation models describing fate and behaviour of pesticides in surface waters

4.5.1 Introduction

To assess the impact of pesticides on aquatic ecosystems it is necessary to know to which concentrations they are exposed. Measuring concentrations in the field is expensive and time-consuming; often simulation models are used to calculate exposure concentrations. In this chapter, simulation models calculating Predicted Environmental Concentrations (PEC) in surface waters (water column as well as sediment) will be summarised in view of their usefulness for regulatory purposes.

A brief overview of the main features of the considered models is presented below (Table 4). A more detailed description for each of these models can be found in Annex 9.5. This Annex also contains brief descriptions of some additional models which, for the various reasons listed are not included in Table 4.

Table 4 Main features of the surface water fate models assessed in this section

	Layout water network	Hydrology	Entry routes	Chemicals simulated* (water col. /sediment)	Pesticide processes					
					water column			sediment		
					degrad	sorption	resusp/sedimentation	degrad	sorption	flow
ABIWAS	one segment	steady state	initial concentration	(1/0)	differentiated (only abiotic)	susp.solids	no	-	-	-
SLOOT. BOX	one segment	steady state	pulse type input	(1/0)	lumped	susp.solids	yes	-	-	-
EXAMS	many segments (incl branches)	steady state	pulse or continuous type inputs	(2/2)	differentiated	susp.solids plankton	no	differentiated	solid phase sediment, benthos	no water flow incl.
WASP	many segments (incl branches)	dynamic	pulse or continuous type inputs	(3/3)	differentiated	susp.solids plankton	yes	differentiated	solid phase sediment,	water flow included benthos
TOXSWA	diff.segments (no branches)	steady state	initial conc. and continuos itype nputs	(1/1)	lumped	susp.solids	no water plants	lumped	solid phase sediment	water flow included

* parent and/or metabolites combined

A model describing the behaviour of pesticides in surface waters generally consists of several parts: hydrology, pesticides, and various ecosystem compartments. In the hydrological part, the flow of water is described in the water column (and sometimes also in the sediment). In the pesticide part, transfer and (dis)appearance of pesticide mass in the water column and also in the sediment are described. In addition, some of the models have separate parts to describe the behaviour of suspended solids, algae or aquatic vegetation.

In the next sections the main characteristics of the simulation models will be compared.

4.5.2 Layout surface water network and hydrology

Aquatic environments are highly variable. Simulation models simplify the variation within the environment by simulating one or more homogeneous segments. The models SLOOT.BOX and ABIWAS contain only one segment in the water column. The TOXSWA model contains several segments distributed along one water course (no branching). WASP and EXAMS allow description of a surface water network with several branches and the water column divided into many segments.

Most of the models have a static hydrology; that is, they do not simulate increases in flow or depth due to surface runoff or lateral flow which may result from storms. The TOXSWA model possesses an interface allowing linkage to a dynamic hydrologic model. The hydrodynamic model DYNHYD is included in WASP, but also other, static models have been used in conjunction with WASP.

Flow of water in the sediment is described in the WASP and TOXSWA models. ABIWAS does not have a sediment layer, while SLOOT.BOX only describes sedimentation and re-suspension; so both ABIWAS and SLOOT.BOX do not calculate PEC in sediments.

4.5.3 Entry routes and frequency of application

Pesticide loadings to the aquatic systems are simulated as pulses or stepwise continuous distributions. Examples of pulse type inputs include spray drift or momentary discharges. Stepwise continuous distributed inputs represent lasting drain discharges, surface runoff, or upward seepage. Simple models may only simulate changes in initial conditions, while more complex models may accept loadings from various sources throughout the simulation.

ABIWAS requires an initial (water) concentration, while SLOOT.BOX can receive pulse type inputs at any time. TOXSWA requires an initial water and sediment concentration in the segments (resulting from an pulse type input) and a stepwise continuous distributed input to the sediment. EXAMS and WASP can accept pulse type and stepwise continuous distributed inputs to water and sediment segments at different times throughout the simulation.

If lateral flow would be important EXAMS or WASP can be applied.

4.5.4 Compartments considered within the modelled system

In the water column all models contain a water phase and suspended solids. EXAMS and WASP distinguish plankton from other suspended solids. TOXSWA is the only model where macrophytes or rooted water plants are present.

Only WASP simulates a dynamic suspended solids' behaviour including deposition and re-suspension. In EXAMS and TOXSWA the concentration of suspended solids is constant, but they move with the water body.

ABIWAS and SLOOT.BOX do not have a sediment layer. EXAMS, WASP and TOXSWA distinguish a solid sediment phase and pore water. In addition, EXAMS and WASP simulate the presence of benthos.

Processes considered in water column:
In the water column all models calculate sorption to suspended solids and degradation. ABIWAS only calculates the abiotic degradation. TOXSWA and SLOOT.BOX use a lumped degradation rate. EXAMS and WASP distinguish between hydrolysis, photolysis, redox reactions and biolysis (in WASP a lumped parameter is also possible). TOXSWA is the only model that simulates sorption to water plants. All models contain volatilisation.

In WASP three chemicals can be modelled and in EXAMS two. In the other models calculations are executed for only one chemical.

ABIWAS and SLOOT.BOX have advective water flow, while the three other models consider advection as well as dispersion. EXAMS, WASP and TOXSWA also calculate the exchange with the sediment by means of advection and diffusion.

Sediment*:*
Of the five models, only EXAMS, WASP and TOXSWA model the sediment and so only these three models calculate PEC in the sediment. The three models all calculate sorption to solid sediment material. TOXSWA simulates degradation using a lumped degradation rate, while EXAMS and WASP again specify the different mechanisms. EXAMS and WASP can handle two chemicals in the sediment. All the three models consider the transport processes of advection, dispersion and diffusion, but bioturbation is only included in EXAMS and WASP.

4.5.5 Predicted Environmental Concentrations in surface water and sediment (PEC$_{sw}$ and PEC$_{sed}$)

All five mentioned models calculate concentrations in the water phase, so a PEC$_{sw}$. Only EXAMS, WASP and TOXSWA simulate pesticide mass in the sediment and so only these three models can provide a PEC$_{sed}$. As both EXAMS and TOXSWA do not simulate re-suspension and sedimentation of suspended solids these models are only able to predict short term PEC$_{sed}$. From an ecotoxicological point of view it is still a point of discussion whether the total pesticide concentration (dissolved plus sorbed) or the pesticide concentration in the pore water represents best the PEC$_{sed}$. Sediment dwelling organisms swallow detritus and therefore they are also exposed to sorbed pesticide and not only to pesticide present in the pore water. The three mentioned models, EXAMS, WASP and TOXSWA, all calculate total concentrations as well as concentrations in pore water.

4.5.6 Usability

ABIWAS and SLOOT.BOX are very easy to use and both have a menu-oriented shell to guide the user. However, they have a rather limited capacity to simulate different types of surface waters and they do not include sediment. EXAMS, WASP and TOXSWA are all less easy to use and interpret. All three models comprise a shell with a help utility to guide input preparation, but these leave still room for questions. Most input data are readily available for the models although they all have data that can only be obtained with difficulties (e.g. indirect photolysis in EXAMS or WASP, or sorption to water plants in TOXSWA).

WASP, EXAMS and TOXSWA have a post-processor to process model output. The post-processor in EXAMS produces rudimentary graphics output and many output tables; some of these output tables can be difficult to interpret or transfer to other software packages. The post-processor of WASP is relatively easy to use and very flexible. TOXSWA produces ASCII data files with the aid of a conversion program and these are loaded into a graphic software package to produce graphs.

The WASP and EXAMS models are both very flexible and can describe many different surface water network configurations and contain many parameters to describe pesticide behaviour. The WASP model is most performing in its hydrology as this is dynamic as well as in its suspended solids' behaviour. TOXSWA is less flexible, it describes only one watercourse. It needs less input parameters. It is the only model which considers sorption to water plants, a process generally more important than sorption to suspended solids.

4.5.7 Use for registration purposes

Of the five models considered four play a role in national registration procedures. In Germany the ABIWAS model is used for calculating (abiotic) degradation rate constants of pesticides. In the United States of America no models are legally required for the pesticide registration process, but actually both EXAMS and WASP are used. Recently there is a shift from using EXAMS to WASP as WASP can also simulate non-steady flow. In the Netherlands calculation of the exposure concentration by SLOOT.BOX is legally required. The SLOOT.BOX model will be replaced in the future by the TOXSWA model.

4.5.8 Validation status

None of the mentioned models has gone through a systematic validation process in the sense that a comparison between model results and reliable experimental data has been done according to pre-defined quantified standards. For SLOOT.BOX as well as ABIWAS no validation has taken place and for both EXAMS and WASP no process attempting to raise their validation status has been executed according to our knowledge. However both models EXAMS and WASP have been extensively applied, but generally speaking in such a way that model parameters have been adjusted to better simulate the studied situations. Parallel to the development of the TOXSWA model four experiments have been performed, providing data for a validation process, which is actually planned for 1996 and 1997.

In order to be able to go through a validation process in a satisfactory way the following *principal parameters* need to be *measured* in validation experiments:

Water course characteristics:
- cross-sectional and longitudinal profile
- mass concentration of suspended solids and their organic matter content
- dry weight of macrophytes per area of sediment and species present

- bulk density of dry bottom material as a function of depth
- organic matter content of sediment as a function of depth
- porosity in sediment as a function of depth
- pH-variation as a function of time
- temperature as a function of time
- light intensity as a function of time
- chlorophyll concentration in the water (so macrophytes plus algae, if possible to be able to calculate the decrease in the light intensity with depth
- redox-conditions of the sediment (if possible).

Hydrology:
- flow velocity or discharge as a function of time
- water depth as a function of time
- (longitudinal) dispersion coefficient.

Pesticide:
- pesticide concentration in incoming water flow
- entry routes with corresponding
    . pesticide concentrations or loads
    . location of entry
    . time and duration of entry
    . volumes of incoming water

these can include spray drift, surface runoff, drainage, groundwater flow and atmospheric deposition
- mass concentration in water column as a function of time (and if relevant space)
- pesticide content of suspended solids (if considered relevant)
- pesticide content of macrophytes as a function of time (and if relevant space) (if macrophytes are considered)
- mass concentration in sediment as a function of depth and time (and if relevant location in water course)
- sorption isotherm for sorption to suspended solids
- sorption isotherm for sorption to sediment (site-specific)
- sorption isotherm for sorption to macrophytes (if considered)
- transformation rate constant for the water column (accounting for biodegradation, hydrolysis and photolysis if relevant)
- transformation rate constant for the sediment (accounting for biodegradation and hydrolysis, if possible for site-specific conditions)
- volatilisation - if possible.

4.5.9 Conclusions and Recommendations

As systematic comparisons between model results and measured data are lacking actually it is difficult to state with which accuracy the models can predict exposure concentrations or loads in or from water courses. Estimating this however it can be said that in general the five mentioned models predict concentrations well within one order of magnitude and that they perform better for static or slowly flowing systems.

The most developed, flexible models, enabling the calculation of PEC in the water column as well as in the sediment appear to be EXAMS, WASP and TOXSWA. Both EXAMS and WASP can be applied to branched systems; WASP can handle dynamic flow conditions, but it is more complicated to use. EXAMS and WASP can simulate metabolites or breakdown products, while TOXSWA cannot. The TOXSWA model can be used in non-branched water courses and accounts for sorption to macrophytes.

A simple model like SLOOT.BOX can be useful for screening or comparing products with a high solubility, so low sorption capacity. The ABIWAS model performs well in calculating (abiotic) degradation rate constants; in fact ABIWAS has been developed for this use and not with the aim of calculating PEC. If SLOOT.BOX or ABIWAS are used to calculate a PEC in the water column, then another method is needed to calculate a PEC in the sediment.

The foregoing implies that there is a need for future research aiming to raise the validation status of applied models.

4.5.10. Other models

In the Annex 9.5 the five models mentioned are described into more detail. Also other models are described there. These are models that for several reasons, stated in their descriptions, were not included, although they might play a role at certain levels of the regulation procedure. Also multi-media models were not assessed. Multi-media models are useful to rank/prioritise substances or to perform a first screening of the risk of substances. At the 15th SETAC Annual Meeting of 1994 in Denver, Colorado a workshop was held on the Application of Multi-media Models for Regulatory Decision Making. Five different multi-media models, SIMPLEBOX, HAZCHEM, CHEMCAN, CALTOX and CemoS were compared independently. The overall conclusion of the workshop was that the different multi-media compartmental models are generally consistent, that the predictions are in accordance with observations and that the results can be used for regulatory purposes. In the Annex 9.5 the compartment model TOPFIT is described.

References:

Mackay, D. and S. Peterson. 1981. Calculating Fugacity. Environmental Science and Technology 15(9):1006-1014.

Parker, R.D. and D.D. Rieder. 1995. The Generic Expected Environmental Concentration Program, GENEEC. Part B, Users Manual. Tier One Screening Model for Aquatic Pesticide Exposure. Environmental Fate and Effects Division, Office of Pesticide Programs, U.S. Environmental Protection Agency.

Rasmussen, D, 1995. surface water model for pesticides - SLOOT.BOX. Technical report V. National Environmental Research Institute, Denmark.

De Vries, D.J.. 1987. IMPAQT, a physico-chemical model for simulation of the fate and distribution of micropollutants in aquatic systems. TOW-IW T250, Delft Hydraulics.

De Vries, D.J. and M.P.J.M. Kroot. 1989. SOM-3, a simple model for estimating fluxes, concentrations and adaptation times of micropollutants in aquatic systems. User's manual, T0632, Delft Hydraulics.

Williams, W.M. and J.M. Cheplick. 1993. RIVWQ Users Manual. Waterborne Environmental, Inc. Waterborne Environmental (987-B Harrison Street, S.E. Leesburg, Virginia 22075, USA.

5. MODEL LIMITATIONS AND DEFICIENCIES

5.1 Spray drift models

Spray drift usually considers only single values for wind speed and wind directions though these meteorological parameters vary highly with place and time. Additional assumptions are made for the spraying system itself: the droplet spectrum and the velocity of droplets are rough simplifications of the real spray drift situation. Finally, some models can handle only a limited number of spray drift situations as listed in the table below.

Table 5 Spray drift model limitations

Model	Limitations due to spray drift situation
IDEFICS	- simulates only field spraying (orchards are not considered) - no simulation of aircraft spraying - no specific pesticide parameters included
MOPED	- only horizontal spraying considered - no simulation of aircraft spraying - no specific pesticide parameters included
PEDRIMO	- no specific pesticide parameters included

None of these models are validated at the moment.

5.2 Drainage models

Some of the most important limitations of the models for calculating inputs to surface waters via drainage systems are listed in Table 6 below.

Table 6 Drainage model limitations

Model	Main limitations/deficiencies
PESTLA 3.0	Non-structured soils only
PESTRAS 2.1	No field drains Non-structured soils only
OPUS 1.63	One-dimensional treatment of solute flux in saturated zone Incomplete documentation Non-structured soils only
CHAIN_2D 1.1	Degradation not affected by water content Difficult to use for routine applications Non-structured soils only
MACRO 3.2	Outputs sensitive to (uncertain) macropore-related parameters
CRACK_P 1.0	Clay soils only Outputs sensitive to (uncertain) macropore-related parameters

Use of OPUS, CHAIN_2D, PESTLA and PESTRAS should be restricted to non-structured sandy soils. CRACK_P is specifically designed for use in clay soils, but should not be applied to lighter-textured, permeable, sandy and loamy soils (clay content c. < 35%).

Outputs from the macropore flow models MACRO and CRACK_P are sensitive to parameters related to the macropore region (e.g. macropore conductivity, volume, spacing), which are, in turn, difficult to estimate. This may lead to high levels of predictive uncertainty, compared to the use of models in non-structured sandy soils.

OPUS suffers from an essentially one-dimensional treatment of pesticide flux in the saturated zone and rather incomplete documentation. The current version of CHAIN_2D is complicated and difficult to use. However, the Windows-based version 2.0 currently under development (released in March 1996) should certainly remove this limitation for the use of the model for management purposes. PESTRAS is designed for use at the regional scale, and does not explicitly treat 'within-field' drainage systems. Empirical parameters are used to calculate lateral saturated flow, rather than any physically-based approach, and this may limit, to some extent, the general applicability of the model.

Model users should be aware of the low validation status of all the available models when used for predicting drainflow concentrations, and that the predictive accuracy of the models may not better one order of magnitude for predicting peak concentrations (i.e. acute exposure) and perhaps a factor two for predicting long-term loads (i.e. chronic exposure).

5.3 Surface runoff models

Most runoff models assume equilibrium partitioning between pesticide sorbed to the soil surface and in the runoff water. As the contact time of the runoff water and the soil surface is too short to reach equilibrium this approach overestimates concentrations in the runoff water.

Runoff events occur in the time frame of hours. Therefore models which have a daily time step (i.e. PRZM, PELMO, GLEAMS) are not able to predict the actual time-course of loading into the surface water. On the other hand models which work with shorter time steps such as OPUS rely on breakpoint weather data, which are not readily available.

Almost all the models can only simulate uniform slopes and land use. All 1-dimensional models calculate the runoff values at the edge of field. Therefore effects of buffer zones will not be taken into account by these models.

The amount of runoff water is estimated by most of the models using the curve number approach. These curve number were empirically derived from studies conducted in the USA. As it is an empirical method it is questionable whether it is valid for estimations in other parts of the world.

5.4 Surface water fate models

In most surface water fate models water flow has been described as a steady state. This assumption of constant water depth and flow velocity is especially less realistic if longer periods are considered and in cases where considerable runoff and/or drainage inputs occur. In case of runoff or drainage dilution will occur and the flow velocity will increase, implying that model results will be too conservative.

All surface water fate models assume instantaneous mixing over the cross-section of the segments. Only WASP and EXAMS allow for the definition of vertically stacked segments in the cross-section of a water course. Experiments of e.g. Crum and Brock (1994) indicate however that in reality it can take 24 hours before pesticides entering via spray drift deposition have reached the lower parts of the water course, especially in the presence of macrophytes. This means that the PEC_{sw} predicted by a model can differ considerably of the real exposure concentration of water organisms during the first day, and this first day exposure is often very important for establishing the acute toxicity.

The longitudinal dispersion coefficient determines to a great extent the spread of the pesticide along the water course. So especially with point-type pesticide inputs and steep concentration fronts it is important to know its value. For smaller or slowly streaming water courses very few research has been done in this area and it would be useful to study dispersion into more detail for these types of water courses.

Most models have schematised the sediment into a few layers in which they calculate pesticide concentrations. This may result in underestimating real pesticide concentrations in the upper sediment part and so this may hamper a good estimation of the PEC_{sed}.

When no water flow, upward or downward seepage, can be simulated real concentration profiles in the sediment may differ considerably from simulated profiles, influencing in a negative way PEC_{sed} estimations.

Most models describe sorption to sediment and suspended solids as an instantaneous and linear process. Experimental work shows however that often sorption is not linear when wide ranges of concentrations are considered. Moreover sorption generally increases with time, while most sorption coefficients have been established in rather short experiments. Considering these factors seems especially important to simulate well exposure concentrations in slowly moving water bodies and in the sediment.

Pesticides do not only sorb to sediment at the water course bottom but they can sorb to organic matter at the walls of the water course as well. In small water courses this can represent a non-negligible area that can influence the concentration with time.

Very few research has been executed so far about the process of sorption, or uptake, of pesticides to macrophytes. Especially when large amounts of macrophytes are present this process affects the pesticide concentration, among others by the effect of retardation.

Most of the models use first order kinetics to describe degradation processes. EXAMS and WASP models make corrections for light intensity, pH or temperature. The TOXSWA model uses a lumped degradation coefficient, which hampers the use of laboratory data on e.g. hydrolysis and photolysis. Under field conditions these environmental factors fluctuate considerably in the water phase and this makes it not easy to apply right values in the model. To perform detailed risk assessments the modeller should make certain that predictions of the amount of material remaining are consistent with available field data.

When large amounts of the pesticide are present in a sorbed phase, e.g. to macrophytes, suspended solids and/or sediment, the degradation rate may be different from a situation with all pesticide in the dissolved phase. This is another reason why model predictions should be compared to available field and laboratory information in order to make sure that these are consistent.

References

Crum, S.J.H. and T.C.M. Brock, 1994. Fate of chlorpyrifos in indoor microcosms and outdoor ditches. In: "Freshwater Field Tests for Hazard Assessment of Chemicals", I.A. Hill, F. Heimbach, P. Leeuwangh and P. Matthiesen (eds), Lewis Publishers, Michigan.

6. EUROPEAN SCENARIOS

6.1 Definition of European Scenarios

A critical component of any modelling procedure is the identification of relevant scenarios to characterize the environmental conditions determining model input parameters. As defined in Chapter 3, a scenario comprises ‘a unique combination of agronomic and environmental conditions that realistically represents significant areas within which conditions are relatively homogeneous with respect to modelling input parameters’. These conditions include climate, hydrogeology, surface water characteristics, soil and topography. However, not all the conditions need to be defined for all PEC_{sw} calculation purposes. For example, within the phased approach recommended in section 2.5, first step calculations require only a very simple definition of surface water and sediment characteristics. In fact full characterisation of all conditions may be necessary only for the most detailed simulations carried out at the step 4 level.

6.1.1 Existing European scenarios: Step 1 calculations

Ideally, when calculating PEC_{sw} for European registration purposes, modellers should be able to draw on a limited number of well defined European scenarios. To date no such scenarios exist although the basic dimensions of some static surface water bodies have been defined for many national registration purposes (see section 2.4) and, in the Netherlands, a simple ‘standard scenario’, defining conditions in a shallow edge of field surface water ditch is used, if necessary in conjunction with drainage inputs calculated using the standard soil and climate scenario defined for leaching models (see the report of the FOCUS leaching group).

All these crude scenarios are clearly intended for use only for the simplest, level 1 ‘worst case loading’ calculations. For these purposes, worst case loadings are based on maximum annual applications and so no specific climate, cropping, topography or soil scenarios are necessary. There is however, a clear need for the existing national surface water scenarios to be harmonised. It is therefore recommended that a single, agreed ‘*Step 1 standard European surface water scenario*’ be defined based on the following elements:

- Dimensions of the water body - *width, surface area, depth of water.*
- Flow regime in the water body - *Static.*
- Suspended solids - *Mass per unit volume, organic carbon fraction.*

For ease of use, the definitions should be as simple as possible and, whilst they should not be unrealistic, need not relate to any real field situation.

6.1.2 Scenario definition for Step 2 calculations

For step 2 calculations, it is proposed that a time sequence of loadings, based on simple but conservative over-estimates, be used in conjunction with a more complex, mechanistic surface water fate model. Calculation of loadings is simply based on sequential application patterns of the compound under investigation so, as with step 1 calculations, no specific climate, cropping, topography or soil scenarios are required.

Again, the development of a single, *'Step 2 standard European surface water scenario'* is recommended. In this case however, the scenario should be more comprehensively defined than that of step 1 and the elements to be considered should be based on the critical input requirements for the chosen model. As described in section 4.5, these input requirements vary according to the model used, but a minimum defined set of characteristics for this level of calculation is as follows:

- Dimensions of the water body - *width, surface area, depth of water.*
- Flow regime in the water body - *Static or steady-state low flow of specific velocity.*
- Suspended solids - *Mass per unit volume, organic carbon fraction.*
- Dimensions of the sediment - *surface area, depth.*
- Sediment characteristics - *Particle-size fractions, organic carbon fraction, bulk density.*

As with step 1, the definitions should be as simple as possible and could be developed by expanding the existing criteria defined for the step 1 standard scenario.

6.1.3 Worst Case Scenarios for Step 3 calculations

For step 3 calculations, a time series of surface water loadings relating to 'worst case inputs' via spray drift, surface runoff or drainage is required. Here, it is recommended that a limited number of 'worst case' climate/spray; climate/topographic or climate/soil scenarios are used in combination with the Step 2 standard European surface water scenario. In each case, the definition of worst case conditions will depend on the critical parameters used in the chosen model. For example, in all the current surface runoff models, a curve number approach is used to calculate runoff and the USLE or MUSLE is used to calculate erosion losses. For these situations, worst case soil conditions can be specified by using soils in hydrologic group D 'poor hydrologic condition' and with a silty topsoil containing low levels of organic matter. Similarly, a worst case weather situation for run off can be specified by identifying areas where specific target crops have extreme climatic conditions (extreme climates may be those with large amounts of annual rainfall or with common high intensity rainfall events) and then selecting periods of weather in which a minimum amount of rain or number of events occurs within a set period of pesticide application. An example of how data relating to such a worst case weather situation can be identified is given in section 6.2.1 below.

Worst case scenarios for calculating step 3 surface water loadings from spray drift, runoff or drainage inputs should be realistic but need not be based on an actual field situation.

Using the type of arguments described above, it is possible to define some characteristics and give guidance on the selection of others that are dependent on the range of target crops and mode of application of the pesticide under investigation. In order to initiate the development of worst case scenarios for step 3 calculations, some basic characteristics are defined below. It is recommended that future work concentrates on the development, expansion and verification of these definitions.

Worst case spray drift scenario:

- Spray characteristics
  1m wide buffer to surface water body.
  95 percentile drift distribution.

Cropping
  Determined from the pesticide specific target crop that has the greatest drift impact for the defined spray characteristics.

Worst case runoff scenario:

- Topography
  Uniform 2 - 3 % slope.
  Runoff from 100% of the field.
  All runoff impacts directly upon the water body.
- Soil
  Soil hydrologic group D.
  Topsoil texture class Silt loam.
  Topsoil organic matter content < 2.0%
- Cropping
  Determined from the pesticide specific target crop and associated management that gives the greatest fraction of applied compound impacting upon the soil.
- Weather
  Data representative of an extreme climate for the identified cropping scenario (either large average annual rainfall or many, high intensity rainfall events).
  Period with a specified minimum amount of rain or number of specific intensity rainfall events within 30 days of pesticide application.

Worst case drainage scenario

- Drains
  Spacing 10m.
  Depth 0.7m.
- Soil
  Slowly permeable, seasonally wet water regime.
  Clay topsoil with average structure.
  Clay subsoil with poor structure (coarse prismatic) and bulk density 1.4 to 1.5.
  Topsoil organic carbon 1.2 to 2.0%; subsoil organic carbon 0.4 to 0.6%.
- Cropping
  Determined from the pesticide specific target crop and associated management that gives the greatest fraction of applied compound impacting upon the soil.

- Weather

  Data representative of an extreme climate for the identified cropping scenario (climates with a large average annual effective rainfall).
  Period with specified minimum amounts of effective rainfall within 30 and 200 days of pesticide application.

6.1.4 Scenarios for Step 4 simulations

Scenarios for carrying out the most detailed simulations of surface water fate should be related to specific and realistic combinations of cropping, soil, weather, field topography and aquatic bodies adjacent to fields. In these cases, typical field situations for target crops need to be identified along with some indication of their spatial distribution.

In order to initiate this process, a possible procedure for identifying typical field situations for target crops is outlined below. Where relevant, the critical parameters that need to be defined for each scenario are suggested.

1. Identify the distribution of target crops.

2. Identify broad surface hydrological situations. An initial proposal for some groupings of these is given below. This proposal needs to be developed and expanded by an expert working group.

   a) *Major groundwater basins*
   Low-lying, level areas with comprehensive field drainage into adjacent ditches which contain water throughout the year. Ditches usually occur on at least two sides of the field and ponds may also be present. Flow regimes are static or very slow moving

   b) *Edges of major groundwater basins, local groundwater areas and spring sites.*
   Low-lying, gently sloping areas with local field drainage into adjacent ditches which in turn drain into larger watercourses. Ditches contain water throughout most or all of the year but usually occur along one side of the field only. Flow regimes are slow to moderate.

   c) *Major plains of slowly permeable or impermeable land with seasonal wetness.*
   Gently sloping to level areas with comprehensive field drainage into adjacent ditches which contain water for varying periods during the autumn winter and spring. Ditches usually occur on at least two sides of the field and ponds are common. Flow regimes are slow to moderate.

   d) *Stream headlands in slowly permeable or impermeable land with seasonal wetness.*
   Gently to moderately sloping areas with local field drainage into adjacent ditches which contain water for varying periods during the autumn winter and spring. Ditches usually occur along one side of the field only. Flow regimes are moderate to rapid.

e) *Stream headlands in hilly areas.*
Gently to moderately sloping areas with no field drains, but ditches along one or two field edges. Ditches connect with larger water courses and carry water for varying but relatively short periods after rainfall events. Flow regimes are moderate to rapid.

3. Define the surface water body in each of the hydrological situations covered by the target crop. At a minimum, the elements to be defined should include:

• Dimensions of the water body	*width, surface area, depth of water.*
• Flow regime in the water body	*Static or steady-state low flow of specific velocity.*
• Suspended solids	*Mass per unit volume, organic carbon fraction.*
• Dimensions of the sediment	*surface area, depth.*
• Sediment characteristics	*Particle-size fractions, organic carbon fraction, bulk density.*
• Biota	*Mass per unit area of macrophytes or fraction of plankton in suspended solids.*

4. Define the field topography adjacent to the selected surface water bodie(s). At a minimum, the elements to be defined should include:

• Dimensions of the field	Width, breadth, surface area
• Slope characteristics	% slope, fraction of field covered by defined slope, presence of buffer strip or level area adjacent to the water body.

5. Identify the range of climates within the selected cropping / surface water scenarios. For this purpose a range of climates within Europe should be defined in terms of the following parameters:

    - Average annual hydraulically effective rainfall
    - Average annual temperature
    - Average winter temperature (during the months of December, January & February)
    - Average summer temperature (during the months of June, July & August)
    - Frequency of rainfall events
    - Intensity of rainfall events

5. Select one or more weather dataset(s) representative of the most common climate(s) for the cropping / surface water scenario.

6. Identify the range of soils within the selected cropping / surface water / climate scenario(s). For this purpose, the soils within Europe should be grouped in terms of the following characteristics:

    - USDA soil hydrologic group: (as defined for the runoff models described in chapter 4.3)

• Topsoil texture group:	Fine sandy Medium or coarse sandy Silty Loamy Clayey
• Topsoil organic matter range:	<1.5% 1.5 - 2.5% 2.51 - 5.0% 5.1 - 10.0% >10.0% (organic or peaty topsoils)
• Subsoil structure	Good Average Poor
• Subsoil texture group	Sandy Silty Loamy clayey

7. Select one or more soil types representative of the chosen cropping / surface water / climate scenario(s). Derive specific model input parameters for the selected soils.

8. Define the specific cropping and management regime, including the width of any spray buffers, for the selected cropping / surface water / climate / soil scenario(s).

In order to implement the procedure outlined above at the European level, an appropriate database of aquatic environments adjacent to agricultural land, topography, soil types, crops and climate is needed. Such a database could also be used to assess the distribution and significance of the ‘worst case’ runoff and drainage scenarios developed for step 3 calculations.

The SEISMIC system (Hollis et al., 1993), an interactive environmental database system for England and Wales designed to facilitate scenario selection and parameter estimation for simulation models, provides an example of how such databases can be used to identify realistic cropping, soil and climate scenarios, although water bodies are not included.

European-scale data on cropping, climate, soil distribution and topography are available as a result of various EU initiatives over a number of years. However the data are disparate and often difficult to access and manipulate. They require collation and expert interpretation before they are suitable for identifying realistic European scenarios on which to base PEC_{sw} calculations. It is recommended that existing data sources within the EU are examined and interpreted to develop an easily accessed database of aquatic environments, cropping, agricultural field topographies, soil types and climates suitable for defining European scenarios for surface water fate modelling.

References

HOLLIS, J.M., HALLETT, S.H. and KEAY, C.A. (1993). The development and application of an integrated database for modelling the environmental fate of pesticides. In: *Proceedings 1993 Brighton Crop Protection Conference - Weeds,* pp. 1355 - 1364.

6.2 Example Scenario Calculation

This section describes a full PEC calculation for surface waters undertaken using some of the models reviewed in chapter 4. First, an example scenario is defined. Inputs to the surface water body via spray drift, surface runoff and drains are then calculated and finally, these calculated values are used to provide input data to calculate PEC's in the surface water body.

The selection of a specific scenario and set of models for this example simulation does not mean that they are to be preferred: They have simply been chosen as examples to illustrate how surface water PEC calculations may be made at the most detailed, highest tier level.

6.2.1 Definition of the scenario

In order to define a suitable scenario for the example PEC calculation, a sequential approach was adopted. Firstly, the characteristics of the pesticide to be simulated were defined.

A herbicide, applied as a surface spray at a rate of 2kg/ha to an autumn-sown cereal crop at early post-emergence stage with no crop interception,, was chosen. The following compound properties were assumed:

half-life in the topsoil	= 50 days,	k_{oc}	= 100 cm^3 g^{-1},
half life in water	= 30 days	*water solubility*	= 50 mg l^{-1},
vapour pressure	= 1.0 x 10^{-6},	*molecular weight*	= 250.

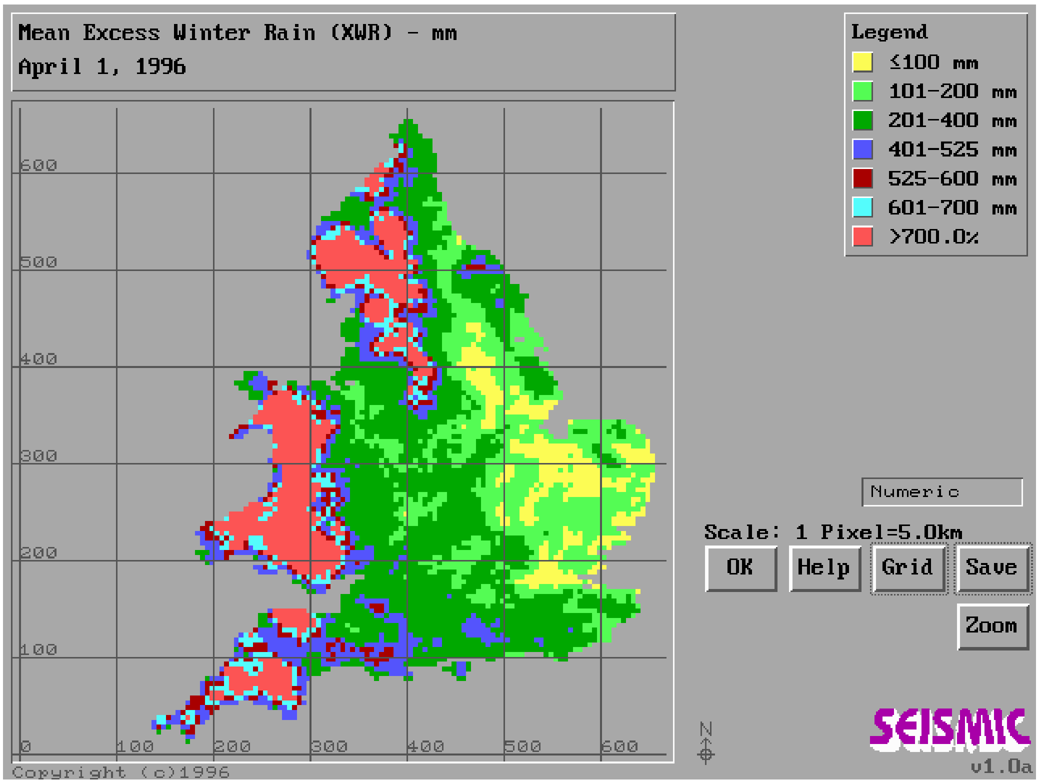
Next, an appropriate 'worst case' weather dataset for the target crop scenario was selected using the following procedure:

1. Patterns of average annual effective precipitation, defined as total rainfall during the 'climatic field capacity' were examined in relation to the proposed use pattern of the compound (autumn application to winter-sown cereals).
2. A long-term (30 year period) weather data set was selected for a site representative of an area with the largest annual effective precipitation in relation to the desired land use.

In order to facilitate this selection procedure, SEISMIC (Hollis et al., 1993), an interactive environmental information database system for England and Wales designed to facilitate scenario selection and parameter estimation for simulation models, was used. The rainfall data set selected was that representative of Rosewarne in the south west peninsular of England (50.22° N; 5.30° W). Rosewarne has an average annual rainfall during the climatic field capacity period of approximately 550mm and Figures 2 and 3, the result of steps 1 and 2 above, show that this represents a realistic, but extreme climatic scenario for cereals in England and Wales.

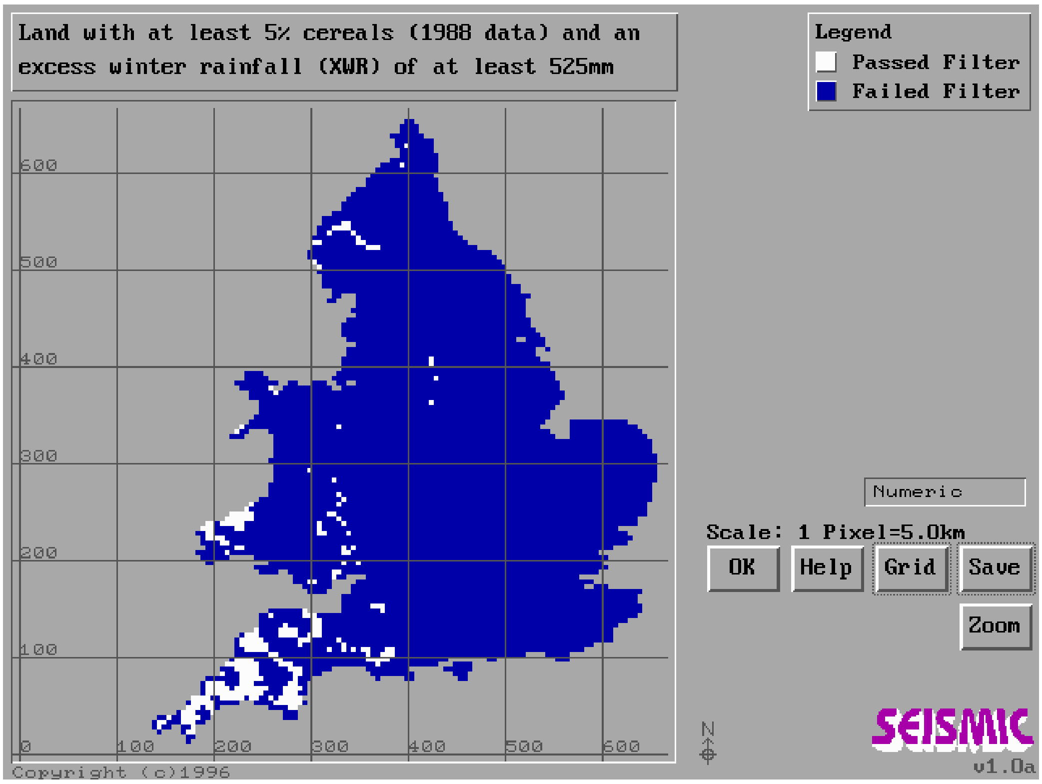
Rosewarne is located at grid intersect 1463 E; 0412 N on the maps shown below.

Fig. 2. Mean Excess Winter Rain (available for leaching and runoff) in England and Wales



Mean Excess Winter Rain (XWR) - mm
April 1, 1996

Fig. 3. Distribution of the chosen cropping and climate scenario in England and Wales



Land with at least 5% cereals (1988 data) and an
excess winter rainfall (XWR) of at least 525mm

Following selection of a cropping and climate scenario, a suitable soil scenario was defined. For this simulation, in which the combined inputs from spray drift, surface run off and drainage were to be simulated, a realistic ‘worst case’ soil for drainflow was selected, again using the SEISMIC system. Hydrologically it is characterized as a slowly permeable, seasonally waterlogged soil over a slowly permeable substrate with negligible storage capacity and its basic properties are summarized as follows:

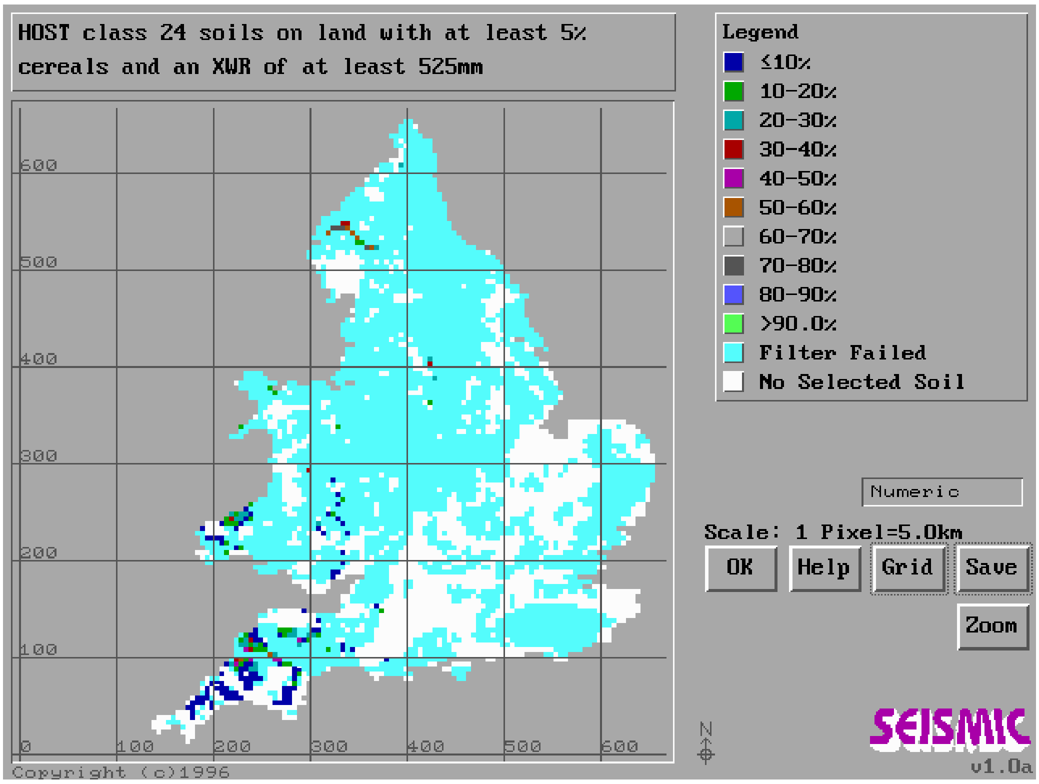
Horizon	**clay %**	**silt %**	**sand %**	**Soil structure**	**Organic C %**	**Bulk density g/cm^3**
Topsoil (0-25 cm)	40	40	20	Average	1.5	1.2
Subsoil (25-80 cm)	50	30	20	Poor	0.4	1.4

In the UK, soils with these physical and hydrological characteristics have a comprehensive field drainage system installed when under arable farming rotations and to reflect this, the following drainage scenario, typical for these soils, was chosen:

Drain spacing	10m intervals
Drain depth	0.8m from the surface

Fig. 4 shows how representative this soil is of the defined cropping and climate scenario.

Fig. 4. Distribution of the chosen soil, cropping and climate scenario in England and Wales



HOST class 24 soils on land with at least 5% cereals and an XWR of at least 525mm

Having defined a realistic combination of cropping, climate and soil, the final stage in scenario characterisation was to select a representative topography and surface hydrology. This stage in the definition process was more difficult because of the lack of access to comprehensive information relating to topographic and hydrological situations.

The broad scenario selected comprises a small square field with a uniform slope. Along the field edge at the base of the slope is a straight, level ditch with very low flow. The parameters which define this scenario are as follows:

Topography

Field size	100m x 100m (1 Ha)
Slope	2%
Spray buffer width	1m

Surface hydrology

Ditch length	100m
Ditch width	2m
Depth of water in ditch	0.5m
Volume of water in ditch	100m^3
Depth of sediment in ditch	5cm
Flow rate in ditch	0.001m/s

Whilst not unrealistic for the defined crop, climate and soil scenario, this is clearly a very idealised situation. Most of the parameters set out above were chosen to avoid complex topographical and hydrological situations. This was partly because the models selected for simulation do not adequately deal with complex topographies and hydrologies, but also because it ensured the relatively rapid and easy preparation of model input data files. It is possible that, in defining such a simple scenario, the flow rate in the ditch is rather slow for the selected soil and topographical conditions, which in reality, usually have somewhat higher flow rates.

Finally it was necessary to identify a suitable simulation period from the 30 years of data within the selected weather dataset. A two year period running from January 1st in year 1 to December 31st in year 2 was considered to be adequate. The criteria set out below, chosen to give a 'worst case' scenario for both drainage and surface runoff, were then used to identify a suitable two year period:

- At least 550mm of rain during the period from October to April.
- A total of 80mm of rainfall within the first 30 days after pesticide application.

The period selected qualified for both these criteria, pesticide being applied on October 24th in year 1.

6.2.2 Simulation of inputs to surface water via spray drift

Drift values for the example scenario defined above were obtained from Table 18 in Ganzelmeier et al. (1995), (see section 4.1 above on determination of drift loads). For a field crop in an early growth stage with a one meter buffer area, the 95th percentile drift is equivalent to approximately 4% relative to the application rate in g/ha. The simulated ditch is 2m wide and the ditch bank furthest from the sprayed field is therefore 3m from sprayer. The 95th percentile drift at the 3m distance from the treated field is approximately 1%. Thus the average load across the ditch is equivalent to 2.5%. With an application rate of 2000g/ha, a surface area of 0.02 ha, and the drift load equal to 2.5% of the application rate, the calculated drift load to the ditch would be 1.0 g.

6.2.3 Simulation of runoff inputs to surface water

The model GLEAMS version 2.03 was used to simulate water, sediment and pesticide runoff at the edge of a field as specified in the previously defined scenario. To run the model, the following options were chosen :

- Beginning of the simulation : 01/01/year 1
- End of the simulation : 30/09/year 2

- Winter crop seeded on the 21/10/year 1 after autumn ploughing on the same day. The growing season is defined as :
  - On the 21/10/ year 1 : seeding
  - On the 9/11/ year 1: the crop reaches 10% of canopy cover
  - On the 22/03/ year 2 the crop reaches 50% of canopy cover
  - On the 10/04/ year 2 the crop reaches 75% of canopy cover
  - On the 29/04/ year 2 the crop reaches 100% of canopy cover
- Crop harvesting on the 20/07/ year 2

- CNII (curve number of the SCS hydrological method) was chosen in the table of the GLEAMS Handbook for small grain, straight row and conservation tillage, hydrologic soil group D in poor hydrologic condition.

- Topography :
  - Slope : 2%
  - Field size : 100 m **Error! Reference source not found.** 100 m

- Monthly net solar radiation (Rn) was calculated from monthly total radiation (Rt) by means of the equation:

Rn = Rt (1- **Error! Reference source not found.**)

which represents the balance of low wavelength energy. The term corresponding to the balance of long wavelength energy was neglected which seems acceptable for monthly balances.

Hydrologic and quality results are shown in the following figures. Total pesticide losses represent 2.7% of the application rate. GLEAMS outputs are presented in tables from which Figures 5 and 6 were realised.

Fig 5 : Predicted runoff and pesticide concentrations in the liquid phase of runoff

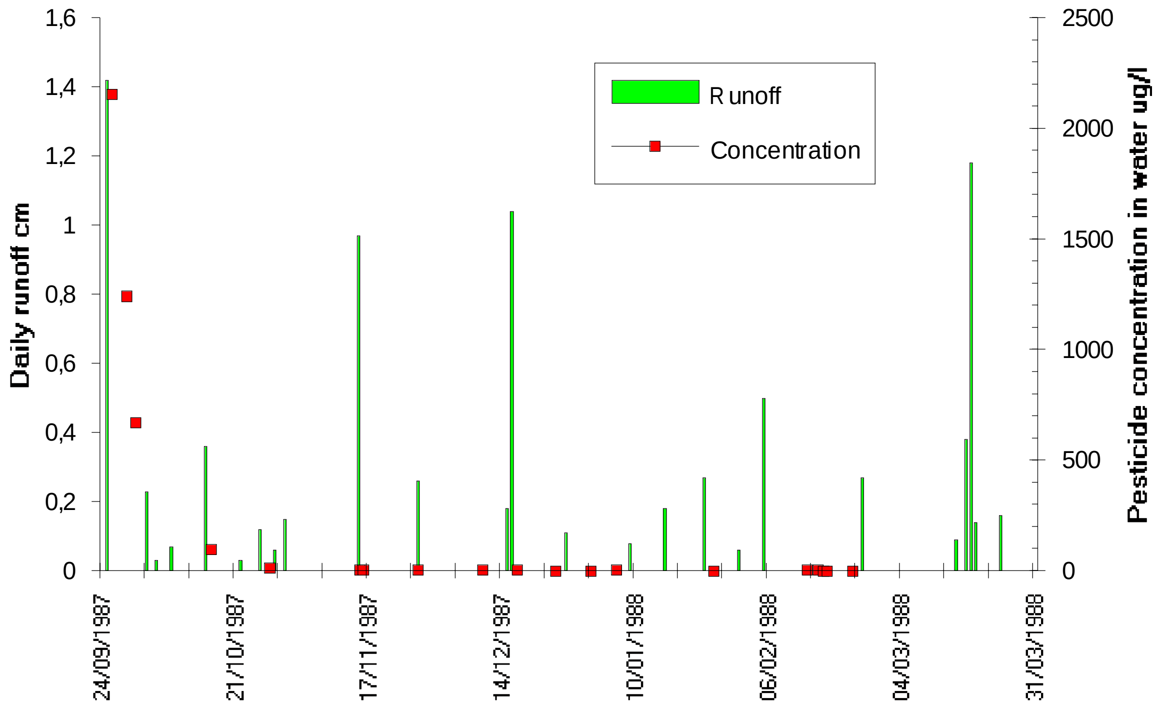
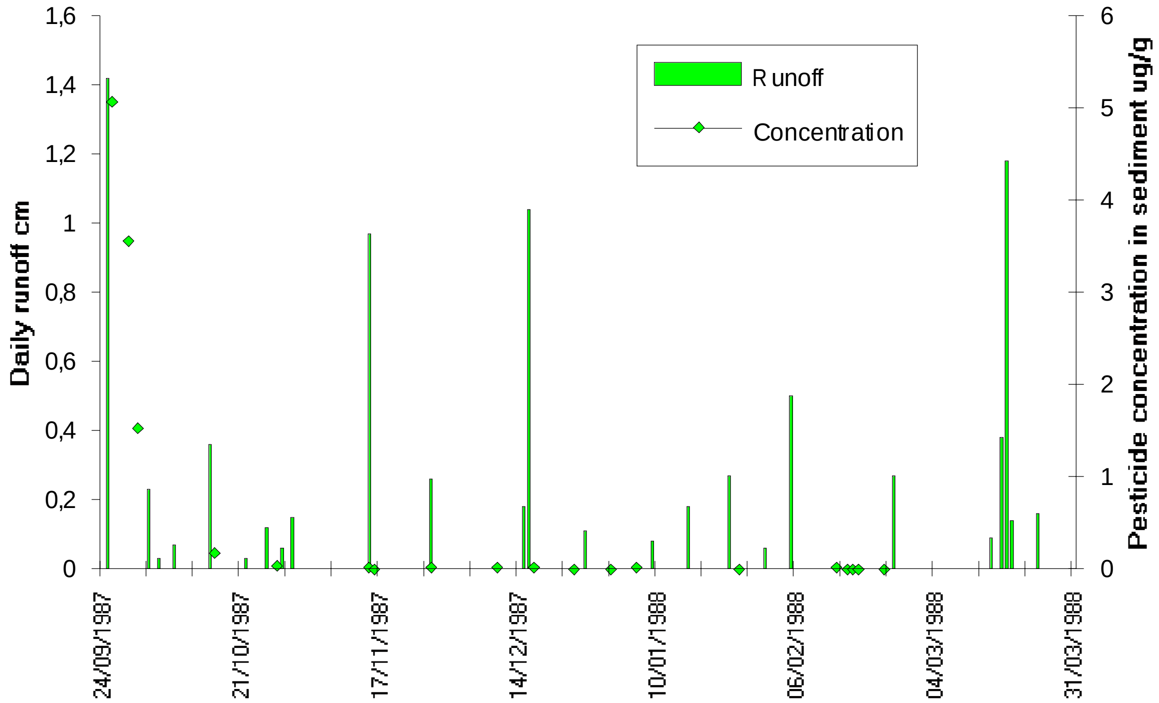


Fig 6 : Predicted runoff and pesticide concentrations in the solid phase of runoff



6.2.4 Simulation of drainflow inputs to surface water

The MACRO model was used to calculate drainflow inputs to surface water using the example scenario defined in section 6.2.1.

The MACRO simulation was run from the 1st January in the year of application (in order to allow time for predictions to become independent of the assumed initial conditions) and finished at harvest of the winter crop the following year (= c. 600 day simulation). A drain depth of 0.8m and a drain spacing of 10m were assumed.

Identical parameter values were selected for those parameters common to MACRO and GLEAMS. Additional parameters required by MACRO (but not GLEAMS) were estimated either as default values in the model, or by using pedo-transfer functions. The simulation was run from the 1st January in the year of application)in order to allow time for predictions to become independent of the assumed initial conditions) and finished on 30/9 the following year.

A reasonable compatibility with the GLEAMS simulation of the surface runoff for the same period was attained by the following procedure: the rainfall input file for the MACRO simulation was adjusted by subtracting the daily runoff values predicted by GLEAMS. The MACRO simulation then predicted sub-surface flow to drains and groundwater, but with no surface runoff, since the values of saturated hydraulic conductivity assumed (e.g. 150 mm.h^{-1} in the topsoil, 20 mm.h^{-1} in the subsoil) were sufficient to ensure that the water table did not reach the soil surface. Figures 7 and 8 show the predicted water flows and concentrations reaching the ditch via field drains respectively.

Fig 7.

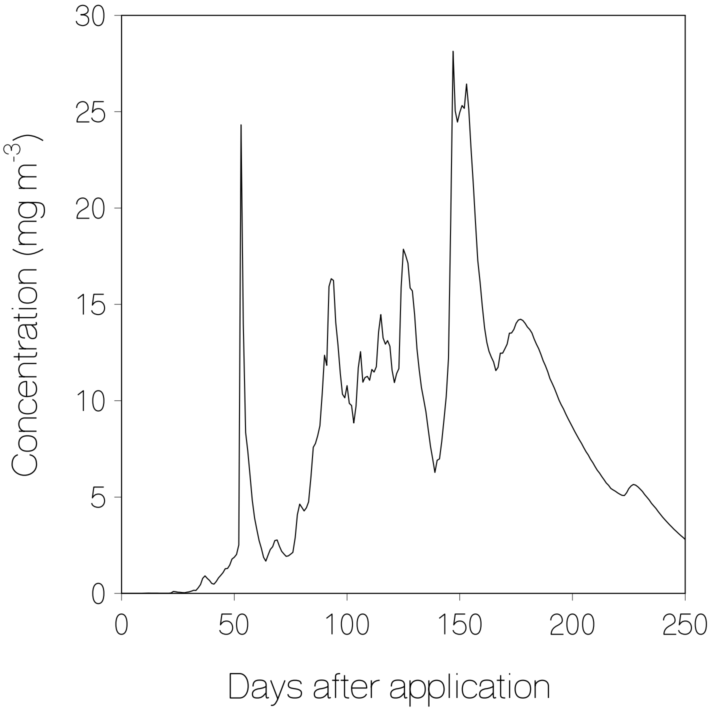
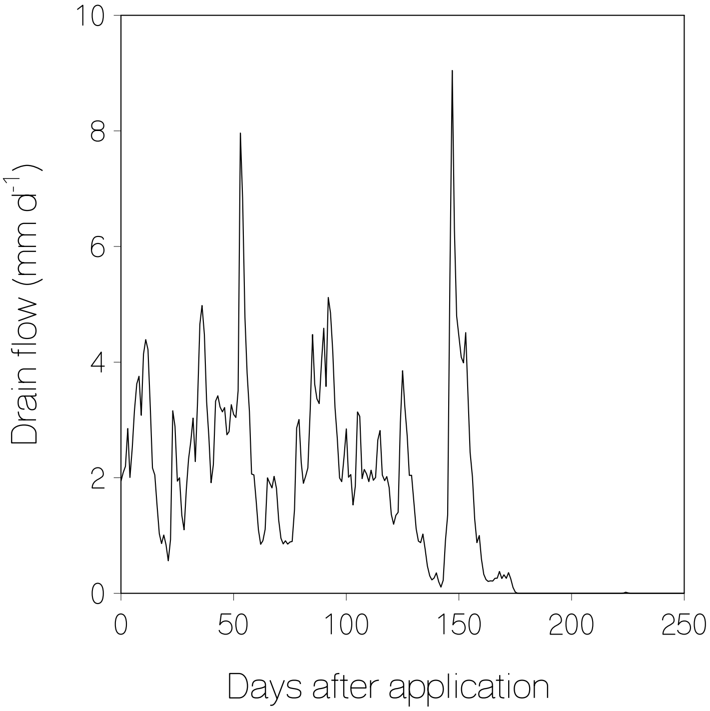


Fig. 8.



The amounts predicted to move to the ditch via general groundwater flow were, as expected for such a heavy clay soil, insignificant, being 2 orders of magnitude smaller than the drainflow contributions. Thus, no figures are presented here for this entry route. There were peak concentrations of c. 25 mg.m^{-3} at the end of December, c. 60 days after application, and again in early April, c. 160 days after application, 0.25% of the application was predicted to move to the ditch in drains. In the entire winter period following application, 1.8% of the applied amount was predicted to be lost to the drains.

6.2.5 Simulation of fate in surface water

The surface water fate of the example compound was modelled using the Exposure Analysis Modelling System (EXAMS version 2.95). The environmental scenario consisted of a field-side ditch with very little flow. Macrophytes and suspended sediment were not simulated. Descriptive information on the parameters used to describe the surface water system and the chemical of interest are summarised below.

Environmental Parameters	
Length	100 m
Width	2 m
Water depth	0.5 m
Volume	100 m3
Flow Rate	0.001 m/s
Sediment layer depth	5 cm

Phys/Chem Parameters

Molecular weight	250
Solubility	50 mg/l
Vapour pressure	10E-6 Pa.
Koc	100 ((mg/kg)/(mg/l))
DT50 in sediment	50 days
DT50 in water	30 days

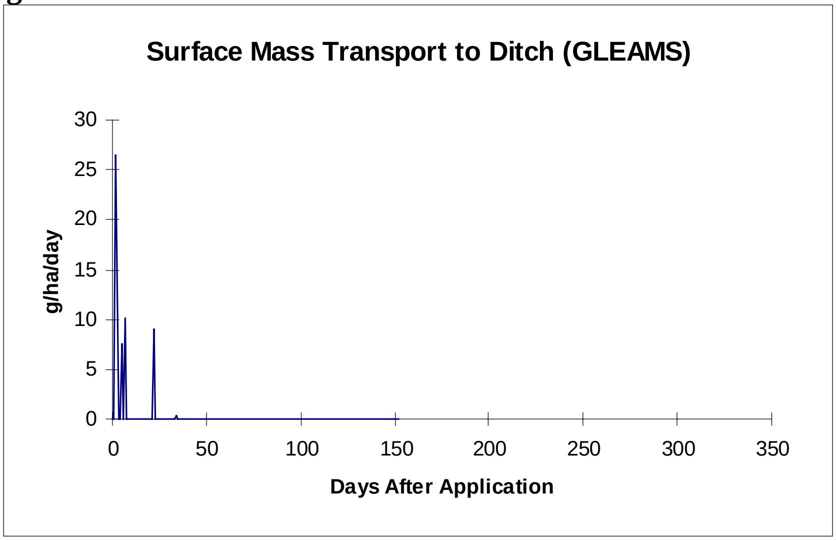
Degradation in water was simulated as the hydrolysis rate under neutral conditions (KNH = 9.63E-04). The aquatic environment scenario had a pH of 7, so acid and base hydrolysis reactions were not simulated (for some compounds these reactions could be quite important and would need to be represented). The degradation rate for sediment was based on the DT50 in soil of 50 days (KBACW = 5.78E-04). This degradation pathway was represented by the benthic bacterial biolysis rate in the model.

Chemical inputs to the ditch from drift, subsurface drainage, and surface runoff were simulated.

The drift load to the aquatic system was taken to be 1.0 g, estimated using the German drift tables of Ganzelmeier et al. (1995), as described in subsection 6.2.2 above. This 1.0 g was added directly to the water segment of the ditch.

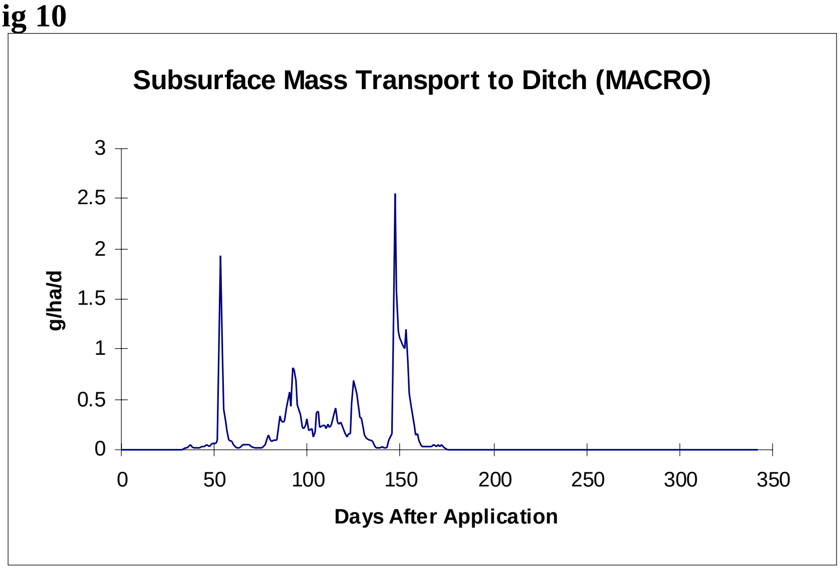
Surface runoff values were taken from the GLEAMS model output, calculated as described in subsection 6.2.3 above and shown graphically in Fig 9. It was assumed that the “catchment” or field area that contributed to the aquatic system was the total field area of one hectare defined in the example scenario. Chemical being transported from the field in the aqueous phase was added directly to the water column. Chemical sorbed to eroded sediments was added to directly to the sediment layer.

Fig. 9



Daily subsurface drainage values that might represent tile drainage from a field were taken from the MACRO model output, calculated as described in subsection 6.2.4 above. They are shown graphically in Fig 10 below.

Fig 10



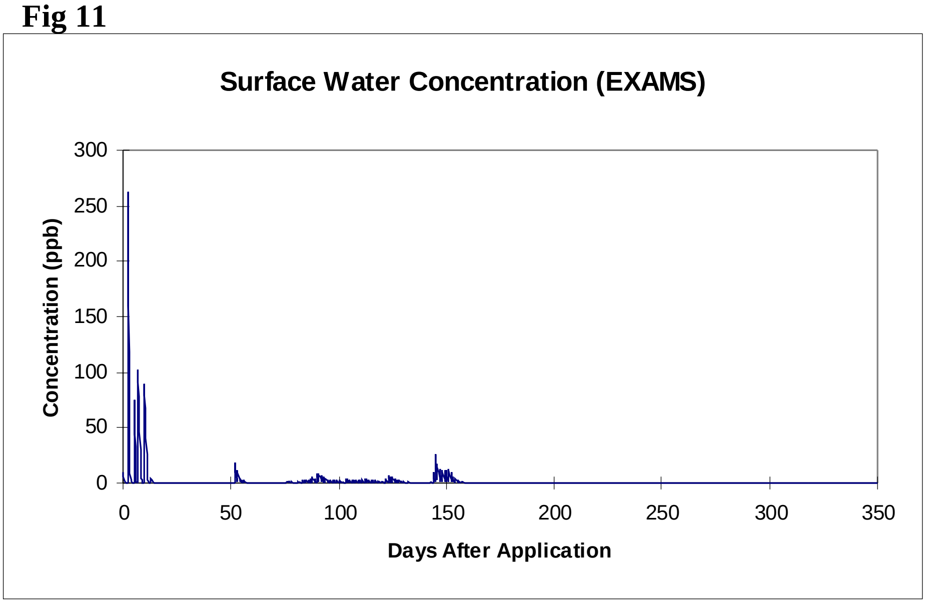
Input loads from both subsurface drainage and surface runoff were added directly to the water column (or to the sediment layer, where appropriate). If loads had occurred on the same day, then they would have been added together and presented as one pulse loading to the system, however, this did not occur. Assuming instantaneous dilution within the aquatic system, an input of 0.1 g to the surface water body would result in a maximum concentration of only one part per billion in the simulated ditch. In order to simplify the EXAMS simulation, all drainage and runoff values less than 0.1 g/ha/d were deleted from the input set. These values would have no significant effects on short or long-term average concentrations in the simulated ditch. All the calculated input load values used in the simulation are given in Table 3 of the EXAMS output report given in Annex 9.6.

Examination of Table 3 in Annex 9.6 shows that, for this example scenario, the calculated contributions to stream loadings from surface runoff far outweighed those from spray drift. Even drainage inputs contributed more to stream loadings than the spray drift input. This may seem surprising given that simple overspray or spray drift scenarios have been used as ‘worst case’, first tier examples when calculating surface water PEC’s for some national registration purposes (see section 2.4). The reason that this situation occurs is that stream load contributions from both surface runoff and drainage are assumed to be derived from the whole field (surface area 1ha) and occur as a number of individual daily events. Contributions from spray drift on the other hand, are derived only from a small strip of land adjacent to the surface water ditch and occur as a single event. These considerations need to be taken into account when developing any tiered approach to calculating surface water PEC’s.

Results

Predicted peak daily aqueous concentrations from the EXAMS simulations are plotted in Figure 11 below. The highest concentrations were seen during the period within approximately twenty days after application and, apart from the initial peak caused by spray drift, resulted from surface water runoff. Concentrations in the range of 0.1 to 20 ppb were predicted to occur in the period between 50 and 160 days after application. These were the result of inputs from subsurface drainage. In the periods between loading events however, concentrations decreased rapidly so that calculated long-term average concentrations were much lower than peak concentrations.

Fig 11



The EXAMS model, when used in mode 3, will automatically calculate average concentrations for 96 hour and 21-day periods for surface water and sediment pore water. These calculated values are presented below as the predicted environmental concentration in water (PECsw) and sediment (PECsed). (By using EXAMS in mode 2, the user can extract daily concentrations from the output file and calculate average concentrations for other time periods.)

	Time Period	
	96 hr	21 d
PECsw (ppb)	49.2	15.3
PECsed (ppb)	0.19	0.06

6.2.6 Conclusions

This example PEC calculation probably represents a very conservative estimate of exposure for two sets of reasons.

Firstly, PEC's are likely to be overestimated because of limitations in the models used. These limitations are discussed in chapter 5, but those which particularly apply to this simulation are:

- GLEAMS assumes equilibrium partitioning between pesticide sorbed to the soil surface and in the runoff water. As the contact time of the runoff water and the soil surface is too short to reach equilibrium, this approach overestimates concentrations in the runoff water.

- Loadings into EXAMS are made as instantaneous pulses. In reality the ditch input loads would be spread throughout a storm period and peak values would not be expected to be as high.
- EXAMS cannot simulate a changing hydrograph that would be associated with precipitation events and so dilution due to runoff and drainage water is not simulated.

Secondly, the scenario defined combines a number of ‘worst case’ features that represent a rather extreme, although not unrealistic, set of circumstances. These are:

- Drift loads were derived from the narrowest possible edge of field buffer (1 m) and the very upper end of drift distribution (95%). Typical loads from spray drift are probably much lower.
- Surface runoff was assumed to be derived from the whole field and all of it routed directly from the edge of the field into the aquatic environment with no buffer or ponding allowed to occur.
- The meteorological scenario is an extreme one in that:
    - The data is representative of one of the wettest areas in which the target crop is grown.
    - The compound was applied in autumn to a soil already at field capacity and with the drains already running with water.
    - Heavy rainstorms immediately followed the simulated pesticide application.
- The soil scenario is a near 'worst-case' for sub-surface drainage inputs, since macropore flow dominates the hydrology of such clay-textured soils.

Finally, the example calculation described in this section was meant to give a general example of how the various models could be used together to calculate PECsw. For many compounds, however, other factors might also need to be included in the modelling to accurately represent their behaviour in aquatic systems. These factors include adsorption to macrophytes and suspended sediments, acid and base catalysed hydrolysis, direct and indirect photolysis, etc.

7. VALIDATION

7.1 Validation Status of Existing Models

7.1.1 Spray drift

The models described in this section have either been calibrated (MOPED using the German drift tables) or validated with a limited number of experiments (PEDRIMO, IDEFICS). But as they are all recently developed these comparisons have been made to only a limited extent.

7.1.2 Drainage

Most of the drainage flow models assessed by the group are only recently developed and have been compared to field data to only a limited extent, if at all. Therefore, the validation status of all of the models must be considered low.

MACRO predictions have been compared with measured drain concentrations for 3 compounds on one soil type in Denmark and for 3 compounds on 3 soil types in the UK. For those measured concentrations above the analytical detection level, MACRO usually gave predictions within one order of magnitude without prior calibration and where some prior calibration of soil hydrology was undertaken, usually within a factor of two.

Predictions from CRACK_P, which was specifically developed for cracking clay soils, have been compared with measured drain concentrations of one compound on this soil type in the UK. The simulation successfully matched observed concentrations for a short period during the winter following autumn application.

PESTLA 3.0 estimates have been compared with measured drain concentrations of two compounds on two sandy soils in the Netherlands. Most predicted concentrations were less than 1.0 $\mu g\ l^{-1}$, but few conclusions can be drawn as to the accuracy of simulation because most of the measured concentrations were below the analytical detection limit.

As far as the authors are aware, predictions of PESTRAS, OPUS and CHAIN_2D have not, as yet, been compared with measurements of pesticide losses in drainage water.

7.1.3 Surface runoff

While all of the models have been widely used, specific studies to validate the models across a wide range of conditions have not been done. Most validation type studies have involved only the hydrology and erosion algorithms and have not included definitive validation of pesticide transport. Attempts have been made to validate the MUSLE and USLE equations with varying degrees of success. Several versions of runoff curve numbers are available and can be used. For most conditions within the United States the curve number concept appears reasonably valid. The validity of the curve numbers to accurately represent conditions within the EU is uncertain.

GLEAMS and PRZM are the most widely used of the models world-wide and in general it is felt that in most cases the models predict runoff losses within one order of magnitude. Some work has been done to attempt to validate PELMO for leaching but no formal work has been done for runoff. Each of these three models, GLEAMS, PRZM, and PELMO has been used for regulatory purposes (although PELMO has not been used for runoff). As deficiencies have become apparent in the models, they have been updated. For example, PRZM2 was found to significantly overestimate runoff of compounds such as Atrazine that had low sorption. A new non-uniform mixing algorithm was developed and has been incorporated into the code and now model results more closely predict what has been seen in field studies (PRZM2.3 is expected to be released in early 1996). The hydrology algorithms in GLEAMS are being updated to be more similar to those used in EPIC which are more accurate in predicting runoff events. EPIC, OPUS, and SWRRBWQ have been used less widely and have not been utilised for regulatory purposes to any great extent.

Currently PRZM and GLEAMS are being validated for both runoff and leaching by the FIFRA Environmental Modelling Validation Task Force. This is a group sponsored by twelve agricultural product companies with advisors USEPA and various academic and government institutions. The intent of this group is to take the models and compare them to data from derived from field studies. Results are expected to be available as early as 1997.

7.1.4 Surface water fate

None of the mentioned models has gone through a systematic validation process in the sense that a comparison between model results and reliable experimental data has been done according to pre-defined quantified standards. For SLOOT.BOX as well as ABIWAS no validation has taken place and for both EXAMS and WASP no process attempting to raise their validation status has been executed according to our knowledge. However both models EXAMS and WASP have been extensively applied, but generally speaking in such a way that model parameters have been adjusted to better simulate the studied situations. Parallel to the development of the TOXSWA model four experiments have been performed, providing data for a validation process, which is actually planned for 1996 and 1997.

7.2 Data requirements for validation of Models

7.2.1 Spray drift models

The following data is recommended for the validation of spray drift models:

- spraying equipment
    - * distribution of droplets (diameters)

  - * nozzle pressure
  - * spraying direction (top to bottom, horizontal)
  - * amount of vehicle
- meteorological parameters
  - * wind speed and wind direction (with time)
  - * temperature
  - * humidity in air
  - * atmospheric stability
- crop parameters
  - * crop height
  - * leaf stage
- pesticide parameters
  - * concentration in formulation
  - * vapour pressure

Output data needed for validation of spray drift models:

- drift deposits dependent on the distance from the agricultural area.

7.2.2 Drainage models

Data requirements for validation of leaching models have been previously presented by the FOCUS leaching group (DOC.4952/VI/95). These requirements are also relevant for models dealing with saturated flow, with the following additional data needed to validate drainage losses to surface waters: drain flow rate should be measured continuously, while concentration samples should be taken flow-proportionally and with as high a time-resolution as possible (e.g. at least several times per day during high flow periods). It is also highly desirable to measure water table heights and soil concentrations with the core sampling method.

7.2.3 Surface runoff models

The following data is recommended for the validation of surface runoff models.

Weather data :
Precipitation
Storm duration
Air temperature
Solar radiation

Soil data :
Depth of each soil layer
Soil texture and organic matter content of each soil layer
Corresponding porosity, field capacity, welting point and saturated conductivity
Soil moisture at the beginning of the simulation

Field management data :
Field area
SCS curve numbers

Soil erodibility, cropping practice factor, cover management factors
Albedo
roughness factors
Slope length and steepness

Cropping data :
Planting date, harvest date, tillage operation
Rooting depth
Leaf area index during the growing season
Albedo

Product chemistry data :
Initial pesticide amount on soil and leaves at the beginning of the simulation
Application dates and rates
Application method and efficiency
Koc, water solubility, washoff fraction
Foliar half-life and soil half-life
Henry's law coefficient
Diffusion coefficient

Output data necessary to validate runoff models :

Runoff volumes
Percolation volumes
Soil moisture
Evapotranspiration
Erosion loads and sediment enrichment with fine particles
Pesticide concentrations in runoff (water and sediment if possible)
Pesticide concentrations in percolation
Pesticide loads in runoff (water and sediment if possible)
Pesticide loads in percolation

7.2.4 Surface water fate models

The following data is recommended for the validation of models describing pesticide fate in surface waters.

Water course including sediment
Cross-sectional and longitudinal profile
Mass concentration of suspended solids and their organic matter content - if possible
Dry weight of macrophytes per area of sediment and species present
Bulk density of dry bottom material as a function of depth
Organic matter content of sediment as a function of depth
Porosity in sediment as a function of depth
Bioturbation - if possible
pH variation with time
Temperature variation with time
Light intensity variation with time
Chlorophyll concentration in the water

Redox conditions in the sediment (if possible)

<u>Hydrology</u>
Flow velocity or discharge as a function of time
Water height as a function of time
(Longitudinal) dispersion coefficient.

<u>Pesticide</u>
Compound entering surface water
Pesticide concentration in incoming water flow
Entry routes with corresponding
    . pesticide concentrations or loads
    . location(s) of entry
    . time and duration of entry
    . volumes of incoming water;
these can include spray drift, surface runoff, drainage, groundwater flow and atmospheric deposition

Sorption isotherm for sorption to suspended solids
Sorption isotherm for sorption to sediment (site-specific)
Sorption isotherm for sorption to macrophytes
Transformation rate constant for the water column (differentiated for biodegradation, hydrolysis and photolysis as a function of temperature, pH and light intensity)
Transformation rate constant for the (site-specific) sediment (differentiated for biodegradation and hydrolysis as a function of pH, redox-conditions and temperature - if possible)
Volatilisation - if possible.

Output data needed for validating surface water models

Discharge and water height as a function of time (if these were not model input)
Mass concentration in water column as a function of time and space
Pesticide content of suspended solids (if considered relevant)
Pesticide content of macrophytes as a function of time (and if relevant space)
Mass concentration in sediment as a function of depth and time and location in water course.

8. CONCLUSIONS AND RECOMMENDATIONS

The need for prediction of environmental concentrations in surface water and sediment with time following initial exposure of these compartments to plant protection products is an implicit requirement of the EU registration directive (Anon., 1991). Models which predict the amount of pesticide entering surface waters (via drift, run-off, drainage or atmospheric deposition) as well as their subsequent fate within the water and associated sediment compartments clearly have an important and increasing role in ecological risk assessment within the pesticide registration process. Relevant (time weighted) PEC values need to be compared with short and long term toxicity values (EC_{50} and NOEC) for fish, aquatic invertebrates (e.g. Daphnia) and aquatic plants (e.g. algae).

To date no one model predicts the amount of a plant protection product entering surface water and sediment via all entry routes and the fate of the pesticide within these compartments. Therefore in order to predict environmental concentrations for comparison with aquatic toxicity values there is sometimes a need to use more than one model. A phased approach (see Figure 1) is recommended starting with simple calculations and developing into more comprehensive and complex modelling. However a more comprehensive approach can always be substituted for a simpler approach.

Because of the potential combination of models (e.g. a model predicting inputs to surface water from drains together with a model of the fate of the plant protection product in the surface water itself) evaluations may consist of a simple but conservative over-estimation of loading coupled with a more complex assessment of fate in surface water using a suitable mechanistic model.

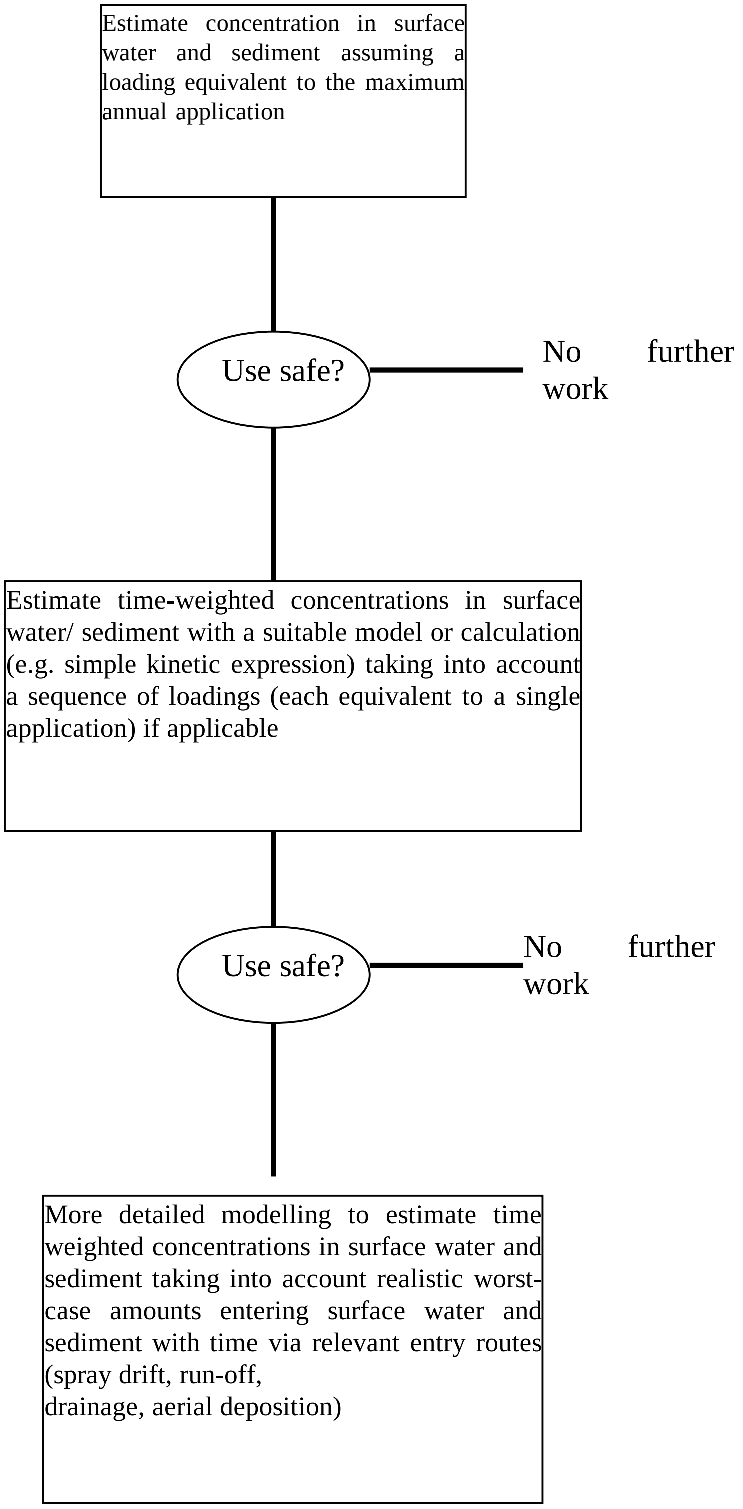
This report has reviewed models which attempt to estimate the inputs of pesticides to surface waters as a result of spray drift, run-off and drainage from fields and from atmospheric deposition and to estimate the fate of pesticides in surface water. However if no concern as to the use of a particular plant protection product exists (i.e. acceptable toxicity exposure ratios) with an assumption that 100% of the maximum annual loading to the normal site of application were to reach a body of water then no model calculations of inputs (loadings) are necessary.

In many cases this will not be the position and some estimate of realistic loadings and fate within surface water will need to be made in order to predict (time-weighted) concentrations for comparison with relevant short- and long-term toxicity assessments.

8.1 Spray drift

In many cases spray drift is the most important component of the total loading of pesticides to surface waters. Its occurrence is not a function of soil type and pesticide properties (unlike drainage and run-off) and spray drift events are often the most likely source of acute effects on non-target organisms.

Figure 12. Stepwise procedure for predicting environmental concentrations in surface water and sediment.



The tables based upon experimental data (e.g. German drift tables of Ganzelmeier (1993) and interpolated in the simple model PSMDRIFT) are recommended for estimates of spray drift with distance from surface water.

However as stated in Chapter 5.1 it is important to note that no table of drift values which consider the weather conditions in Southern European Countries are available. This group recommends that either such data are generated or that current or developing spray drift models be expanded or adapted and validated to enable them to be used for extrapolation to the wide range of agro-environmental situations existing within the European Community.

8.2 Drainage

The loading of pesticides to surface water via drains should be considered when the use and type of pesticide indicate that contamination via this route is likely:

- Compounds applied to drained soils
- Products applied just before or whilst drains are flowing to surface water (i.e. autumn/winter).
- Persistent compounds applied in late spring and summer.
- Weakly adsorbed compounds with high water solubility.

Due to the complex nature of the processes involved in the transport of solutes via drains a more complex model (PESTLA, CRACK_P or MACRO) is recommended where initial assessments indicate that concentrations in surface water as a consequence of drainage are of concern. The model MACRO is considered the most generally applicable model to a wide range of soil types. Also the version MACRO D_B contains a series of databases and estimation routines which can be used to parameterise many of the inputs from simple physical properties of the soil.

Validation tests with the models MACRO and CRACK_P have resulted in predicted concentrations in drainflow to within one order of magnitude, and total loadings within a factor of two. The group recommends continuing validation at a community level. In order to place the contribution of contamination of surface waters by pesticides as a result of drainage throughout European Community in context, the development of an appropriate database of soil types, crops and climate is needed. This will enable assessments to be made where the distribution of ‘realistic worst case scenarios’ (if any) following use of a plant protection product can be established.

8.3 Runoff

The loading of pesticides to surface water as a result of surface run-off (dissolved in water and adsorbed to sediment) should be considered when the use and type of pesticide indicate that contamination via this route is likely:

- Compounds applied to soils vulnerable to run-off events (e.g. silty soils).

- Persistent compounds.
- Compounds applied at times when typical climatic conditions indicate high probability of run-off events (e.g. increased occurrence of storms or excess winter rain).

Alternatively a simple assumption of the percentage run-off from a field based on expert judgement can be made if some justification for the value chosen can be given. If levels of concern are not exceeded then further modelling is not necessary.

All existing models for prediction of losses of water (run-off) and sediment (erosion) use the common foundations of run-off curve numbers (RCN) and the modified universal soil loss equation (MUSCLE). However the validity of the curve numbers (developed by US Department of Agriculture) to accurately represent climatic and agronomic conditions within the EU is uncertain. It is strongly recommended that validation of the run-off curve number approach at the community level is urgently addressed.

Whilst taking into account the above , as stated in Chapter 5.3, on the basis of history and breadth of usage GLEAMS, PRZM and PELMO appear to be the most suitable models to be used in providing ‘edge of field’ concentrations of pesticides in run-off water and eroded sediment.

The predicted concentrations at the edge of field are extremely dependent upon the choice of a number of key soil and climatic factors including run-off curve numbers, intensity of rainfall and slope. Therefore in order to develop typical scenarios for run-off within the EU and subsequently assess the distribution of ‘realistic worst case scenarios’ (if any) following use of a plant protection product the development of an appropriate database of soil types, topography, crops and climate is needed. In the meantime, recommendations for the selection of modelling scenarios relevant to run-off simulations are given in Chapter 4.3.

8.4 Surface water fate

The need for surface water fate model calculations can be eliminated if the initial concentration equivalent to the maximum annual application rate is below the level of concern.

Where this is not the case then simple calculations of loss from the water column and associated sediment at least are needed. Models such as ABIWAS and SLOOT.BOX can be used for calculating PEC’s in surface water. If the time weighted PEC values for a static body of water are below the level of concern then no further assessments are needed. However if PEC values are also required for flowing water (e.g. ditches and streams) then one of three models are recommended (EXAMS, WASP and TOXSWA).

Surface water fate models have, in general, a low validation status. This group recommends as a matter of urgency that the validation of these models is fully supported and other projects initiated to extend validation status to other models and different agro-environmental situations.

The type of surface water surrounding European agricultural locations varies widely from almost static ponds, to drainage ditches and canals to fast flowing shallow, headwater streams. In order to calculate PEC's with a degree of harmonisation, the definition of standard scenarios, based on data of the typical aquatic environments in close proximity to agricultural land is needed.

8.5 Main recommendations of the working group

- It is strongly recommended that validation of the run-off curve number approach at the community level is urgently addressed.

- In order to develop typical scenarios for surface water fate modelling including inputs from drainage and run-off within the EU and to subsequently assess the distribution of 'worst case scenarios' following use of a plant protection product the development of appropriate EU databases of aquatic environments adjacent to agricultural land, soil types, topography, crops and climate is needed.

- This group recommends that the validation of promising models is fully supported and other projects initiated to extend validation status to other models and different agro-environmental situations.

- The group recommends continuing validation of drainage models at the European community level.

- This group recommends that either spray drift data are generated in southern European countries or that current or developing spray drift models be expanded or adapted and validated to enable them to be used for extrapolation to the wide range of agro-environmental situations existing within the European Community.

- Whilst standard scenarios are not available for the assessment of PEC's in surface water and sediment, it is recommended that all model calculations make careful and reasoned consideration of the definition of the scenario(s). Justification for all selections must be made.

- Standard scenarios for the European Union should be developed.

- Because there is no model available describing all the input routes and the fate in surface water, it is recommended that such a model should be developed. An important part of the model development should be the validation of the model. It is therefore important to work already on a dataset to be used for the validation by detailing existing datasets and/or start monitoring programmes suitable for validation purposes.

References

Anonymous (1991) “Council Directive of 15th July 1991 concerning the placing of plant protection products on the market (91/414/EEC)”, Official Journal of the European Communities, No L 230, pp. 1-32.

Ganzelmeier (1995) “Studies on the spray drift of plant protection products, Mitteilungen aus der Biologischen Bundestanstalt für Land-. und Forstwirtschaft, Berlin, Heft 305.

ANNEX 1 Spray Drift Models

1a. IDEFICS

1a.1. General information

Name of model:
*IDEFICS (**I**MAG program for **D**rift **E**valuation from **F**ield Sprayers by **C**omputer **S**imulation)*

Major aim of the model:
Simulation of spray drift from conventional boom sprayers in cross wind

Most recent release:
No public release planned

Intended use of the model:
computations on demand; for internal use only

Model developers:
H.J. Holterman

Sponsoring institution:
Ministry of Agriculture, Nature and Fisheries

Date of most recent release:
version 2.5, March 1995

1a.2. Documentation and systems considerations

1a.2.1 User manual

Availability:
for internal use only

Language:
Dutch (in preparation)

1a.2.2 Other documentation

Kind of documentation:
extensive report (in preparation)

Conceptual model description:
included

Mathematical model description:
extensive description included

Sensitivity analysis:
included

Assistance in determining model parameters:
included

Text examples:
included

References:
included

Source code availability:
not available

1a.2.3 System considerations:

Hardware requirements:
PC 386 (or higher); co-processor required; MS-DOS

Run time for standard scenario:
10 hours (486DX2/66MHz); strongly dependent on input parameters

Reliability:
no problems known

Clarity of error messages:
good

1a.2.4 Support

Method of support:
(irrelevant)

1a.2.5 Model input / pre-processor

User friendliness:
menu oriented input of parameters

On-line help utility:
not available

Data range checking:
yes

On-line standard scenario:
not available (default parameter setting)

Flexibility:
wide flexibility

1a.2.6 Output / post-processor

Nature of output:
various tables

Data processing:
additional programs (tools) to process data tables into graphs; standard Lotus worksheets

Flexibility:
various output tables on request

Documents input parameters:
yes

Clarity of output reports:
good

1a.3. Model science

1a.3.1 Model philosophy

3D random-walk model, locally 2D. Computation of droplet path through air, starting from the (moving) nozzle outlet until droplet reaches ground or downwind boundary. Final position is recorded. Droplet path is affected by gravity, wind, turbulence, evaporation, driving speed. A large number of drops per nozzle must be simulated. Standard output: tabulated cumulative deposits. Optional: table of final position of each drop.

1a.3.2 Compartments considered

1a.3.3 Input parameters

Conceptual parameters:
Geometric parameters:
crop height, ditch geometry

Application related parameters:
driving speed, boom height above the crop, nozzle position, nozzle type, top angle of spray cone, drop size distribution, liquid pressure;

Atmospheric parameters:
mean wind speed, turbulence intensity, atmospheric stability, air temperature, relative humidity;

Numerical parameters:
number of drops per nozzle, time step limitation, resolution of ground deposits
frequency of application:

1a.3.4 Numerical technique

Basic algorithm:
numerical estimate of droplet trajectories.

Stability:
no problems known

1a.3.5 Air module

Local turbulences:
included

Atmospheric stability:
including unstable - neutral - stable

Wind speed and direction:
wind speed is input parameter; wind direction: cross wind

Temperature and humidity:
input parameters

1a.3.6 Application equipment

Drop size distribution:
mono-sized, or array of 50 classes according to drop diameter (directly obtained from actual measurement)

Liquid pressure:
input parameter

Driving speed and direction:
driving speed is input parameter; direction parallel to edge of crop (perpendicular to mean wind direction) or optionally perpendicular to edge of crop (upwind).

Local turbulence due to equipment:
not considered

Initial drop speed and direction:
depending on liquid pressure and nozzle type

Interactions between drops:
entrained air phenomenon considered empirically

1a.3.7 Pesticide module

Concentration of pesticide in spray liquid:
input parameter

Volatilization:
evaporation of water from drops during their flight (solid-core assumption); pesticide itself considered involatile during the time of application.

1a.3.8 Crop module

Crop height:
input parameter

Geometry of agricultural field:
crop height and ditch geometry

Interception:
crop penetration dependent on drop size

1b. MOPED

1b.1. General information

Name of model
__MO__del for __P__esticide __D__rift

Name or number of most recent release
Oct 1993, English version of the user shell in preparation.

Intended use of model
Model simulates the spray drift of pesticide in major crops during application

Model developers
M. Klein

Sponsoring institution
Umweltbundesamt Berlin

Date of most recent release:
Version 2.0 Oct 1993

1b.2. Documentation and Systems considerations

1b.2.1 User manual

Availability
User manual available at the Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, D-57392 Schmallenberg.

Language
Available languages: German (English manual in preparation)

Clarity
good

Model limitations
Model assumptions are described

Includes conceptual model description
Yes

Includes mathematical model description
yes, but not very detailed

Includes sensitivity analysis
No

Provides assistance in determining model parameters
No

Provides test examples
Yes

Provides references
Yes

1b.2.2 Other documentation considerations

Tightness of version control
Only one version exists, no further development planned

Availability of source code
Available on request

1b.2.3 System considerations

Hardware requirements
PC with MS-DOS

Run time for standard scenario
not more than one minute (386 DX, 25 MHz)

Reliability
no problems known

Clarity of error messages
no error messages

1b.2.4 Support

Method of support
provided by M. Klein (Fraunhofer-Institut, D-57392 Schmallenberg)

Availability of information about bugs, corrections, and new versions
no information is systematically distributed

Training for users
Available on request

1b.2.5 Model Input/Pre-processor

User friendliness
very good (menu oriented shell)

Help utility
Information on function keys available

Data range checking
No

Availability of standard scenarios
Yes, standard data for some crops given

Availability of needed data
Data are readily available.

Flexibility
Limited flexibility

1b.2.6 Output/Post-processor

Nature of output
Tables and graphic

User friendliness
Very good (menu oriented shell)

Help utility
Information on function keys available

Sample files
Provided together with the programme on floppy

Flexibility
No flexibility

Documents input parameters
Yes

Clarity of output reports
good (but at present only in German language)

1b.3. Model science

1b.3.1 Model philosophy

Box type model, Moving point source (spraying system) ist modelled by a non-moving line source parallel to the driving lane and perpendicular to the direction of wind velocity. The deposition rate which linearly increases with increasing atmospheric concentration is calculated by summing up the depositions caused by spraying in different lanes.

*1b.*3.2 Compartments considered

Multi compartment model
(air compartments with fixed height of 0.5 m and length of 1 m)

1b.3.3 Input

Entry routes and application
Model only needs the rate of application.

Frequency of application
not possible to consider

1b.3.4 Numerical technique

Adequacy of algorithm
calculation of concentrations in the air and deposition to the surface is performed numerically.

Stability
no problems known

1b.3.5 Air Module

Local turbolences or variation in wind velocity
Not considered.

variation of windspeed and direction of wind speed
not considered

Temperature and Air moisture during spraying
not considered

1b.3.6 Spraying system

droplet spectrum of the nozzle
eight classes of droplets according to their diameter can be considered

nozzle pressure
not considered

velocity of spraying equipment in the field
not considered

Local turbolences because of the spraying equipment
not considered

1b.3.7 Pesticide module

Volatilization
not considered

1b.3.8 Crop module

Height of the crop
considered

Geometrie of the agricultural field
roughly considered, the model needs the distance between to crop rows

Interception
considered by an overall factor considering also the leaf stage

1c. <u>PEDRIMO</u>

1c.1. General information

Name of the model:
*PEDRIMO (**Pe**sticide **dr**ift **mo**del)*

Major aim of the model:
Simulation of spray drift (sediment and loss to the air) for field sprayers and aircrafts

Most recent release:
*For aircrafts: Nachrichtenbl. Deut. Pflanzenschutzd., **47** (2), S 36-49, 1995*
*Public release for field sprayers is planned in „Nachrichtenbl. Deut. Pflanzenschutzd., **48** (1), 1996“*

Intended use of the model:
Comparison of plant protection equipments for assessment of drift potential; Assessment of weather conditions and technological parameters in its influence on drift

Model developers:
P. Kaul, S. Gebauer, R. Neukampf

Sponsoring Institution:
BBA

Date of most recent release:
June 1995

1c.2. Documentation and systems considerations

1c.2.1 User manual

Availability:
Not necessary, the program explains itself

Language:
English

1c.2.2 Other documentation

Kind of documentation:
Only above mentioned publications

Mathematical model description:
included

Sensitivity analysis:
included

Assistance in determining model parameters:
included in the programme

Test examples:
Examples for calculations are part of the publications, they can used as test examples.

References:
included

Source code available:
not available

Validation in comparison with field experiments
included

1c.2.3 System considerations

Hardware requirements:
PC 386; co-processor; MS DOS; printer

Run time for standard scenario:
aircraft: about 5 minutes; field sprayer: about 10 minutes. It depends on input parameters.

Reliabilities:
no problems

Clarity of error messages:
A lot of error messages are included.

1c.2.4 Support

Method of support:
Windows technics; Turbo Pascal

1c.2.5 Model input / pre-processor

User friendliness:
menu and windows-technics oriented input and output

On-line help utility:
not necessary

Data range checking:
included

On-line standard scenarios:
not available

Flexibility:
parameter like in reality

1c.2.6 Output / post-processors

Nature of output:
in connection with calculations: tables of results
output in menu: tables and graphs
by using Windows: printing of input and output in tables and graphs

Data processing:
Words and Paintbrush (under Windows) for printing

Flexibility:
up to 4 calculations can be shown in 1 table and 1 graph

Documents input parameters:
yes

Clarity of output reports:
table and graph with all of parameters

1c.3 Model science

1c.3.1 Model philosophy

The simulation model PREDIMO is based on systems of equations describing drop evaporation, drop movement and the spread of contaminated air clouds. It describes the way of drift of the droplet clouds formed under the sprayer boom and in the wake of the sprayer vehicle / around the wings of the aircraft. The outputs are the amounts of chemicals which settle on areas neighbouring the treated one and those which remain suspended in the air.

1c.3.2 Input parameters

Conceptual parameters:

Geometric parameters:
height of vehicle, working wide, space between the nozzles (field machines), wing wide (aircrafts), crop height

Application related parameters:
height of application above crops, moving speed, droplet size distribution

Atmospheric parameters:
wind speed, atmospheric stability, air temperature, relative humidity or wet bulb temperature

Numerical parameters:
time step in dependence of actual droplet diameter

Frequency of application

1c.3.3 Numerical technique

Basic algorithm:
step by step calculation for droplet diameter, droplet movement and evaporation, cloud concentration and expansion, superposition of sediment and evaporated amount

Stability:
problems became solved by finding a dependence of time steps and droplet diameter, so calculations are fast and stable

1c.3.4 Air module

Local turbulences:
included for the wake behind the sprayer vehicle

Atmospheric stability:
including unstable, stable and neutral

Wind speed and direction:
input parameter and cross wind

Temperature and humidity:
input parameters

1c.3.5 Application equipment

Drop size distribution:
like measured for the used nozzles, some nozzles from fine to coarse are offered (mean diameter and other informations are given)

Liquid pressure:
is not used, is not relevant for describing the physicle process

Driving speed and direction:
moving speed is an input parameter, direction is cross wind

Local turbulence due to equipment:
considered

Initial drop speed and direction:
it can be considered in the expansion of the starting cloud
it is the same with air assistence

Interaction between droplets:
not considered

1c.3.7 Pesticide module

Concentration of pesticide in spray liquid:
Calculation is done for water or oil. Influence of pesticides concentration on evaporation of droplets are not considered. Because results are given in percent of applied amount (water or chemical) this parameter is not relevant.

Volatilization:
considered for water droplets in air

1c.3.8 Crop module

Crop height:
input parameter

Geometry of agricultural field:

Interception:
not considered

ANNEX 2 Drainage models

2a. MACRO

2a.1. General Information

Name of model

MACRO

Name or number of most recent release

Version 3.2. Database version (MACRO_DB) to be released in 1996.

Intended use of model

MACRO was designed to predict the fate and mobility of pesticides in a wide range of soil types, including structured soils. The program can calculate fluxes to groundwater and to surface waters via field drains.

Model developer

Nicholas Jarvis
Department of Soil Sciences
Swedish University of Agricultural Sciences (SLU)
Box 7014
750 07 Uppsala
Sweden

Sponsoring institution

Swedish Environmental Protection Agency for versions up to and including 3.1.
SLU for version 3.2
Swedish Chemicals Inspectorate, SLU and Soil Survey and Land Research Centre (U.K.) for upcoming database version (MACRO_DB).

Date of most recent release

February 1996.

2a.2. Documentation and system considerations

2a.2.1 Users manual

Availability

A technical description of the model is freely available (distributed with the model). Brief installation and start-up instructions are also supplied.

Jarvis, N.J. 1994. The MACRO Model (Version 3.1). Technical Description and Sample Simulations. Reports and Dissertations no. 19, Dept. Soil Sciences, Swedish University of Agricultural Sciences, Uppsala, Sweden, 51 pp.

Language

English.

Clarity

Good, but rather technical for management applications.

Defines model limitations

Model assumptions are given.

Includes conceptual model description

Yes.

Includes mathematical model description

Yes.

Includes sensitivity analysis

No, but included in an earlier report describing version 3.0 of the model.

Jarvis, N.J. 1991. MACRO - A model of water movement and solute transport in macroporous soils. Reports and Dissertations no. 9, Dept. Soil Sciences, Swedish University of Agricultural Sciences, Uppsala, Sweden, 58 pp.

Provides assistance in determining model parameterS

Some discussion included in earlier report describing version 3.0 (see above).

Provides test examples

Hypothetical test data sets are supplied with the model.

Provides references

Yes.

2a.2.2 Other documentation considerations

Tightness of version control

Tight version control by author.

Availability of source code

Program is normally distributed as executable file. Source code supplied on request, but only by special agreement for approved purposes.

2a.2.3 System considerations

Hardware requirements

IBM-PC compatible computer, preferably 486 processor (or 386 with math co-processor), 550 K free memory, c. 2 MB hard disk space.

Run-time for standard scenario

On a 486 machine (66 MHz), c. 5-10 mins. per year, strongly depending on the layer thicknesses chosen.

Reliability

Very high.

Clarity of error messages
Not applicable (system highly unlikely to crash).

Operating system
MS-DOS

2a.2.4 Support

Method of support
Through contacting author.

Availability of information about bugs, corrections, and new versions
Information is distributed by the author, as and when necessary, through an estabilished mailing list.

Training for users
No regularly scheduled training specifically in using MACRO, although a bi-annual post-graduate modelling course (which includes some aspects of MACRO) is held at Uppsala.

2a.2.5 Input/Preprocessor

User-friendliness
High.

Help utility
Included in system. On-line help is included for all user options, model parameters and outputs.

Data range checking
Yes. Warnings and errors are given when unreasonable parameter values are chosen.

Sample input files
Yes. Supplied with model.

Database included
No.

Availability of needed data
`Difficult' parameters must be estimated using pedo-transfer functions, or else default values supplied with the model can be used.

Flexibility
Very flexible, due to user options or `switches'.

2a.2.6 Output/Postprocessor

Nature of output
Outputs are selected by the user from a choice of over 200 variables. Two files are produced - a summary file with options/parameter values and a file which is used as input to a supplied graphics program (PG).

User-friendliness
High.

Help utility
Yes.

Sample files
Can be produced from sample input files supplied with model.

Flexibility
High.

Documents input parameters
Yes, in summary file.

Clarity of output reports
Good.

2a.3. Model science

2a.3.1 Compartments considered

Plant surfaces, soil unsaturated and saturated zones. Two-region model with micropores and macropores.

2a.3.2 Input

Input routes
Spray to soil surface, or incorporated on day 1 of simulation.

Application
Single or multiple applications (of one compound), pulsed.

2a.3.3 Numerical technique

Types of algorithm
Explicit finite difference in micropore domain, implicit elimination technique in macropores.

Definition of lower hydrologic boundary condition

Set by user. Choice of five possibilities.

Stability
Always stable.

Numerical dispersion
Corrected.

Time increments
Variable, but maximum 1 hour. Set automatically internally.

Space increments
Set by user, with a maximum of 15 layers.

Verification of numerical technique

Yes. For water flow, by comparison with another estabilished numerical model (SOIL). For solute, by comparison with analytical solutions.

2a.3.4 Hydrology model

Unsaturated water flow

Richards' equation in micropores. Capacitance approach in macropores.

Drain flow

Seepage potential theory. Drain flow treated as a sink term to vertical water flow (quasi-2D approach).

Runoff and erosion

Runoff is considered, but only as a means to remove excess water at the soil surface. Not recommended for predictive use (no dependence on slope or topography).

Evapotranspiration

Either meteorological variables or potential evapotranspiration can be used as driving data. Actual evapotranspiration calculated as a function of the root distribution (assumed logarithmic with depth) and soil water content.

Preferential flow

Considered (two-region model with macropores).

2a.3.5 Solute transport

Unsaturated zone

Convection-dispersion equation in micropores with dispersivity set by user. Mass flow only in macropores.

Saturated zone

Solute loss to drains calculated assuming mass flow only and complete mixing in the horizontal dimensions in each pore region.

2a.3.6 Sorption

Type of model

Linear isotherm, instantaneous reversible equilibrium, in each pore region. Sorption sites partitioned between macro- and micropores.

Dependency on environmental parameters

Set by user for each layer.

2a.3.7 Degradation

Metabolites

Only one chemical considered in version 3.2. Possibility to simulate parent compound and single metabolite will be included in version 4.

Type of mode
First-order kinetics.

Dependency on environmental parameters
Rate constants are corrected for temperature and water content effects using a modified Arrhenius equation and an empirical response function respectively. Soil temperatures are calculated from air temperatures using the heat conduction equation.

Mechanisms considered
Only one mechanism considered (i.e. lumped degradation rate constant).

Compartments considered
Rate constants specified for four compartments (micropores, macropores, solid/liquid phases).

2a.3.8 Other transformations/losses

Volatility
Not considered.

Plant uptake
Passive uptake in transpiration stream, with `exclusion factor'.

Degradation on plant surfaces
Considered (first-order kinetics).

Foliar washoff
Considered.

Runoff and erosion
Only runoff is considered. Loss is calculated from the equilibrium solution concentration in a surface layer using a `mixing depth' approach. However, it is not recommended to use MACRO for this purpose, since runoff is not dependent on slope or topography and erosion is not considered.

2b. OPUS

2b.1. General Information

Name of model
OPUS

Name or number of most recent release
Version 1.63

Intended use of model
OPUS was designed to predict the field-scale movement of material (including pesticides) in soil and surface water, and the potential pollution risk from agricultural management practice

Model developer
Roger Smith
U.S.D.A - A.R.S.
Water Management Research Unit
AERC CSU
Fort Collins, CO 80523
U.S.A.

Sponsoring institution
See author's address above.

Date of most recent release
May 1995.

2b.2. Documentation and system considerations

2b.2.1 Users manual

Availability
Both a technical description of the model and manual are freely available (distributed with the model).

Smith, R.E. 1992. OPUS, An integrated simulation model for transport of non-point source pollutants at the field-scale, Volume I, Documentation, ARS-98, 120 pp.

Ferreira, V.A. and Smith, R.E. 1992. OPUS, An integrated simulation model for transport of non-point source pollutants at the field-scale, Volume II, User manual, ARS-98, 200 pp.

Language
English.
Clarity
Generally good, but some sections of model description for pesticides lack detail.

Defines model limitations
Model assumptions are given and some limitations briefly discussed.
Includes sensitivity analysis
No, but has been published separately.

Smith, R.E. 1993. `Simulation experiments on the role of soil hydraulic characteristics in agro-ecosystems'. Modeling Geo-Biosphere Processes, 2, 1-14.

Provides assistance in determining model parameters
Yes.

Provides test examples
Yes.

Provides references
Yes.

2b.2.2 Other documentation considerations

Tightness of version control
So far, only one minor update of first version.

Availability of source code
Program is distributed as executable file. Source code is available on request.

2b.2.3 System considerations

Hardware requirements
IBM-PC compatible 386DX or better, with math co-processor.

Run-time for standard scenario
c. 1 minute per year of simulation on 50 MHz 486 DX, running all options (= slowest), 16 seconds per year on 90 MHz Pentium.

Reliability
Good.

Clarity of error messages
Only for input data screening.

Operating system
MS-DOS

2b.2.4 Support

Method of support
Through contacting author.

Availability of information about bugs, corrections, and new versions
Information is distributed by the author, as and when necessary.

Training for users
None available.

2b.2.5 Input/Preprocessor

User-friendliness
Moderate/Low.

Help utility
None.

Data range checking
Yes.

Sample input files
Yes. Supplied with model.

Database included
Some parameter values suggested in users manual.

Availability of needed data
`Difficult' parameters can be estimated using in-built pedo-transfer functions, or default values can be internally calculated.

Flexibility
High. Wide range of user options.

2b.2.6 Output/Postprocessor

Nature of output
Outputs are ASCII-files. Level of detail selected by the user.

User-friendliness
Moderate.

Help utility
No.

Sample files
Yes, can also be produced from sample input files supplied with model.

Flexibility
High. A range of options is available. A graphical run-time display version is available from the author on request.

Documents input parameters
Yes.

Clarity of output reports
Good.

2b.3. Model science

2b.3.1 Compartments considered

Plant surfaces, soil unsaturated and saturated zones, soil surface.

2b.3.2 Input

Input routes

Spray either to crop or soil surface, or injected into the soil.

Application

Single or multiple applications of up to 10 different compounds.

2b.3.3 Numerical technique

Types of algorithm

Implicit finite difference.

Definition of lower hydrologic boundary condition

Either elastic head boundary if water tables are deep, or water table boundary controlled by drainage tiles.

Stability

Always stable.

Numerical dispersion

Yes. Solute transport is by mass flow only.

Time increments

Variable, but maximum 1 day. Set automatically internally.

Space increments

Set internally, considering soil horizon boundaries given by user. Maximum of 20 layers.

Verification of numerical technique

Not known.

2b.3.4 Hydrology model

Unsaturated water flow

Richards' equation for redistribution of water. For each rainfall event, approximate wetting profiles are calculated from infiltrated amount and antecedent water contents.

Drain flow

Hooghoudt's equation. Drain flow treated as a sink term to vertical water flow (quasi-2D approach).

Runoff and erosion

With only daily rainfall data, runoff is estimated from the SCS curve number method and erosion is calculated with the modified USLE. If detailed rainfall intensity data is available, runoff and erosion are calculated using physically-based approaches.

Evapotranspiration

Potential evapotranspiration calculated from radiation and temperature using a simplified Penman equation. Actual evapotranspiration also depends on *plant cover, leaf area and mulch cover, but apparently not on soil water status.*

Preferential flow
Not considered.

2b.3.5 Solute transport

Unsaturated zone
Mass flow only (i.e. dispersion not explicitly modelled). Numerical dispersion included.

Saturated zone
Solute loss to drains calculated assuming mass flow only, pesticide originating from soil layer at drain depth, and complete mixing in the horizontal dimensions.

2b.3.6 Sorption

Type of model

Linear isotherm, with choice of instantaneous equilibrium or kinetic sorption.
Dependency on environmental parameters
Assumed directly proportional to organic carbon.

2b.3.7 Degradation

Metabolites
Not considered.

Type of model
First-order kinetics.

Dependency on environmental parameters
Rate constants are corrected for temperature and water content effects using the Arrhenius equation and an empirical water response function (Walker's approach). Soil temperatures are calculated from air temperatures using the heat conduction equation, and also allowing for heat convection with flowing water.

Mechanisms considered
Only one mechanism considered (i.e. lumped degradation rate constant).

Compartments considered
Lumped rate constant for each soil layer. Unclear how rate constants vary with depth in the soil.

2b.3.8 Other transformations/losses

Volatility
Not considered.

Plant uptake

Not considered.

Degradation on plant surfaces

Yes. First-order kinetics assumed.

Foliar washoff

Considered.

Runoff and erosion

Concentrations in runoff and eroded material calculated from the known solution and sorbed concentrations in a surface layer using the `mixing depth' approach.

2c. **CRACK-P**

2c.1. General Information

Name of model
CRACK_P

Name or number of most recent release
Version 1.0

Intended use of model
CRACK_P is designed to predict the movement of pesticides in cracking clay soils. The program is primarily intended for calculating fluxes to surface waters via field drains.

Model developer
Adrian Armstrong/Andrew Portwood
ADAS Land Research Centre
Gleadthorpe, Meden Vale
Mansfield, Notts. NG20 9PF
U.K.

Peter Leeds-Harrison
Silsoe College, Cranfield University
Dept. Agricultural Water Management, Silsoe Campus
Silsoe, Bedford MK45 4DT
U.K.

Sponsoring institution
Ministry of Agriculture, Fisheries, Food (U.K.)

Date of most recent release
Autumn 1995.

2c.2. Documentation and system considerations

2c.2.1 Users manual

Availability
Armstrong, A.C., Matthews, A.M., Portwood, A.M. and Jarvis, N.J. 1995. (available from first author).

CRACK_P. A model to predict the movement of water and solutes from cracking clay soils. Version 1.0. Technical description and users guide.

Language
English.

Clarity
Good.

Defines model limitations
Yes.

Includes conceptual model description
Yes.

Includes mathematical model description
Yes.

Includes sensitivity analysis
No.

Provides assistance in determining model parameters
No.

Provides test examples
Yes.

Provides references
Yes.

2c.2.2 Other documentation considerations

Tightness of version control
Strict control.

Availability of source code
Program distributed as executable file, subject to agreements.

2c.2.3 System considerations

Hardware requirements
IBM-PC compatible computer, preferably 486 processor (or 386 with math co-processor).

Run-time for standard scenario
10 minutes.

Reliability
Low. Can occasionally crash. Work in progress to make program more robust.

Clarity of error messages
Low. Work in progress to improve this.

Operating system
MS-DOS

2c.2.4 Support

Method of support
Through contacting author.

Availability of information about bugs, corrections, and new versions

Not yet known.

Training for users

Not available, except by special request.

2c.2.5 Input/Preprocessor

User-friendliness

Moderate/High, via edit screens.

Help utility

None.

Data range checking

None.

Sample input files

Yes.

Database included

No.

Availability of needed data

In principle, all parameters can be independently measured. Library of reference values will be provided.

Flexibility

Low.

2c.2.6 Output/Postprocessor

Nature of output

Tabular. Graphical output can be obtained by separate post-processor program.

User-friendliness

Low.

Help utility

No.

Sample files

Yes.

Flexibility

Low.

Documents input parameters

Yes.

Clarity of output reports

Good.

2c.3. Model science

2c.3.1 Compartments considered

Soil unsaturated and saturated zones. Two-regions with aggregates and cracks.

2c.3.2 Input

Input routes
Spray to soil surface, or soil incorporated on day 1 of simulation.

Application
One compound, single application.

2c.3.3 Numerical technique

Types of algorithm
Explicit finite difference for diffusion in aggregates. Accounting procedure to track wetting fronts in the cracks.

Definition of lower hydrologic boundary condition
Zero percolation flux. Field drains.

Stability
May become unstable, if chosen time step is too large.

Numerical dispersion
Not known, but thought to be minimal with small time steps.

Time increments
Constant and set by user. Typically of the order of minutes.

Space increments
Set by user, with a maximum of 10 layers.

Verification of numerical technique
Not known.

2c.3.4 Hydrology model

Unsaturated water flow
Hagen-Poisseille's equation in cracks. Philips's infiltration equation for water entry into aggregates.

Drain flow
Seepage potential theory. Drain flow treated as a sink term from saturated cracks.

Runoff and erosion
Runoff is considered, but only as a means to remove excess water at the soil surface. Not recommended for predictive use (no dependence on slope or topography).

Evapotranspiration

Potential evapotranspiration input by user. Actual evapotranspiration is calculated as a function of the root distribution (assumed logarithmic with depth) and soil water content.

Preferential flow

Explicitly considered by this model : two-region model with cracks.

2c.3.5 Solute transport

Unsaturated zone

Diffusion in aggregates. Mass flow only in cracks.

Saturated zone

Solute loss to drains calculated assuming mass flow only from the cracks and complete mixing in the horizontal dimensions.

2c.3.6 Sorption

Type of model

No sorption in the cracks. Linear isotherm with instantaneous equilibrium in aggregates.

Dependency on environmental parameters

Set by user for each layer.

2c.3.7 Degradation

Metabolites

Only one chemical considered.

Type of model

First-order kinetics.

Dependency on environmental parameters

Rate constants are corrected for temperature and water content effects using the Arrhenius equation and an empirical response function (Walker's approach). Soil temperatures are calculated from air temperatures using empirical relations.

Mechanisms considered

Only one mechanism considered (i.e. lumped degradation rate constant).

Compartments considered

Aggregates only. Degradation in cracks assumed negligible.

2c.3.8 Other transformations/losses

Volatility

Not considered.

Plant uptake

Not considered.

Degradation on plant surfaces

Not considered.

Foliar washoff

Not considered.

Runoff and erosion

Although runoff is considered, it is not recommended to use CRACK_P for this purpose, since runoff is not dependent on slope or topography and erosion is not considered.

2d. CHAIN-2D

2d.1. General Information

Name of model
CHAIN_2D

Name or number of most recent release
Version 1.1 (October 1994), version 2.0 to be released in spring 1996.

Intended use of model
CHAIN_2D is designed to simulate two-dimensional variably-saturated water flow, heat transport, and the transport of solutes involved in sequential first-order decay reactions.

Model developer
Jirka Simunek/Rien van Genuchten
U.S. Salinity Laboratory, USDA-ARS
450 Big Springs Rd.
Riverside, CA 92 507
U.S.A.

Sponsoring institution

USDA-ARS

Date of most recent release

October 1995.

2d.2. Documentation and system considerations

2d.2.1 Users manual

Availability
Available on request.

Language
English.

Clarity
Good, but rather technical for management applications.

Defines model limitations
Yes.

Includes conceptual model description
Yes.

Includes mathematical model description
Yes.

Includes sensitivity analysis
No.

Provides assistance in determining model parameters
No.

Provides test examples
Yes.

Provides references
Yes.

2d.2.2 Other documentation considerations

Tightness of version control
Tight control.

Availability of source code
Available for version 1.1

2d.2.3 System considerations

Hardware requirements
Any computer capable of compiling and linking FORTRAN source code. Version 2.0 - IBM PC compatible, running MS Windows 3.1 or MS Windows 95.

Run-time for standard scenario
No standard scenario.

Reliability
Can crash for highly non-linear physical properties or for high fluxes into dry soils.

Clarity of error messages
Version 1.1 - low. Version 2.0 - high

Operating system
Version 1.1 is independent of OS. Version 2.0 requires MS Windows 3.1 or MS Windows 95.

2d.2.4 Support

Method of support
Through contacting authors.

Availability of information about bugs, corrections, and new versions
Available through authors.

Training for users
Not available except by special request.

2d.2.5 Input/Preprocessor

User-friendliness

Version 1.1 - low. Version 2.0 - high (Windows environment).

Help utility

Version 1.1 - none. Version 2.0 - online interactive help.

Data range checking

Version 1.1 - no. Version 2.0 - yes.

Sample input files

Yes.

Database included

Not in version 1.1. Small catalogue of soil hydraulic properties in v. 2.0

Availability of needed data

In principle, all parameters can be independently measured.

Flexibility

High.

2d.2.6 Output/Postprocessor

Nature of output

Tabular. Version 2.0 will provide graphical output in the form x-y graphs, contour and spectral maps, velocity vectors, as well as other features.

User-friendliness

Version 1.1 - low. Version 2.0 - high.

Help utility

Version 1.1 - none. Version 2.0 - online interactive help.

Sample files

Yes.

Flexibility

Version 1.1 - low. Version 2.0 - high.

Documents input parameters

Yes.

Clarity of output reports

Good.

2d.3. Model science

2d.3.1 Compartments considered

Unsaturated and saturated soil zones.

2d.3.2 Input

Input routes
Time dependent or independent Dirichlet, Neumann or Cauchy boundary conditions. Any time intervals are allowed.

Application
See above.

2d.3.3 Numerical technique

Types of algorithm

Finite elements for spatial distribution and implicit finite differences for temporal discretization of Richards equation for water flow. Finite elements for spatial distribution and Crank-Nicholson finite differences for temporal discretization of the convection-dispersion equation for solute transport.

Definition of lower hydrologic boundary condition
5 different options, including field drains.

Stability
May become unstable for extremely non-linear cases.

Numerical dispersion
Can be eliminated.

Time increments
Self-adjusting variable time steps optimized within the program.

Space increments
Set by user (up to many thousands of nodes).

Verification of numerical technique
Verified against analytical solutions and existing numerical models.

2d.3.4 Hydrology model

Unsaturated water flow
Richards equation.

Drain flow
Simplified representation of nodal drains using results of electrical analogue experiments.

Runoff and erosion
Not considered.

Evapotranspiration
Potential evapotranspiration is input by user. Actual evapotranspiration is calculated as a function of root distribution and soil water pressure head.

Preferential flow
Not considered.

2d.3.5 Solute transport

Unsaturated zone
Convection-dispersion-diffusion in the liquid phase, diffusion in the gaseous phase.

Saturated zone
Convection-dispersion-diffusion.

2d.3.6 Sorption

Type of model
Linear or non-linear (Freundlich or Langmuir). One or two-site (equilibrium and kinetic sites) sorption model.

Dependency on environmental parameters
Set by user. Can be dependent on temperature (Arrhenius equation).

2d.3.7 Degradation

Metabolites
Up to ten solutes involved in first-order decay reactions.

Type of model
First- and zero order kinetics.

Dependency on environmental parameters
Set by user. Can be dependent on temperature (Arrhenius equation).

Mechanisms considered
Can be considered separately for each phase (solid, liquid, gaseous).

Compartments considered
Both saturated and unsaturated soil zones.

2d.3.8 Other transformations/losses

Volatility
Considered.

Plant uptake
Considered.

Degradation on plant surfaces
Not considered.

Foliar washoff
Not considered.

Runoff and erosion
Not considered.

2e PESTLA

2e 1. General Information

Name of model
PESTLA

Name or number of most recent release
v.3.0

Intended use of model
PESTLA predicts the behaviour of pesticides in non-structured soils.

Model developer
Jos Boesten and Joop Kroes
Winand Staring Centre
P.O. Box 125
6700 AC Wageningen
Netherlands

Sponsoring institution
SC-DLO

Date of most recent release
Version 3.0 is to be released in March 1996. The drainage routines included in this version of PESTLA are taken directly from the existing TRANSOL model, also developed at the Winand Staring Centre.

2e 2. Documentation and system considerations

2e 2.1 Users manual

Availability
Not yet available. A description of the forerunner model TRANSOL is available: J.G. Kroes, "TRANSOL V. 2.3. A dynamic model for transport and transformation of solutes in soils. User's guide". Winand Staring Centre, Interne Mededeling 110 (July 1994).

Language
English.

Clarity
Not yet known.

Defines model limitations
Yes.

Includes conceptual model description
Yes.

Includes mathematical model description
Yes.

Includes sensitivity analysis
Probably not, but sensitivity analyses using earlier versions of PESTLA have been published.

Provides assistance in determining model parameters
Yes.

Provides test examples
Yes.

Provides references
Yes.

2e 2.2 Other documentation considerations

Tightness of version control
Very tight (as for the 2.3 version).

Availability of source code
Probably not for the water flow submodel, but yes for the pesticide submodel.

2e 2.3 System considerations

Hardware requirements
IBM compatible PC.

Run-time for standard scenario
A few minutes per simulated year for 486 machine.

Reliability
High.

Clarity of error messages
Low.

Operating system
MS-DOS

2e 2.4 Support

Method of support
Through contacting authors.

Availability of information about bugs, corrections, and new versions
Yes.

Training for users
No, except upon special request.

2e 2.5 Input/Preprocessor

User-friendliness
Moderate.

Help utility
None.

Data range checking
Yes.

Sample input files
Yes.

Database included
No.

Availability of needed data
All input data can be measured or estimated independently.

Flexibility
Low.

2e 2.6 Output/Postprocessor

Nature of output
Tabular. Graphical output by separate post-processor program.

User-friendliness
Low.

Help utility
No.

Sample files
Yes.

Flexibility
Low.

Documents input parameters
Yes.

Clarity of output reports
Good.

2e 3. Model science

3.1 Compartments considered

Soil unsaturated and saturated zones.

2e 3.2 Input

Input routes
Spray to soil surface, or soil incorporated.

Application
One compound, multiple application.

2e 3.3 Numerical technique

Types of algorithm
Explicit finite difference for pesticide submodel.

Definition of lower hydrologic boundary condition
6 different options.

Stability
Prevented through control of the time step.

Numerical dispersion
Minimal.

Time increments
Set by program (variable), typically 0.1 day.

Space increments
Set by user (maximum of 40 layers).

Verification of numerical technique
Yes.

2e 3.4 Hydrology model

Unsaturated water flow
Richards equation.

Drain flow
Ernst equation. Sink term to Richards' equation

Runoff and erosion
Runoff is considered, but only to remove excess water at the surface. Not recommended for predictive use.

Evapotranspiration
Potential evapotranspiration is input. Actual values calculated by the model.

Preferential flow
No.

2e 3.5 Solute transport

Unsaturated zone
Convection-dispersion equation in liquid phase, diffusion in gas phase.

Saturated zone
Concept of perfectly mixed reservoir.

2e 3.6 Sorption

Type of model
Two-site model (equilibrium and kinetic sites) using the Freundlich equation.

Dependency on environmental parameters
Set by user for each layer.

2e 3.7 Degradation

Metabolites
Yes, via sequential metabolism scheme.

Type of model
First-order kinetics.

Dependency on environmental parameters
Temperature, water content.

Mechanisms considered
Only one (lumped rate constant).

Compartments considered
Two options for each soil compartment: either total soil system or liquid phase only.

2e 3.8 Other transformations/losses

Volatility
Yes.

Plant uptake
Yes.

Degradation on plant surfaces
Not considered.

Foliar washoff
Not considered.

Runoff and erosion
Not considered.

2f. PESTRAS

2f.1. General Information

Name of model
PESTRAS

Name or number of most recent release
v.2.1

Intended use of model
PESTRAS was developed to estimate regional patterns of the vulnerability of soils to pesticide leaching and accumulation.

Model developer
A. Tiktak, A.M.A van der Linden and F.A. Swartjes
National Institute of Public Health and Environmental Protection
Antonie van Leeuwenhoeklaan 9
P.O. Box 1
3720 Bilthoven
Netherlands

Sponsoring institution
National Institute of Public Health and Environmental Protection

Date of most recent release
August 1994.

2f.2. Documentation and system considerations

2f.2.1 Users manual

Availability
A technical description of the model is available (price 30 dfl.). Brief installation and startup instructions are also supplied.

A. Tiktak, A.M.A. van der Linden and F.A. Swartjes (1994): PESTRAS: a one-dimensional model for assessing leaching and accumulation of pesticides in soil. Report no. 715501003, RIVM, Bilthoven, Netherlands, 99 pp.

Language
English.

Clarity
Good.

Defines model limitations
Model assumptions are given.

Includes conceptual model description
Yes.

Includes mathematical model description

Yes.

Includes sensitivity analysis

Yes, sensitivity of pesticide leaching and accumulation to variations in pesticide properties, soil temperature, soil water fluxes and transport parameters is discussed comprehensively (see also: A. Tiktak, F. A. Swartjes, R. Sanders and P.H.M. Janssen. 1994: Sensitivity analysis of a model for pesticide leaching and accumulation. In: J. Grasman and G. van Straten (eds.) : Predictability and non-linear modelling in natural sciences and economics. Kluwer, Dordrecht 1994, 471-484).

Provides assistance in determining model parameters

No specific assistance is given. The manual merely points out that the required input parameters can be derived from standard soil and vegetation characteristics, by transfer functions, or taken from standard databases.

Provides test examples

Yes. A realistic test example is provided which is based on the Dutch standard scenario.

Provides references

Yes.

2f.2.2 Other documentation considerations

Tightness of version control

Tight version control by authors.

Availability of source code

Yes, the program is distributed as source code and compiled by the user after installation.

2f.2.3 System considerations

Hardware requirements

Any computer platform where a FORTRAN-77 or FORTRAN-90 compiler is available. The model has currently been integrated into a GIS (ARC/INFO) environment (A.Tiktak, A.M.A. van der Linden and I.Leine 1995: Application of GIS to the modelling of pesticide leaching on a regional scale in the Netherlands. Submitted to J. Environ. Qual.).

Run-time for standard scenario

Approx. one minute for three years (PC 486DX 33 Mhz machine).

Reliability

Very high.

Clarity of error messages

User must specify a label and dimensions for input. If these are not correct, an error message is printed indicating the input line. Range checking is included where possible.

Operating system

Any computer platform where a FORTRAN-77 or FORTRAN-90 compiler is available.

2f.2.4 Support

Method of support

A help-desk is not available, but the user can ask incidental questions concerning the model through e-mail.

Availability of information about bugs, corrections, and new versions

Distributed with the floppy-disk.

Training for users

No. The manual is self-supporting. The model was developed for skilled users.

2f.2.5 Input/Preprocessor

User-friendliness

Moderate. All input is through ASCII files. Files consist of records which can be input in any order. This feature provides very flexible coupling of the model to external systems (i.e. a GIS or a package for sensitivity analysis).

Help utility

None.

Data range checking

Yes, where possible.

Sample input files

Yes.

Database included

The information system GeoPESTRAS can be obtained on request.

Availability of needed data

Most data can be obtained from standard soil characteristics using pedo-transfer functions.

Flexibility

Moderate/High. The user can either let the model simulate water and heat flow or provide data calculated with any other model.

2f.2.6 Output/Postprocessor

Nature of output

Output variables are specified by the user, as well as depth and time intervals for output. The user can choose between either a single file for all output or separate files for each sub-model. A spreadsheet interface and visualization tool are also available for output processing.

User-friendliness

High.

Help utility

A Demo and manual are available in Dutch (English translation will be available in the near future).

Sample files

Can be produced with the sample input files supplied with the model.

Flexibility

High.

Documents input parameters

Yes, if required.

Clarity of output reports

Good.

2f.3. Model science

2f.3.1 Compartments considered

Plants, soil unsaturated and saturated zones.

2f.3.2 Input

Input routes

Spray to soil surface, soil incorporated or injection.

Application

One or multiple applications of one or several pesticides.

2f.3.3 Numerical technique

Types of algorithm

Half-implicit finite difference for water flow submodel.

Implicit finite difference for heat transport.

Explicit finite difference for solute transport.

Definition of lower hydrologic boundary condition

Flux or pressure head boundary condition, either constant or varying with time.

Stability

Good, as long as the Peclet number is satisfied.

Numerical dispersion

Corrected for.

Time increments

Set by program (variable).

Space increments

Set by user (may be different for water, heat and solute flow sub-models).

Verification of numerical technique

Yes, for solute transport, by comparing to an analytical solution.

2f.3.4 Hydrology model

Unsaturated water flow

Richards equation.

Drain flow

Drainage is treated as a sink term to Richards equation in the saturated zone. The user can choose between two approaches, both of which rely on the hydraulic conductivity of the soil and an empirical parameter. Total lateral flow comprises 'fast' and 'slow' components.

Runoff and erosion

Not considered.

Evapotranspiration

Potential evapotranspiration is calculated according to Makkink's approach, modified by a crop factor. Actual values are calculated by the model, depending on interception, root density and soil water content.

Preferential flow

No.

2f.3.5 Solute transport

Unsaturated zone

Convection-dispersion equation.

Saturated zone

Convective flow only and instantaneous complete mixing in each layer.

2f.3.6 Sorption

Type of model

Freundlich equation, instantaneous and reversible.

Dependency on environmental parameters

Sorption assumed dependent on soil organic matter.

2f.3.7 Degradation

Metabolites

Yes.

Type of model

First-order kinetics.

Dependency on environmental parameters

Temperature, water content and depth.

Mechanisms considered

Only one (lumped rate constant).

Compartments considered

Total soil system only.

2f.3.8 Other transformations/losses

Volatility

Not considered in PESTRAS 2.1, but is included in the new release 3.0 that will be available at the end of 1995.

Plant uptake

Yes.

Degradation on plant surfaces

Not considered.

Foliar washoff

Not considered.

Runoff and erosion

Not considered.

2g. Other models considered but not assessed in detail

2g.1 WAVE

2g.1 1. General Information

Purpose of the model:

WAVE is an integrated mechanistic model for the description of transport and transformation of agrochemicals at the local scale in non-cracking soils.

Authors and Affiliation:

Vanclooster, M., Viaene, P., Diels, J. & Christiaens, K.
Inst. for Land and Water Management
Catholic University of Leuven
Vital Decosterstraat 102
B-3000 Leuven
Belgium

Version 2.0 of the model was released in December 1994, and includes treatment of water and nitrogen fluxes/turnover. Although the model does include treatment of drainage systems which is currently on general release. Nevertheless, a description of the pesticide version of the model is given below, since this is planned to be released in 1996 (M. Vanclooster, pers. communication).

2g.1 2. System considerations

The model runs on PC, UNIX or Macintosh machines, preferably with extended memory.

2g.1 3. Model science

2g.1 3.1 Compartments considered

Vertical soil column, divided into layers. Mobile and immobile water.

2g.1 3.2 Input

Input routes
Spray to soil surface.

Application
One compound.

2g.1 3.3 Numerical technique

Types of algorithm
Implicit finite difference.

Definition of lower hydrologic boundary condition
7 different options, including groundwater table.

Stability
Controlled by adjustment of the time step.

Numerical dispersion
Corrected for in program.

Time increments
Smaller than one day, dynamically changed in program.

Space increments
Set by user.

Verification of numerical technique
Water flow checked against quasi-analytical evaporation and infiltration models. Solute transport checked against analytical CDE.

2g.1 3.4 Hydrology model

Unsaturated water flow
Richards equation.

Drain flow
Hooghoudt equation.

Runoff and erosion
Runoff as excess to infiltration capacity, maximum ponding depth considered.

Evapotranspiration
Potential reference evapotranspiration is input.

Preferential flow
Macropore flow (by-pass flow) not considered. Preferential solute transport accounted for in the 2-region (mobile-immobile) approach. Preferential water flow in matrix can be modelled with multi-modal soil hydraulic functions.

2g.1 3.5 Solute transport

Unsaturated zone
Convection-dispersion equation, with mobile-immobile water.

Saturated zone
Convective transport to drains.

2g.1 3.6 Sorption

Type of model
Linear, equilibrium, on mobile and immobile sites.

Dependency on environmental parameters
Organic matter content.

2g.1 3.7 Degradation

Metabolites
One.

Type of model
First-order.

Dependency on environmental parameters
Temperature, humidity.

Mechanisms considered
Lumped.

Compartments considered
All soil compartments.

2g.1 3.8 Other transformations/losses

Volatility
Not considered.

Plant uptake
Not considered.

Degradation on plant surfaces
Not considered.

Foliar washoff
Not considered.

Runoff and erosion
Not considered.

2g.2. SOILFUG model Version 0.9

2g.2.1 Overview

Purpose of model:
A screening model using the fugacity concept and predominantly physico-chemical parameters to determine concentrations of pesticide in surface waters.

Authors and Affiliations:
Antonio Di Guardo
Institute of Agricultural Entomology
University of Milan
Via Celoria 2,
20133 Milan
Italy

2g.2.2 Model Algorithms

The model divides the soil into four compartments (soil air, soil water, soil organic matter, soil mineral matter) and uses the fugacity concept to partition the pesticide between them.

Degradation and volatilisation of the compound occur according to first order kinetics but there is no account taken of temperature or soil moisture effects.

The effect of rain is examined with the "rain event" concept. The total rain falling and the water leaving the system during the event are required as input data. Incident rain is added to the soil water compartment up to saturation of the soil and the partitioning recalculated. Excess water is ignored and thus there is no consideration of surface run-off. The amount of water leaving the system is then used to calculate the concentration of pesticide in the receiving water.

The model can be used at scales ranging from single drains to the catchment.

2g.2.3 Software features

Runs under Windows 3.1 on an MS-DOS system (386 computer or above). Graphical or tabular representation of the results can be obtained on screen or printed out but currently cannot be saved in the system.

Input screens are user friendly requiring only that values are entered in the dialogue boxes. A default set of parameters are provided and an extremely limited database of the required properties of pesticides is also present in the program.

2g.2.4 Availability and Support

The program is available from the author. A preliminary user-manual exists and a description of the model has been published (A. Di Guardo, D. Calamari, G. Zanin, A. Consalter and D. Mackay (1994) Env. Sci. Poll. Res. 1 (3) 151-160). However, some of the equations in this paper are stated incorrectly.

2g.2.5 Validation reported

The model has been validated using data from Rosemaund Farm, Herefordshire, UK (A. Di Guardo, R. Williams, P. Matthiessen, D. Brooke and D. Calamari (1994) Chemosphere 28 (3) 511) and from two sites in Northern Italy (A. Di Guardo, D. Calamari, G. Zanin, A. Consalter and D. Mackay (1994) Env. Sci. Poll. Res. 1 (3) 151-160). In general the model is said to overestimate the field results by a factor 10 for undissociated pesticides. However, it is less accurate for dissociated compounds.

2g.2.6 Critical Assessment

SoilFug is a relatively simple model requiring few inputs (and mostly those which are easily available). It is easy and quick to use and provides results as an average concentration over a rain event. Validations reported using 14 different pesticides in three different catchment areas (all clayey soils) indicate that the model generally overpredicts the experimental results by a factor of only ten. This would make it fairly accurate by current standards and this may be due to the effect of validating it on a large experimental area where the fluctuations that occur in the experimental data over a small area are smoothed out by the size of the catchment.

The model requires that the amount of water leaving the soil system is used as an input. This can be difficult to obtain experimentally and hence in practice a constant percentage (e.g. 60 %) of the incident rainfall is likely to be used as a default value (whichever value is used, the pesticide concentration in the drainage water does not alter since the concentration is calculated in the soil water. Hence only the total amount lost is affected). This data input removes the neccessity of obtaining a water balance for the system but has an adverse effect on the ability and flexibility of the model to be used for predictive purposes, particularly for long-term (i.e. seasonal, single or multiple year) simulations. It is also important to note that the model treats the soil compartment in a `lumped' fashion and therefore implicitly assumes very short travel times for pesticide to surface waters (effectively, always within the rain event). Therefore, SoilFug represents an `extreme worst-case' for preferential flow and should only be appropriate to those soils where preferential flow dominates input to surface waters (i.e. clay soils). This limitation of the model is not apparently recognized by the authors.

SoilFug is a useful screening model, but is not designed for dynamic (long-term) modelling of pesticide fate and behaviour.

2g.3. SWAT (Surface Water Attenuation model)

2g.3.1 Overview

Purpose of model:

A screening model used to predict the peak concentration of pesticide in all waters moving from the field into an adjacent water body. It is based on empirically derived relationships between soil characteristics and short term stream response to rainfall events, and uses attenuation factor concepts to determine the decrease in topsoil water concentrations of pesticide taking place between field application and loss in water moving from the field into surface waters.

Authors and Affiliations:
John M. Hollis and Colin D. Brown
Soil Survey and Land Research Centre,
Cranfield University
Silsoe,
BEDS.
MK45 4DT
UK

2g.3.2 Model Algorithms

All soils are grouped into a number of hydrologically distinct Runoff Potential classes based on their predicted stream response coefficients derived from empirical regression analysis using soil distributions and measured stream response in 800 catchments within Great Britain (Boorman et al 1995). Soils with the largest predicted stream response coefficients require only small amounts of rain to induce response in adjacent water bodies and vice versa.

Based on this concept, Minimum Standard Rainfall volumes are defined for each Runoff class. For each Soil Runoff Class, no water from the soil is predicted to contribute to the adjacent water body unless the minimum standard rainfall or more is recieved during a single event or daily time step.

Following pesticide application, the concentration of pesticide in the topsoil is calculated at the time of each subsequent rainfall event with a volume equal to that of the minimum standard rainfall volume for the soil under investigation.

Topsoil water concentrations are calculated using the retardation factor concept to calculate the depth penetrated during the time between pesticide application and the rainfall event and partititon and attenuation factors to account for sorption and degradation occuring during that time. Time-dependent partitioning and first order kinetics for degradation and volatilisation are assumed. There is no variation of degradation rates to take into account changes in soil temperature or moisture.

At the time of each rainfall event, rainfall infiltrates the soil, displaces and mixes with the mobile soil water fraction in the top 1mm of soil and dilutes the concentration of pesticide moving rapidly through the soil by a factor equal to the ratio of the unit volume of mobile water in the top 1mm of soil divided by the minimum standard rainfall volume.

The displaced mobile water fraction, now mixed with the minimum standard rainfall volume, is then assumed to move to surface waters, either via by-pass flow through the soil to drains, via topsoil lateral throughflow, via overland flow or by some combination of these. Calculation of the concentration of pesticide in soil water impacting upon the adjacent water body is then based upon a topsoil partition factor applied to the concentration of pesticide in the displaced soil water following dilution by the rainfall.

2g.3.3 Software features, availability and support

SWAT was developed as an MS-EXCEL spreadsheet and is not yet available as a software package. Although very easy to use, it has no customised screens or areas for data entry or graphical presentation of results. There is no user manual or support, although a full description of the model including model evaluation against field data has been published (BROWN, C.D. & HOLLIS, J.M. (1996). SWAT - A semi-empirical model to predict concentrations of pesticides entering surface waters from agricultural land. *Pesticide Science*. accepted for publication in 1995/96).

2g.3.4 Validation reported

The model has been evaluated using field data from 3 sites in the UK (Brown & Hollis, 1996). The data used for validation include fifteen individual pesticides and four different soil types with three Runoff potentials. Using literature values for the mean half lives and Koc values of the pesticides studied, the evaluation showed that the model is capable of predicting transient peak concentrations of a wide range of pesticides in water moving to streams in response to rainfall events.

Almost all the predicted concentrations were within one order of magnitude of measured values. Predicted concentrations were too great when rainfall initiated water movement to streams very soon after pesticide application, particularly for the more mobile compounds. Some predictions for very strongly sorbed pesticides were also poor.

2g.3.5 Critical Assessment

SWAT is a simple model with a novel approach to predicting peak loadings to surface water bodies from combined surface runoff and drainage following rainfall events. It is easy to use and requires few input parameters, mostly those that are easy to obtain. The most difficult parameters to obtain are the mobile water fraction, the retained water fraction and the hydraulic conductivity at 5 kPa for the topsoil. However, providing that the soil type can be identified, the model will use default values for these parameters.

The model uses empirically derived relationships linking soil characteristics with stream response and, as these have been derived at a national level, they may be less valid when applied to specific local situations. In addition, the retardation and attenuation factor concepts used in the model are relatively simple and are more applicable to laboratory rather than field conditions. Nevertheles, the evaluation undertaken shows that the model is robust and gives predictions within one order of magnitude for a variety of field conditions and pesticide characteristics. In this respect, its accuracy compares well with most other more mechanistic models dealing with soil drainage or surface runoff.

SWAT can be used in the UK with relative confidence, but care should be taken when using it for other European situations where the rainfall - stream response relationships upon which it is based may not hold true. This is particularly the case for southern European situations.

SWAT is a useful screening model that could be used to give a preliminary assessment of worst case loadings to surface water bodies from soil drainage and runoff. Because it only predicts peak concentrations impacting on water bodies, it should only be used to calculate PEC_{sw} for acute exposure.

ANNEX 3 Surface runoff models

3a. EPIC

3a.1. General Information

Name of model
Environmental Policy Integrated Climate

Name or number of most recent release
Version 3090NRCS94a

Intended use of model
Model is designed to determine the effect of field-level management alternatives on water quality at the edge of the field and the bottom of the root zone.

Model developers
J. Williams, C. Jones, P. Dyke.

Sponsoring institution
USDA Agricultural Res. Service and Texas Agricultural
Experiment Station, Temple, Texas, USA

Date of most recent release
October 1994

3a.1. 2. Documentation and systems considerations

3a.1. 2.1. User manual

Availability
Requests for copies of the model and documentation should be made to:
Bill Boyd, Environmental Engineer
Midwest National Technical Center
100 Centennial Mall North, Room 152
Lincoln, Nebraska 68508-3688 USA
voice: 402 437-5318
fax: 402 437-538

Language
English

Clarity
Good. However, the user manual and user documentation do not completely document the input editor program (UTIL), software loading, model execution, or pesticide processes.

Defines model limitations
Yes.

Includes conceptual model description
Yes.

Includes mathematical model description
A mathematical description is included.

Includes sensitivity analysis
Yes.

Provides assistance in determining model parameters
Tables are provided with typical input parameters for US scenarios.

Provides test examples\
Yes.

Provides reference
Extensive list is provided in the manual.

3a.1. 2.2. Other documentation considerations

Tightness of version control
Tight version control

Availability of source code
It is supplied on program diskette.

3a.1. 2.3. System considerations

Hardware requirements
IBM PC-AT or IBM-compatible systems. Use of an math coprocessor chip will execute programs much more rapidly.

Run time for standard scenario
low (about 50 seconds per simulated year when simulating a scenario with four basins using a 80386 machine with math coprocessor)

Reliability
Programs perform without problems if input data are correct.

Clarity of error messages
Not very specific

3a.1. 2.4. Support

Method of support
Support provided by:
Bill Boyd, Environmental Engineer
Midwest National Technical Center
100 Centennial Mall North, Room 152
Lincoln, Nebraska 68508-3688 USA
voice: 402 437-5318

fax: 402 437-5381

Availability of information about bugs, corrections and new version
No information about bugs is systematically distributed to users

Training for users
Training is occasionally available from various sources.

Contact Bill Boyd (see above).

3a.1. 2.5. Input/preprocessor

User friendliness
Parameter editor (UTIL) assists in developing input parameter files.

Help utility
Generalised help tables provided

Data range checking
Yes, if UTIL editor is used.

Sample input files
Yes

Databases included
Generalised help tables, including information on pesticide properties, are provided.

Availability of needed data
All input parameters are obtainable from soil and weather data bases. Obtaining access to such information is difficult in some countries.

Availability of standard scenarios
None

Flexibility
The wide range of options makes the program quite flexible but developing input data is somewhat daunting to occasional users. This model is more flexible, but at the same time more data intensive than most other models.

3a.2.6. Output/Postprocessor

Nature of output
Tabular

User friendliness
Minimal

Help utility
None.

Sample files
One included in user manual.

Flexibility
Somewhat flexible.

Documents input parameters
Yes.

Clarity of output reports
Good.

3a.3. Model Science

3a.3.1. Compartments considered

Plant (foliar washoff and degradation, plant uptake), soil surface (runoff and erosion), soil (soil and soil water including lateral flow), and percolation

3a.3.2. Numerical technique

Adequacy of algorithm
Not known

Definition of lower boundary conditions
A water table is simulated that can rise and fall in response to rainfall, runoff, and potential evaporation is simulated.

Stability
Stable

Numerical dispersion
Not known

Time increments
1 day

Verification of numerical technique
Not reported

3a.3.3. Input Parameters

Weatherdata
Daily precipitation, air temperature, and solar radiation data are needed. Model contains a weather generator for use with US weather sets which probably could be adapted for use in EU regions.

Soils data
Bulk density, wilting point, field capacity, sand, silt and clay content, organic carbon content, depth for each layer, albedo, minimum and maximum depth to water table.

Field management data

SCS runoff curve numbers, roughness factors, return flow travel time, USLE factors, slope length and steepness

Cropping data

Planting date, harvest date, tillage operation, maximum leaf area index.(EPIC can simulate many different tillage practices.)

Product chemistry data

Application dates, Koc, washoff fraction, foliar half-life, soil half-life, application efficiency, water solubility.

3a.3.4. Hydrology model

Spatial distribution

The surface distribution is homogenous.

Infiltration model

Storage routing capacity technique.

Evapotranspiration model

Two options are available: Priestley-Taylor and Penman equations.

Capillary rise

Where saturated conductivity for a layer is exceeded, a "back pass" is executed from that layer to the layer above.

Runoff model

Runoff volume is estimated using a modification of the USDA Soil Conservation Service curve number technique. Peak runoff rates can be calculated either by using a modification of the Rational formula. In addition, lateral subsurface flow is considered.

Preferential flow

Crack flow is considered.

3a.3.5. Erosion model

Spatial distribution

Takes into account overland flow.

Soil Erosion

Can be calculated using USLE, MUSLE, or Onstad-Foster modifications of USLE for precipitation and MUSLE for furrow irrigation scenarios. The model also contains a wind erosion submodel.

Particle transport model

Sediment transport can be simulated in channels.

Agronomy model

Includes parameters for MUSLE relative to soil erodibility and agricultural management. Many different types of tillage practices and equipment can be simulated.

3a.3.6. Pesticide model

Number of molecules considered

Metabolites
Not considered

Sorption
Linear sorption

Dependency on environmental parameters
Koc, specified along with organic carbon for each depth horizon

Type of model
First order kinetic

Dependency on environmental parameters

No correction for temperature or soil moisture content. The decay rate can vary with depth.

Mechanisms considered
Only one degradation process considered (no distinction between biotic and abiotic mechanisms).

Compartment considered
Model uses overall degradation rate in soil.

Dispersion in soil
Dispersion set by program (modelled by numerical dispersion)

Dispersion in concentrated runoff
Not considered

Volatilization
Not considered

Plant up take
Not simulated.

Degradation on plant surfaces
First order kinetic

Foliar washoff
Remaining dislodgeable residues are washed to soil based on a function of rainfall amount and user defined washoff fraction.

Runoff and erosion
Mass balance approach based on results from hydrology and erosion model. Pesticide uptake from soil to runoff is calculated by an empirical extraction coefficient. The model uses the fine particles enrichment ratio calculated by the erosion model to calculate pesticide concentration on eroded soil particles.

Agronomy models
Cultivation
Not considered for pesticide simulation unless through the partition of pesticide foliar application.

Irrigation

The program has the ability to automatically trigger irrigation due to a drop in the soil moisture content.

Pesticide application

Frequency of applications

Multiple applications throughout the simulated period can be simulated.

Application technique

Applications may be foliar sprays, applied to soil surface, or incorporated into the soil.

3a.3.7. Plant model

Foliage

Purpose

Partition of foliar application between soil and foliage, partition of evapotranspiration between evaporation and transpiration. Water,temperature and other stress effects on plant biomass and yield can be simulated.

Description

Leaf area index is used for partition of foliar application.

Flexibility

Parameters set by user

Rooting depth

Purpose

Used for hydrology and evapotranspiration model.

Description

Constant during a cropping period

Flexibility

User specifies value for each cropping period

3a.3.8. Heat model

Purpose

Soil temperatures simulated for use in nutrient cycling and hydrology but are not used for pesticide simulations

Description

Calculated from the previous days temperature, that days temperature, soil surface temperature, depth, bulk density, and a lag coefficient.

3b. GLEAMS

3b.1. General Information

Name of model
Groundwater Loading of Agricultural Management System

Name or number of most recent release
Version 2.03

Intended use of model
Model is intended to 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.

Model developers
R.A. Leonard, W.G. Knisel, D.A. Still

Sponsoring institution
USDA/ARS Southeast Watershed Laboratory, USA

Date of most recent release
January 1992

3b.2. Documentation and systems considerations

3b.2.1. User manual

Availability
It is included as a word perfect file with the source code.

Language
English

Clarity
Good

Defines model limitations
Limited discussion

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.

Includes mathematical model description
A mathematical description of the submodels is included.

Includes sensitivity analysis
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.

Provides assistance in determining model parameters
The user manual provides extensive assistance.

Provides test examples
The user manual does not provide a test example.

Provides references
Extensive list

3b.2.2. Other documentation considerations

Tightness of version control
Tight version control

Availability of source code
It is supplied on program diskette.

3b.2.3. System considerations

Hardware requirements
IBM PC-AT or IBM-compatible systems having 512K or greater RAM. Program compilation requires at least 384K of RAM, more than 384K is preferable. Use of the 8-87 Arithmetic chip will execute programs much more rapidly.

Run time for standard scenario
low (about 30 seconds per simulated year)

Reliability
Programs perform without problems if input data are correct.

Clarity of error messages
Not very specific

3b.2.4. Support

Method of support
Franck Davis, USDA and Walter Knisel, University of Georgia

Availability of information about bugs, corrections and new versions
No information about is systematically distributed to users

Errors correction and maintenance provided by
W.G. Knisel

Training for users
Training is available upon request for 8-15 participants on a fee basis from UGA- Biological and Agricultural Engineering Department at Athens or Tifton (Georgia, USA), depending upon scheduling and computer availability.

3b.2.5. Input/preprocessor

User friendliness
Parameter editor files have been developed to assist in developing input parameter files.

Help utility
Generalised help tables provided

Data range checking
Yes, if editor is used.

Sampler input files
Yes

Databases included
Generalised help tables, including information on pesticide properties, are provided to assist in developing.

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.

Availability of standard scenarios
None

Flexibility
The wide range of options makes the program quite flexible but developing input data is somewhat daunting to occasional users.

3b.2.6. Output/Postprocessor

Nature of output
Tabular

User friendliness
Minimal

Help utility
Help tables included for selecting output variables

Sample files
Yes

Flexibility
Output variables are selected individually. For a specific variable, frequency of reports can be daily, monthly, or annual.

Documents input parameters
Some of the input parameters

Clarity of output reports
Good, but there is no explanation of output reports in the manual.

3b.3. Model Science

3b.3.1. Compartments considered

Plant (foliar washoff and degradation, plant uptake), soil surface (runoff and erosion), and soil (soil and soil water)

3b.3.2. Numerical technique

Adequacy of algorithm
Not known

Definition of lower boundary conditions
Automatically set by program to unsaturated flow

Stability
Stable

Numerical dispersion
Not known

Time increments
1 day

Verification of numerical technique
Not reported

3b.3.3. Input Parameters

Weather data
Daily precipitation and air temperature are needed. Model contains a weather generator for use with US weather sets which could probably be adapted for use in EU regions.

Soils data
Bulk density, wilting point, field capacity, sand, silt, and clay content, organic carbon content, depth for each layer

Field management data
SCS runoff curve numbers, MUSLE factors, slope length and steepness.

Cropping data
Planting date, harvest date, maximum leaf area index.

Product chemistry data
Application dates, rates, Koc, washoff fraction, foliar half-life, soil half-life, application efficiency.

3b.3.4. Hydrology model

Spatial distribution
The surface distribution is global and the soil distribution in different homogeneous layers is set by user.

Infiltration model
Capacity model

Evapotranspiration model

Calculated from daily or monthly temperature data and monthly radiation data. Evaporation and transpiration are distinguished (see 3.6.).

Capillary rise

Not considered

Runoff model

Soil Conservation Service curve number technique

Preferential flow

Not considered

3b.3.5. Erosion model

Spatial distribution

Takes into account overland, canal, canal-canal, impoundment flow.

Soil Erosion

Uses a Modified Universal Soil Loss Equation for inter rill and rill erosion.

Particles transport model

The model uses the Yalin equation for the particles transport in canals and includes a deposition/detachment module by means of a capacity of transport. It makes a classification of suspended particles according to their size. The model calculates an enrichment ratio of sediment with fine particles.

Agronomy model

Includes a rotation for the parameters of the MUSLE relative to soil erodibility and agricultural management and for parameters relative to canals characteristics.

3b.3.6. Pesticide model

Number of molecules considered

Up to ten (including metabolites)

Metabolites

Up to two per parent molecule

Sorption

Type of model

Linear sorption

Dependency on environmental parameters

Koc specified along with organic carbon for each depth horizon

Degradation in soil

Type of model

First order kinetic

Dependency on environmental parameters

No correction for temperature or soil moisture content. The decay rate can vary with depth.

Mechanisms considered

Only one degradation process considered (no distinction between biotic and abiotic mechanisms).

Compartment considered

Model uses overall degradation rate in soil.

Dispersion in soil

Dispersion set by program (modelled by numerical dispersion)

Dispersion in concentrated runoff

Not considered

Volatilization

Not considered

Plant up take

Simple model used

Degradation on plant surfaces

First order kinetic

Foliar washoff

Remaining dislodgeable residues are washed to soil when rainfall exceeds a threshold value.

Runoff and erosion

Mass balance approach based on results from hydrology and erosion model. Pesticide uptake from soil to runoff is calculated by an empirical extraction coefficient. The model uses the fine particles enrichment ratio calculated by the erosion model to calculate pesticide concentration on eroded soil particles.

Agronomy models

Cultivation

Not considered for pesticide simulation unless through the partition of pesticide foliar application (see 3.6.).

Irrigation

The program has the ability to automatically trigger irrigation due to a drop in the soil water content. The time window for irrigation is set by user.

Pesticide application

Frequency of applications

Multiple applications throughout the simulated period can be simulated for up to 10 pesticides. The program has an option which automatically allows the same crop to be grown each year with the same pesticide applications.

Application technique

Applications may be foliar sprays, applied to soil surface, incorporated into the soil or applied via chemigation.

3b.3.7. Plant model

Foliage

Purpose

Partition of foliar application between soil and foliage, partition of evapotranspiration between evaporation and transpiration.

Description

Partition of foliar aplication by user. Leaf area index data used for partitioning evapotranspiration.

Flexibility

Parameters set by user

Rooting depth

Purpose

Used for hydrology and plant uptake model

Description

Constant during a cropping period

Flexibility

User specifies value for each cropping period

3b.3.8. Heat model

Purpose

Soil temperatures simulated but are not used for pesticide simulations

Description

Calculated from air temperature using a moving five-day daily average.

3c. OPUS

3c.1. General information

Name of model
OPUS (no acronym)

Most recent release
Version 1.6

Intended use of model
Principle purpose is to calculate pesticide and water movement in small catchments

Model developers
Roger E. Smith
U.S. Department of Agriculture
Agricultural Research Service
Water Management Research Unit
Fort Collins, CO 80523, USA
roger@lily.aerc.colostate.edu

Virginia A. Ferreira
USDA ARS
Great Plains systems research group
Fort Collins, CO 80522, USA

Sponsoring institution
USDA

Date of most recent release
September 1995

3c.2. Documentation and systems considerations

3c.2.1 User manual

Availability
Available from USDA (Manual dated July/December '92)

Language
English

Clarity
Good

Defines model limitations
Specified in model documentation

Includes conceptual model description
Lengthy description

Includes mathematical model description
Yes

Includes sensitivity analysis
No

Provides assistance in determining model parameters
Default values and tables with model parameters listed in user manual

Provides test examples
Example input files are distributed

Provides references
Extensive list

3c.2.2 Other documentation considerations

Tightness of version control
Version specified on output

Availability of source code
Source code distributed upon request

Source code quality
Clearly structured, few comments

3c.2.3 Systems considerations

Hardware requirements
386 or higher with numeric coprocessor 1 MB hard disk storage

Run time for standard scenario
Depends on options selected about 3 min for 10 year simulation on Pentium PC

Reliability
Program performs without problems if input data are correct

Clarity of error messages
Good

3c.2.4 Support

Method of support
Roger Smith can be contacted for support

Availability of information about bugs, corrections and new versions.
New version is sent to registered user

Training for users
No

3c.2.5 Input/Preprocessor

User friendliness
No preprocessor

Help utility
None

Data range checking
Yes

Sample input files
Distributed with model

Database included
None (manual provides tables for most parameters)

Availability of needed data
Availability of weather data depends on option selected. Soil data readily available.

Flexibility
Low

3c.2.6 Output/Postprocessor

Nature of output
Tabular form only

User friendliness
Medium

Help utility
None

Sample files
Distributed with model

Flexibility
High, content of output can be controlled by user

Documents input parameters
Yes

Clarity of output reports
Good

3c.3. Model science

3c.3.1 Compartments considered

Crop, soil surface, soil (soil and soil water)

3c.3.2 Numerical technique

Adequacy of algorithm

Not known

Definition of lower boundary conditions

Set by user, can reflect drainage tiles, ground water, or other conditions

Stability

Stable

Numerical dispersion

Not known

Time increments

Time step is dependent on current conditions for both soil water and surface water.

Verification of numerical technique

Data reported in manual.

3c.3.3 Input Parameters

Weather data

Daily values of precipitation or breakpoint data. Monthly data of radiation and temperature

Soils data

Core depth, soil texture, organic carbon content, saturated hydraulic conductivity (optional), van Genuchten parameter (optional)

Field management data

Field slope, field length, soil erodibility, cropping 'practice' factor, cover management

Cropping data

Leaf area index, max. rooting depth, max. yield, max. dry matter, max. ground cover, temperature effect on growth rate parameter, emergence, mature, harvest

Product chemistry

Foliar decay coefficient, soil decay coefficient, activation energy of decay (optional), adsorption coefficient, kinetic adsorption coefficient (optional)

Previous pesticide concentrations considered

Yes

Application methods

Foliar, soil surface, incorporated

Application frequency

Max. 15 appl. per year

Irrigation considered

Furrow, sprinkler, can trigger irrigation based on soil moisture

Buffers or other edge of field management considered

Tillage, terracing, buffer strips

3c.3.4 Hydrology Model

Spatial distribution

Up to 10 soil horizons can be specified

Infiltration model

Partitioning between runoff and infiltration is calculated using curve numbers, if weather input is daily. If breakpoint data are used, then the calculations are based on the kinematic wave approach.

Evapotranspiration model

Potential evapotranspiration is calculated from radiation and temperature using a simplified Penman equation. Actual evapotranspiration depends on plant cover, leaf area, and mulch cover.

Capillary rise

Considered

Runoff model

Curve number is used for daily input of actual or simulated weather data. If breakpoint or pluvigraph data are available, then the model is able to simulate dynamic distributed surface hydraulics (kinematic wave hydraulics) to simulate variations in time and space and produce hydrographs and sediment concentration graphs.

Preferential flow

Not considered

3c.3.5 Erosion model

Spatial distribution

Catchment can be subdivided into several identical units

Soil erosion

MUSLE is used with the daily hydrology option. A second option allows erosion to be calculated based on shear force caused by runoff water.

Agronomy model

Taken into account by MUSLE management factors.

3c.3.6 Pesticide model

Number of molecules considered

Up to 10

Metabolites
No

Sorption
Type of model
Linear or kinetic

Dependency on environmental parameters
Organic carbon

Degradation in soil
Type of model
First order

Dependency on environmental parameters
Soil temperature, soil moisture

Mechanisms considered
Lumped degradation rate

Compartments considered
Soil and soil water

Volatilization
No

Plant up-take
Simple model used

Degradation on plant surfaces
Simple model used

Foliar washoff
Yes, user defined but data are included in manual for various pesticides

Runoff and erosion
Mass balance approach based on hydrology and erosion results.

Agronomy models
Cultivation
Many options are simulated

Irrigation
Many options are simulated

Pesticide application
Frequency of application
Multiple applications can be simulated

Application technique
Many options are simulated

3c.3.7 Plant model

Foliage
Purpose

Partition of evapotranspiration and evaporation, partition of foliar application between leaves and soil.

Description
Various options allow simulation of a wide variety of plants and growing conditions including plant stress, grazing, senescence, etc..

Flexibility
Very flexible

Rooting depth
Purpose
Used for hydrology and uptake model

Description
Root mass changes over time for plants

Flexibility
Very flexible

3c.3.8 Heat model

Purpose
Soil temperatures are simulated and can affect pesticide degradation.

Description
Calculated based on air temperature.

3d. PELMO

3d.1. General Information

Name of model

PELMO Pesticide Leaching Model

Name or number of most recent release

Version 2.01

Intended use of model

Principle purpose is to calculate the pesticide movement in surface and subsoils. The model also considers runoff, and erosion losses.

Model developer

Michael Klein
PO Box 1260
D-57377 Schmallenberg
Germany
Phone +49 2972 302317

Date of most recent release

May 1995

3d.2. Documentation and systems considerations

3d.2.1. User manual

Availability

Publication of Fraunhofer Institut

Language

German

Clarity

Good

Defines model limitations

Short description

Includes conceptual model description

Short description

Includes mathematical model description

A mathematical description of the submodels is included.

Includes sensitivity analysis

No

Provides test examples

Yes

Provides references
Yes

3d.2.2. Other documentation considerations

Tightness of version control
Tight version control

Availability of source code
It is supplied on program diskette.

3d.2.3. System considerations

Hardware requirements
PC with math coprocessor, DOS

Run time for standard scenario
Depends on options selected (typically less than 1 minute per year).

Reliability
Programs perform without problems if input data are correct.

Clarity of error messages
Difficult to understand

3d.2.4. Support

Method of support
Staff at Fraunhofer are helpful in resolving problems

Availability of information about bugs, corrections and new versions.
No informations systematically distributed to users

Training for users
Training sessions possible on request

3d.2.5. Input/preprocessor

User friendliness
Medium

Help utility
On-line help build within preprocessor

Data range checking
No

Sample input files
Included with source code.

Databases included

Crop data base included, limited number of soil and weather scenarios for Germany

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.

Availability of standard scenarios

Stanard scenario for Germany supplied with program.

Flexibility

User can specify different options for soil hydrology and pesticide related processes

3d.2.6. Output/Postprocessor

Nature of output

Tabular and graphical representation of concentration profile in soil and leachate data

User friendliness

Medium

Help utility

No on-line help is available.

Sample files

Included with source code.

Flexibility

Daily, monthly or yearly reports of water hydrology and pesticide behaviour

Documents input parameters

Yes

Clarity of output reports

Good

3d.3. Model Science

3d.3.1. Compartments considered

Plant (foliar washoff and degradation, plant uptake), soil surface (runoff, erosion, volatilization), and soil (soil and soil water)

3d.3.2. Numerical technique

Adequacy of algorithm

Model uses backward difference implicit technique

Definition of lower boundary conditions
Automatically set by program to unsaturated flow

Stability
Stable

Numerical dispersion
Used to simulate physical dispersion

Time increments
1 day

Verification of numerical technique
Not reported

3d.3.3. Input Parameters

Weather data
Daily values for precipitation, humidity, temperature and daily temperature variation. An estimate of average storm duration is also needed.

Soils data
Core depth, bulk density, soil texture, field capacity, wilting point, organic carbon are required.

Field management data
Field slope, soil erodibility, cropping practice factor, runoff curve numbers, cover management factors.

Cropping data
Emergence, maturation, and harvest dates. Maximum interception rate for water (storage) and pesticide. Rooting depth. Conditions of crop after harvest (residue removed or left in field). Plant uptake can be simulated if data are available. On-line database included.

Product chemistry
Soil/pesticide adsorption coefficient, decay rate Henry s law coefficient, diffusion coefficient

3d.3.4. Hydrology model

Spatial distribution
Distribution is homogeneous across surface and within any given soil layer. Initial distribution can be set by user.

Infiltration model
Capacity model

Evapotranspiration model
Calculated either using daily temperature or pan evaporation data with and appropriate correction factor or daily temperature and humidity

Capillary rise
Not considered

Runoff model
Uses a modification of the USDA Soil Conservation Service curve number approach. Curve numbers are continuously adjusted each day as a function of soil moisture in the upper soil layers.

Preferential flow
Not considered

3d.3.5. Erosion model

Spatial distribution
Homogeneous erosion across simulated area.

Soil Erosion
Uses the Modified Universal Soil Loss Equation (MUSLE).

Particles transport model
The model calculates a peak runoff rate using a trapezoidal hydrograph and a user input storm duration. An enrichment factor is then calculated using an empirical approach.

Agronomy model
Cropping and management parameters can be modified to influence the erosion model as rotation occurs.

3d.3.6. Pesticide model

Number of molecules considered
One

Metabolites
None

Sorption
Type of model
Freundlich adsorption isotherm and / or sorption increasing with time

Dependency on environmental parameters
User can specify Kd for each depth horizon or enter the Koc along with organic carbon for each depth horizon.

Degradation in soil
Type of model
First order kinetic

Dependency on environmental parameters
Correction for temperature or soil moisture content. The decay rate can vary with depth.

Mechanisms considered

Only one degradation process considered

Compartments considered

Generally described as a lumped degradation rate.

Dispersion in soil

Set by user or simulated using numerical dispersion

Dispersion in concentrated runoff

Not known.

Volatilization

Volatilization loss simulated using Ficks law

Plant uptake

Uptake is linked to the transpiration rate and can be adjusted by user.

Degradation on plant surfaces

Lumped first order degradation rate

Foliar washoff

A foliar extraction coefficient is supplied by user (% washoff per cm of rainfall).

Runoff and erosion

Mass balance approach based on results from hydrology and erosion submodels. The model uses the fine enrichment factor calculated by the erosion model to calculate pesticide concentration on eroded soil particles. The concentration in the runoff water is proportional to the concentration in the surface soil water depending on the soil moisture at beginning of runoff event.

Agronomy models

Cultivation

Not considered.

Irrigation

Not considered; can be added to precipitation

Pesticide application

Frequency of applications

Multiple applications (up to 50)

Application technique

Applications may be foliar sprays, applied to soil surface, or incorporated into the soil.

3d.3.7. Plant model

Foliage

Purpose

Partition of foliar application between soil and foliage, volatilization and degradation can occur on the leae surface.

Description

Interception varies as a percentage between essentially zero at crop emergence and some user specified maximum value. Either a linear or non-linear approach can be selected.

Flexibility

Parameters set by user.

Rooting depth

Purpose

Used for hydrology and plant uptake model.

Description

Constant during a cropping period. A triangular shaped root distribution is assumed with water drawn from surface soil layers if it is available.

Flexibility

User specifies value for each crop.

3d.3.8. Heat model

Purpose

Soil temperatures are used for correction of soil degradation rate

Description

Empirical model based on air temperature

3e. PRZM-2

3e.1. General Information

Name of model

PRZM-2 (A model for predicting pesticide fate in the crop root zone and unsaturated soil zones)

Name or number of most recent release

Version 2.2

Intended use of model

Principle purpose is to calculate the pesticide movement in surface and subsoils. The model also considers volatility, runoff, and erosion losses.

Model developers

R.F. Carsel
Environmental Research Laboratory
US Environmental Protection Agency
Athens, Georgia 30605-2720 USA

J.A. Mullins, J.E. Scarbrough, and A.M. Ivery
ASciI Corporation
Athens, Georgia 30605-2720 USA

Date of most recent release

October 1994

3e.2. Documentation and systems considerations

3e.2.1. User manual

Availability

It is included as a word perfect file with the source code or available from USEPA.

Language

English

Clarity

Good

Defines model limitations

Limitations of each module are specified in the user manual.

Includes conceptual model description.

Lengthy description of model and submodels.

Includes mathematical model description

A mathematical description of the submodels is included.

Includes sensitivity analysis

Traditional sensitivity analyses are not included in the user manual, however, *the model has a feature for simulating the effect of variability on input parameters.*

Provides test examples
Example input files are listed in the manual.

Provides references
Extensive list

3e.2.2. Other documentation considerations

Tightness of version control
Tight version control

Availability of source code
It is supplied on program diskette.

3e.2.3. System considerations

Hardware requirements
'386 or '486 IBM-PC compatible system. MS DOS 3.3 or higher, 640K base memory, 4MB of extended memory, 4.5MB hard disk storage.

Run time for standard scenario
Depends on options selected (typically less than 30 seconds per year).

Reliability
Programs perform without problems if input data are correct.

Clarity of error messages
List of error messages is provided in user manual.

3e.2.4. Support

Method of support
Model is supported by USEPA Center for Exposure Assessment Modelling. Contact telephone numbers are provided in the user manual.

Availability of information about bugs, corrections and new versions
No information about bugs systematically distributed to users. New versions can be obtained from USEPA Center for Exposure Assessment Modeling (see R.F. Carsel address under "Model Developers") or using the Internet

Training for users
No training is offered.

3e.2.5. Input/preprocessor

User friendliness
No preprocessor. Model requires input in fixed format (specific rows and columns) to run.

Help utility

No on-line help but many tables and figures are provided in manual.

Data range checking

No.

Sampler input files

Included with source code.

Databases included

Generalised help tables, includin information on pesticide properties, are provided to assist in developing model scenarios. Examples, however, are oriented towards US situations.

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. Input data for certain optional parameters (such as microbial degradation rates) may be difficult to obtain.

Availability of standard scenarios

None.

Flexibility

The wide range of options makes the program quite flexible but developing input data is somewhat daunting to occasional users.

3e.2.6. Output/Postprocessor

Nature of output

Tabular form only, program has the ability to produce files that are compatible with standard graphics packages after minimal file processing.

User friendliness

Minimal

Help utility

No on-line help is available. Some help for selecting output parameters is available in the manual.

Sample files

Included with source code.

Flexibility

Able to produce a wide range of reports. Snapshot feature is especially good for comparing predictions with field measurements at specific points in time.

Documents input parameters

Some of the input parameters

Clarity of output reports

Good, but there is no explanation of output reports in the manual.

3e.3. Model Science

3e.3.1. Compartments considered

Plant (foliar washoff and Degradation, plant uptake), soil surface (runoff, erosion, volatilization), and soil (soil and soil water)

3e.3.2. Numerical technique

Adequacy of algorithm
Not known

Definition of lower boundary conditions
Root zone model can be coupled with vadose zone model to simulate representative boundary conditions.

Stability
Stable

Numerical dispersion
May be a problem with systems exhibiting significant advection, however, the user can select a "method of characteristics" option to limit the effect.

Time increments
1 day

Verification of numerical technique
Not reported

3e.3.3. Input Parameters

Weather data
Daily precipitation, pan evaporation, temperature, wind speed and solar radiation, storm duration

Soils data
Core depth, bulk density, field capacity, wilting point, organic carbon

Field management data
Field slope, soil erodibility, cropping "practice" factor, "runoff curve" numbers, cover management factors.

Cropping data
Emergence, maturation, and harvest dates. Max. interception rate for water (storage) and pesticide.Rooting depth.

Product chemistry
Soil/pesticide adsorption coefficient, dissolved, adsorbed, and vapor phase decay rates (frequently dissolved and adsorbed are set to equal values to simulate first-order degradation). Henry's law coefficient. Information on transformation rates if metabolites are simulated.

3e.3.4. Hydrology model

Spatial distribution
Distribution is homogeneous across surface and within any given soil layer. Initial distribution can be set by user.

Infiltration model
Capacity model

Evapotranspiration model
Calculated either using daily temperature and solar radiation data or pan evaporation data with and appropriate correction factor.

Capillary rise
Not considered

Runoff model
Uses a modification of the USDA Soil Conservation Service curve number approach. Curve numbers are continuously adjusted each day as a function of soil moisture in the upper soil layers.

Preferential flow
Not considered

3e.3.5. Erosion model

Spatial distribution
Homogeneous erosion across simulated area.

Soil Erosion
Uses the Modified Universal Soil Loss Equation (MUSLE).

Particles transport model
The model calculates a peak runoff rate using a trapezoidal hydrograph and a user input storm duration. An enrichment factor is then calculated using an empirical approach.

Agronomy model
Cropping and management parameters can be modified to influence the erosion model.

3e.3.6. Pesticide model

Number of molecules considered
Up to three (including metabolites)

Metabolites
Up to two with one parent molecule

Sorption
Type of model
Linear sorption based on Kd. Dependency on environmental parameter. User

can specify Kd for each depth horizon or enter the Koc along with organic carbon for each depth horizon.

Degradation in soil
Type of model
First order kinetic

Dependency on environmental parameters
No correction for temperature or soil moisture content. The decay rate can vary with depth.

Mechanisms considered
Hydrolysis, volatilization, microbial degradation.

Compartments considered
Generally described as a lumped degradation rate. If data are available then sorbed, soil water, and vapor phase degradation may be entered separately. Also microbial degradation can be modelled.

Dispersion in soil
Dispersion and diffusion on vapor phase descibed using Fick's law.

Dispersion in concentrated runoff
Concentration in the water above the surface layer is assumed to be equal to the dissolved concentration of the pesticide in the surface soil layer.

Volatilization
Volatilization loss simulated using Jury's boundary layer model.

Plant uptake
Uptake is linked to the transpiration rate and can be adjusted by user.

Degradation on plant surfaces
Lumped first order degradaton constant (note that volatilization from leaf surfaces is calculated elsewhere).

Foliar washoff
A foliar extraction coefficient is supplied by user (% washoff per cm of rainfall).

Runoff and erosion
Mass balance approach based on hydrology and erosion submodels. The model uses the fine particles enrichment factor calculated by the erosion model to calculate pesticide concentration on eroded soil particles. The water layer directly in contact with the surface soil is assumed to have the same concentration as the soil pore water in the uppermost soil layer.

Agronomy models
Cultivation
Not considered.

Irrigation
Furrow irrigation, flood irrigation, and over and under canopy sprinklers are simulated. The program has the ability to automatically trigger irrigation due to a drop in the soil water content. The time window for irrigation is set by user.

Pesticide application

Frequency of applications

Multiple applications throughout the simulated period can be simulated for up to 3 pesticides. Current version can accept 400 applications during a simulation (for example, 10 applications each year for 40 years).

Application technique

Applications may be foliar sprays, applied to soil surface, or incorporated into the soil.

3e.3.7. Plant model

Foliage

Purpose

Partition of foliar application between soil and foliage, volatilization and degradation can occur on the leafe surface.

Description

Interception varies as a percentage between essentially zero at crop emergence and some user specified maximum value. Either a linear or non-linear approach can be selected.

Flexibility

Parameters set by user.

Rooting depth

Purpose

Used for hydrology and plant uptake model.

Description

Constant during a cropping period. A triangular shaped root distribution is assumed with water drawn from surface soil layers if it is available.

Flexibility

User specifies value for each crop.

3e.3.8. Heat model

Purpose

Soil temperatures are simulated and are used to correct the Henry's law constant for temperature effects.

Description

Calculated using user supplied data for air temperature, albedo, and wind velocity.

3f. SWRRBWQ

3f.1. General Information

Name of model
Simulator for Water Resources in Rural Basins - Water Quality

Name or number of most recent release
Version 3210SCS94a

Intended use of model
Model is intended to predict the effect of management decisions on water and sediment yields with reasonable accuracy on large, ungaged, rural watersheds. Model can simulate multiple subbasins and includes a simple river and lake water quality model. Note: SWRRBWQ is now being incorporated into (and will be replaced by) the Soil and Water Assessment Tool (SWAT) currently under development by USDA/ARS in Temple, Texas.

Model developers
J. Arnold, N. Sammons, J. Williams, A. Nicks.

Sponsoring institution
USDA Agricultural Res. Service and Texas Agricultural
Experiment Station, Temple, Texas, USA

Date of most recent release
April 1994

3f.2. Documentation and systems considerations

3f.2.1. User manual

Availability
Requests for copies of the model and documentation should be made to:
Salvador Palaly
USDA Natural Resources Conservation Service
Northeast National Technical Center
160 East 7th Street
Chester, Pennsylvania 19013 USA
voice: 610 490-6063
fax: 610 490-6009

Language
English

Clarity
Good

Defines model limitations
Limited discussion

Includes conceptual model description

Yes.

Includes mathematical model description

A mathematical description is included.

Includes sensitivity analysis

No.

Provides assistance in determining model parameters

Some tables are provided for a limited set of input parameters.

Provides test examples

Yes.

Provides references

Extensive list is provided in the manual.

3f.2.2. Other documentation considerations

Tightness of version control

Tight version control

Availability of source code

It is supplied on request.

3f.2.3. System considerations

Hardware requirements

IBM PC-AT or IBM-compatible systems. Use of an math coprocessor chip will execute programs much more rapidly.

Run time for standard scenario

Low (about 50 seconds per simulated year when simulating a scenario with four basins using a 80386 machine with math coprocessor)

Reliability

Programs perform without problems if input data are correct.

Clarity of error messages

Not very specific

3f.2.4. Support

Method of support

Support provided by
Nancy Sammons
USDA, ARS
Grassland Soil and Water Research Laboratory
808 East Blackland Road

Temple, Texas 76502 USA
email: sammons@arssun1.tamu.edu
voice: 817 770-6512
fax: 817 770-6561

Availability of information about bugs, corrections and new versions
No information about bugs is systematically distributed to users

Training for users
Training is occasionally available from various sources. Contact Nancy Sammons (see above).

3f.2.5. Input/preprocessor

User friendliness
Parameter editor files have been developed to assist in developing input parameter files.

Help utility
Generalised help tables provided

Data range checking
Yes, if UTIL editor is used.

Sampler input files
Yes

Databases included
Generalised help tables, including information on pesticide properties, are provided.

Availability of needed data
All input parameters are obtainable from soil and weather data bases. Obtaining access to such information is difficult in some countries.

Availability of standard scenarios
None

Flexibility
The wide range of options makes the program quite flexible but developing input data is somewhat daunting to occasional users.

3f.2.6. Output/Postprocessor

Nature of output
Tabular

User friendliness
Minimal

Help utility
None.

Sample files
Yes, in user manual.

Flexibility
Somewhat flexible.

Documents input parameters
Yes.

Clarity of output reports
Good, but there is no explanation of output reports in the manual.

3f.3. Model Science

Compartments considered
Plant (foliar washoff and degradation, plant uptake), soil surface (runoff and erosion), soil (soil and soil water), subsurface flow, simplistic consideration of river and lake concentrations.

3f.3.2. Numerical technique

Adequacy of algorithm
Not known

Definition of lower boundary conditions
Unsaturated flow

Stability
Stable

Numerical dispersion
Not known

Time increments
1 day

Verification of numerical technique
Not reported

3f.3.3. Input Parameters

Weather data
Daily precipitation and temperature data. Model contains a weather generator for use with US weather sets which probably could be adapted for use in EU regions.

Soils data
Bulk density, available water capacity, saturated conductivity, clay content, organic carbon content.

Field management data

SCS curve numbers, overland flow N value, return flow travel time, USLE factors, slope length and steepness

Cropping data

Planting date, harvest date, tillage operation, maximum leaf area index.

Product chemistry data

Application dates, Koc, washoff fraction, foliar half-life, soil half-life, application efficiency, water solubility.

3f.3.4. Hydrology model

Spatial distribution

The surface distribution is homogenous within each of up to 10 subbasins.

Infiltration model

Storage routing technique.

Evapotranspiration model

Calculated from daily or monthly temperature data and monthly radiation data. Evaporation and transpiration are distinguished (see 3.6.).

Capillary rise

Not considered

Runoff model

Runoff volume is estimated using a modification of the USDA Soil Conservation Service curve number technique. Peak runoff rates can be calculated either by using the modified Rational formula or the SCS TR-55 method. In addition, lateral subsurface flow is considered.

Preferential flow

Crack flow is considered. Tendency of water to flow through cracks is a function of soil water and clay content.

3f.3.5. Erosion model

Spatial distribution

Takes into account overland flow.

Soil Erosion

Uses a Modified Universal Soil Loss Equation for inter-rill and rill erosion.

Particle transport model

Sediment transport can be simulated in channels and a reservoir.

Agronomy model

Includes parameters for MUSLE relative to soil erodibility and agricultural management.

3f.3.6. Pesticide model

Number of molecules considered

Up to ten.

Metabolites

Not considered

Sorption

Type of model

Linear sorption

Dependency on environmental parameters

Koc specified along with organic carbon for each depth horizon

Degradation in soil

Type of model

First order kinetic

Dependency on environmental parameters

No correction for temperature or soil moisture content. The decay rate can vary with depth.

Mechanisms considered

Only one degradation process considered (no distinction between biotic and abiotic mechanisms).

Compartment considered

Model uses overall degradation rate in soil.

Dispersion in soil

Dispersion set by program (modelled by numerical dispersion)

Dispersion in concentrated runoff

Not considered

Volatilization

Not considered

Plant up take

Not simulated.

Degradation on plant surfaces

First order kinetic

Foliar washoff

Remaining dislodgeable residues are washed to soil based on a function of rainfall amount and user defined washoff fraction.

Runoff and erosion

Mass balance approach based on results from hydrology and erosion model. Pesticide uptake from soil to runoff is calculated by an empirical extraction coefficient. The model uses the fine particles enrichment ratio calculated by the erosion model to calculate pesticide concentration on eroded soil particles.

Agronomy models

Cultivation

Not considered for pesticide simulation unless through the partition of pesticide foliar application.

Irrigation

The program has the ability to automatically trigger irrigation due to a drop in the soil moisture content and a crop stress factor.

Pesticide application

Frequency of applications

Multiple applications throughout the simulated period can be simulated for up to 10 pesticides.

Application technique

Applications may be foliar sprays, applied to soil surface, or incorporated into the soil.

3f.3.7. Plant model

Foliage

Purpose

Partition of foliar application between soil and foliage, partition of evapotranspiration between evaporation and transpiration. Water and temperature stress effects on plant biomass and yield can be simulated.

Description

Leaf area index is used for partition of foliar application. Biomass affects evapotranspiration.

Flexibility

Parameters set by user

Rooting depth

Purpose

Used for hydrology and evapotranspiration model.

Description

Constant during a cropping period

Flexibility

User specifies value for each cropping period

3f.3.8. Heat model

Purpose

Soil temperatures simulated but are not used for pesticide simulations

Description

Calculated from air temperature and adjusted using soil bulk density, crop residue, and snow cover.

ANNEX 4 Surface water fate models

4a. SLOOT.BOX

4a.1. General Information

Name of model
SLOOT.BOX

Name or number of most recent release
1.1

Intended use of model
Estimation of the short and long term concentration in surface water according to drift after application of pesticides

Model developers
J.B.H.J. Linders
RIVM-ACT
P.O. Box 1
NL-3720 BA Bilthoven
The Netherlands
tel. + 31 30 274 31 64
fax. + 31 30 274 44 01
e-mail: Jan.Linders@rivm.nl

Sponsoring institution
National Institute for Public Health and Environmental Protection

Date of most recent release
May 1993

4a.2. Documentation and Systems considerations

4a.2.1. User manual

Availability
Documentation and floppy disk available directly from the author

Language
Manual in Dutch, program in English

Clarity
Good

Defines model limitations
Model assumptions and limitations have been describes clearly.

Includes conceptual model description.
Yes

Includes mathematical model description
Yes

Includes sensitivity analysis
No

Provides assistance in determining model parameters
Defines changeable default values

Provides test examples
No

Provides references
Yes

4a.2.2. Other documentation considerations

Tightness of version control
No

Availability of source code
Yes

4a.2.3. Systems considerations

Hardware requirements
PC with MS-DOS and LOTUS 1-2-3

Run time for standard scenario
Few seconds

Reliability
Good

Clarity of error messages
Yes

4a.2.4. Support

Method of support (Existence of responsible institution?)
Provided by Jan Linders (RIVM-ACT)

Availability of information about bugs, corrections, and new versions
No

Training for users
No

4a.2.5. Input/Preprocessor

User friendliness
Good

Help utility
No

Data range checking
No

Sample input files
No

Database included
No

Availability of needed data
Default values are provided, other data are collected from registration data for the substance

Availability of standard scenarios
Yes, determined by registration authorities in The Netherlands, which use the model in process of registration evaluation

Flexibility
Parameters and scenarios are easily changed

4a.2.6. Output/Postprocessor

Nature of output
Tabular with additional text

User friendliness
Good

Help utility
No

Sample files
No

Flexibility
No

Documents input parameters
Yes

Clarity of output reports
Good

4a.3. Model Science

4a.3.1. Compartments considered

Water, suspended solids

4a.3.2. Entry routes

Entry routes
Drift

Application Type
Pulse

Frequency of application
Single, multiple

4a.3.3. Numerical technique

Adequacy of algorithm
Good: analytical solution to first order reaction kinetics

Definition of lower boundary condition of sediment
Not applicable

Stability
Good

Numerical dispersion
No

Time increments
Not applicable

Space increments (direction of flow for water, depth for sediment)
Not applicable

Verification of numerical technique
Not applicable

4a.3.4. Surface water model (vertical and horizontal heterogeneity)

Standard environment of completely mixed ditch

4a.3.5. Surface water hydrology model (static/dynamic)

No hydrologic model included

4a.3.6. Surface water pesticide model

Metabolites
Treated as active ingredient

Adsorption to suspended solids
Type of model (linear, nonlinear, kinetics). Freundlich constant. Dependency on environmental parameters (i.e. temperature, pH)
No

Adsorption to water plants
Type of model (linear, nonlinear, kinetics)
Not applicable

Dependency on environmental parameters (i.e temperature, pH, plant characteristics)
Not applicable

Degradation in surface water
Type of model (first order, power law, Menten)
First order

Dependency on environmental parameters (i.e. pH, light intensity, microbacterial activity temperature)

Mechanisms considered:
not applicable

Compartments considered:
not applicable

Advection in surface water
Yes

Dispersion in surface water
No

Volatilization
Yes

Inhomogenuity of distribution (e.g. layer of pesticides at water surface)
No

Exchange with sediment (diffusion, advection)
Yes: sedimentation and resuspension

4a.3.7. Suspended solids model (static/dynamic)

Static

4a.3.8. Aquatic vegetation model

Plant species
Not applicable

Characterised by dry mass or surface area
Not applicable

Type of model (static, dynamic: first order, power law, Menten)
Not applicable

4a.3.9. Sediment model (horizontal and vertical heterogeneity)

Not applicable

4a.3.10. Sediment hydrology model (static/dynamic)

Not applicable

4a.3.11. Sediment pesticide model

Metabolites
Not applicable

Adsorption to solid bottom material
Type of model (linear, nonlinear, kinetics)
Not applicable

Dependency on environmental parameters (i.e. temperature, pH)
Not applicable

Degradation in sediment
Type of model (first order, power law, Menten)
Not applicable

Dependency on environmental parameters (i.e. pH, microbacterial activity, temperature)

Mechanisms considered:
Not applicable

Compartments considered:
Not applicable

Advection in sediment
Not applicable

Diffusion in sediment
Not applicable

Dispersion in sediment
Not applicable

Bioturbation
Not applicable

Inhomogenuity of distribution (e.g. layer of pesticides at sediment surface)
Not applicable

Exchange with surface water (diffusion, advection)
Yes: sedimentation and resuspension

4b. TOXSWA

4b.1. General Information

Name of model
TOXic substances in Surface WAter

Name or number of most recent release
Version 1.0 Released April, 1996.

Intended use of model
Model simulates pesticide movement and degradation in a ditch including its sediment

Model developer
P.I. Adriaanse
Fate and Effects Pesticides Department
DLO Winand Staring Centre for Integrated Land, Soil and Water Research
P.O. Box 125
6700 AC Wageningen
The Netherlands
Tel: +31.317.474760
E-mail: IN%"p.i.adriaanse@sc.dlo.nl"

Sponsoring institution
DLO Winand Staring Centre for Integrated Land, Soil and Water Research

Date of most recent release
23 April, 1996

4b.2. Documentation and Systems considerations

4b.2.1. User manual

Availability
User manual and report on the theoretical background of the model has been published at the DLO Winand Staring Centre for Integrated Land, Soil and Water Research in April 1996

Language
English

Clarity
Good

Defines model limitations
Model assumptions and limitations have been clearly described

Includes conceptual model description
Yes

Includes mathematical model description
Yes

Includes sensitivity analysis
Will be published separately, probably end 1996

Provides assistance in determining model parameters
Information about input related to numerical solution (time and space steps) is provided

Provides test examples
Yes

Provides references
Yes

4b.2.2. Other documentation considerations

Tightness of version control
Tight version control

Availability of source code
Available on request

4b.2.3. Systems considerations

Hardware requirements
The program runs at PC (486 or Pentium) a version running at a mainframe computer (actually an Alpha AXP system) will be available on request.

Operating system
MS-DOS resp. Vax VMS.

Run time for standard scenario
At the mainframe computer: About 4 minutes for a system consisting of 1 water sub-system and 39 sediment sub-systems (run of 1600 timesteps). The same run takes 35 minutes at the PC 486 (33 mHz) and 10 minutes at a PC Pentium).

Reliability
Too early to state

Clarity of error messages
Reasonable in conjunction with the theoretical report

4b.2.4. Support

Method of support (Existence of responsible institution?)
Provided by P.I. Adriaanse and W.H.J. Beltman of DLO Winand Staring Centre

Availability of information about bugs, corrections, and new versions
Information will be systematically distributed

Training for users
Training available on request

4b.2.5. Input/Preprocessor

User friendliness
Good

Help utility
Yes

Data range checking
Yes

Sample input files
Yes

Database included
No

Availability of needed data
Most data are readily available. An exception is the slope of the sorption isotherm for water plants. Dry weight of water plants and dispersion coefficient of the pesticide in slowly flowing water need to be estimated

Availability of standard scenarios
Standard scenarios for The Netherlands will be available end 1996

Flexibility
The wide range of options (especially concerning entry routes) makes the program quite flexible, but not easy to use for the occasional user

4b.2.6. Output/Postprocessor

Nature of output
Tabular as well as graphs

User friendliness
Minimal

Help utility
None

Sample files
Yes

Flexibility
User can specify time intervals of output and number and location of sediment subsystems

Documents input parameters
Yes

Clarity of output reports
Good

4b.3. Model Science

4b.3.1. Compartments considered

Water, water plants, suspended solids, sediment-solid bottom material, sediment water

4b.3.2. Entry routes

Entry routes and application

Model can handle distributed pulse inputs (e.g. drift, overspray, runoff, discharge via drains), point-type pulse inputs (e.g. single drain with momentary outflow), continuous distributed input (in sediment, e.g. leaching; not in water itself, e.g. atmospheric deposition) and continuous point-type input (in sediment, e.g. leaching; not in water, e.g. atmospheric deposition). In the sediment an initial concentration profile needs to be defined

Frequency of application

Single application of pulse inputs have been modelled, (multiple applications will be implemented in the future). Continuous input in the sediment by seepage has been defined on daily basis

4b.3.3. Numerical technique

Adequacy of algorithm

Finite difference scheme of which user can define exact type, all types ranging from implicit to explicit and from backward to forward can be selected with the aid of numerical weight factors. In TOXSWA 1.0 only the central explicit calculation scheme can be applied

Definition of lower boundary condition of sediment

Different options: Upward seepage of water with defined pesticide concentration; downward seepage with calculated pesticide concentration; no seepage with no pesticide mass transport

Stability

Model provides error message when stability condition (or in fact the stricter condition of positivity) of solution has not been met. Guidelines are provided concerning possible time and space increments

Numerical dispersion

Numerical dispersion correction implemented

Time increments

Set by user

Space increments (direction of flow for water, depth for sediment)

Set by user

Verification of numerical technique

Simulations will be checked against simulations with different types of finite difference scheme and simulations have been checked with halved time and *space increments. Results of pesticide algorithms are checked against analytical solutions*

4b.3.4. Surface water model (vertical and horizontal heterogeneity)

Surface water subsystem divided into homogeneous slices containing water, suspended solids and water plants

4b.3.5. Surface water hydrology model (static/dynamic)

Actually a static hydrology has been described in one of the input files, but linkage to a suitable dynamic hydrologic model is planned for 1996, 1997

4b.3.6. Surface water pesticide model

Metabolites
No metabolites are considered

Adsorption to suspended solids
Type of model (linear, nonlinear, kinetics)
Freundlich adsorption

Dependency on environmental parameters (i.e. temperature, pH)
None

Adsorption to water plants
Type of model (linear, nonlinear, kinetics)
Linear

Dependency on environmental parameters (i.e temperature, pH, plant characteristics)
None

Degradation in surface water
Type of model (first order, power law, Menten)
First order kinetics

Dependency on environmental parameters (i.e. pH, light intensity, microbacterial activity, temperature)
None (so only one value for rate constant possible)

Mechanisms considered
Only one degradation process considered (no distinction between biotic and abiotic mechanisms)

Compartments considered
Model uses overall degradation rate

Advection in surface water
Set by user (no flow is possible)

Dispersion in surface water
Set by user

Volatilization

Liss-Slater method; across water-air interface

Inhomogenuity of distribution (e.g. layer of pesticides at water surface)

None

Exchange with sediment (diffusion, advection)

Diffusion and advection across interface

4b.3.7. Suspended solids model (static/dynamic)

Static (so constant concentration of suspended solids, but moving with water body)

4b.3.8. Aquatic vegetation model

Plant species
Not differentiated

Characterised by dry mass or surface area
Dry mass

Type of model (static, dynamic: first order, power law, Menten)
Static

4b.3.9. Sediment model (horizontal and vertical heterogeneity)

Homogeneous sediment, but many parameters can be varied with depth

4b.3.10. Sediment hydrology model (static/dynamic)

Semi-stationary hydrology (upward or downward seepage on daily basis)

4b.3.11. Sediment pesticide model

Metabolites
One chemical considered

Adsorption to solid bottom material
Type of model (linear, nonlinear, kinetics)
Freundlich adsorption

Dependency on environmental parameters (i.e. temperature, pH)
None

Degradation in sediment
Type of model (first order, power law, Menten)
First order kinetics

Dependency on environmental parameters (i.e. pH, microbacterial activity, temperature)
None

Mechanisms considered
Only one degradation process considered (no distinction between biotic and abiotic mechanisms)

Compartments considered
Model uses overall degradation rate

Advection in sediment
Set by user

Diffusion in sediment
Set by user

Dispersion in sediment
Set by user

Bioturbation
Not included

Inhomogenuity of distribution (e.g. layer of pesticides at sediment surface)
None

Exchange with surface water (diffusion, advection)
Diffusion and advection across interface

4c. WASP5

4c.1. General Information

Name of model

WASP5 (Water Quality Analysis Simulation Program Modeling System)

Name or number of most recent release

Version 5.10

Intended use of model

WASP is a generalized modeling framework for contaminant fate and transport in surface waters. Three submodels are included in the WASP model. TOXI (toxic chemical model) predicts dissolved and sorbed phase chemical concentrations in the bed and overlying waters. EUTRO (eutrophication model) predicts dissolved oxygen, biochemical oxygen demand, phytoplankton, chlorophyll-a, carbon, ammonia, nitrate, organic nitrogen, and orthophosphate. DYNHYD is a simple link-node hydrodynamic program that predicts flows, volumes, velocities, and depths.

Model developer

Robert B. Ambrose, Jr., P.E.
Environmental Research Laboratory
US Environmental Protection Agency
960 College Station Road
Athens, Georgia 30605-2700 USA
Phone +1 706 546 3323
AMBROSE.ROBERT@EPAMAIL.EPA.GOV

Sponsoring institution

US Environmental Protection Agency
Athens Environmental Research Laboratory
Center for Exposure Assessment Modeling

Date of most recent release

September 1993

4c.2. Documentation and Systems considerations

4c.2.1. User manual

Availability

The manual is distributed in WordPerfect 5.1 with the model. The model and manual can be obtained on diskette from the sponsoring institution or by way of the world wide web (internet):

ftp://earth1.epa.gov/epa_ceam/wwwhtml/ceam_home.html/

Language

English

Clarity
Good

Defines model limitations
Yes.

Includes conceptual model description
Yes.

Includes mathematical model description
Yes, the first part of user manual contains equations describing how the model works.

Includes sensitivity analysis
No.

Provides assistance in determining model parameters
The User Manual contains some literature references and summary tables for parameters used in the model.

Provides test examples
Several test data sets are included.

Provides references
Yes

4c.2.2. Other documentation considerations

Tightness of version control
Controlled by model author.

Availability of source code
Included in distribution of earlier versions. Now only available by special request. Code is written in Lahey FORTRAN 77.

4c.2.3. Systems considerations

Hardware requirements
IBM-PC compatible computer, 80386 or 80486, 640 base memory and 4mb of free extended memory, program files require approximately 6mb hard disk space, input and output files will use 10 or more mb.

Run time for standard scenario
Run time is dependent on the complexity of the scenario being simulated. Using a 50 Mhz 486 computer, it requires approximately 30 seconds per year to simulate toxicant concentrations in a simple pond. A very complex settling basin scenario required 3 minutes per year of simulation. On a 50 MHz '486 it requires approximately 0.5 to 3.0 minutes per year to run the model (depending on the complexity of the scenario being modelled).

Reliability
High

Clarity of error messages

Errors generated within the program to describe problems in data input and output are clear. Errors generated by the compiler (for example if your computer has insufficient memory) are generally unclear.

4c.2.4. Support

Method of support

US Environmental Protection Agency Center for Exposure Assessment Modeling continues to support this model.

Availability of information about bugs, corrections, and new versions

No information is systematically distributed

Training for users

Training is routinely offered (contact model developer).

4c.2.5. Input/Preprocessor

User friendliness

Good preprocessor for hydrodynamic files. Input files for TOXI and EUTRO are in fixed format files that are difficult to use and interpret.

Help utility

Included in WISP (a shell to run WASP) for overall file and program management.

Data range checking

None.

Sample input files

Several are included.

Database included

A limited database for some parameters is included in the user manual.

Availability of needed data

Data are generally available for simple assessments. Data may not be readily available for some parameters (for example indirect photolysis rates) used in some assessments.

Availability of standard scenarios

Some simple scenarios are included with model.

Flexibility

Very flexible, can represent flowing and static systems with various configurations, linkages, and loadings.

4c.2.6. Output/Postprocessor

Nature of output

Text (ASCII) report files. Postprocessor very useful for seeing on screen graphs of many variables over time.

User friendliness

Post processor is easy to use. Can ask for specific graphs on screen.

Help utility

None

Sample files

Sample output files can be produced easily using the sample input files.

Flexibility

Flexible. Can import output files into spreadsheets for additional data analysis.

Documents input parameters

Yes.

Clarity of output reports

Generally good. Some parameters are difficult to interpret without guidance from the manual.

4c.3. Model Science

4c.3.1. Compartments considered

Water, suspended solids, plankton, sediment pore water, sediment, benthos.

4c.3.2. Entry routes

Entry routes and application

Chemical loads can be applied to water and sediment segments.

Frequency of application

Loads can be either constant (length of time specified) or pulsed. Realistic simulations of nonpoint source loadings can be made by linking WASP with a surface runoff model (for example PRZM).

4c.3.3. Numerical technique

Adequacy of algorithm

Algorithms appear to be adequate for task.

Definition of lower boundary condition of sediment

Solid - no seepage allowed. But multiple sediment segments can be simulated so seepage to a deeper sediment layer can be simulated.

Stability

Model is stable with appropriate input parameters.

Numerical dispersion

For simple scenarios numerical dispersion is not a problem. A section in the User's Manual discusses the magnitude of numerical dispersion for different scenarios and provides guidance on how to estimate and reduce the magnitude of any dispersion.

Time increments

Model automatically adjusts the integration interval (or it can be defined by user). Reporting interval for output can be specified by user.

Space increments (direction of flow for water, depth for sediment)

Size of model segments, direction of flows, and communication between segments are defined by used.

Verification of numerical technique

Unknown.

4c.3.4. Surface water model (vertical and horizontal heterogeneity)

Model assumes instantaneous mixing and homogeneity within any given segment. Transfer of chemicals between segments can be defined by user.

4c.3.5. Surface water hydrology model (static/dynamic)

Hydrology model is dynamic. While the hydrodynamics model DYNHYD5 is included with WASP5, other models such as RIVMOD and SED3D have also been used in conjunction with WASP5 (contact model developer). Not only is water flow and velocity simulated but also sediment deposition, resuspension, and pore water movement.

4c.3.6. Surface water pesticide model

Metabolites

A total of three chemicals can be modeled (for example one parent and two metabolites, or two parents, one of which has a metabolite).

Adsorption to suspended solids

Type of model (linear, nonlinear, kinetics)

Linear (reversible) sorption based on user specified partition coefficient.

Dependency on environmental parameters (i.e. temperature, pH)

None

Adsorption to water plants

Type of model (linear, nonlinear, kinetics)

Linear model of biosorption to phytoplankton.

Dependency on environmental parameters (i.e. temperature, pH, plant characteristics)

Affected by temperature.

Degradation in surface water

Type of model (first order, power law, Menten)

Simple first-order reaction.

Dependency on environmental parameters (i.e. pH, light intensity, microbacterial activity, temperature)

pH, light intensity, temperature, and microbial activity, are all considered.

Mechanisms considered

Hydrolysis, photolysis (direct and indirect), oxidation, reduction, transformation, volatilization, biolysis, are all considered. The user can also supply a single lumped first order decay to represent all mechanisms.

Compartments considered
Dissolved and sorbed components calculated separately.

Advection in surface water
Set by user.

Dispersion in surface water
Set by user.

Volatilization
User may select from five options including defining the volatilization rate directly, or use of various common methods (O'Connor, MacKay, or Covar) for determining reaeration and volatilization.

Exchange with sediment (diffusion, advection)
Diffusion and advection can be defined across the interface. Also transport may occur as pore water is exchanged between sediment segments.

4c.3.7. Suspended solids model (static/dynamic)

Dynamic. Sediment resuspension and deposition is simulated.

4c.3.8. Aquatic vegetation model

Plant species
Not differentiated, only plankton are modelled.

Characterized by dry mass or surface area
Dry mass of plankton (mg/L) subjected to biosorption.

Type of model (static, dynamic: first order, power law, Menten)
Static in terms of sorption. However, by utilizing the EUTRO model, phytoplankton densities can be dynamic in response to environmental

4c.3.9. Sediment model (horizontal and vertical heterogeneity)

Homogeneous sediment within any given segment.

4c.3.10. Sediment hydrology model (static/dynamic)

Seepage loads for both water and chemicals can be modelled.

4c.3.9. Sediment pesticide model

Metabolites
One parent and one metabolite/degradate can be modelled.

Adsorption to solid bottom material
Type of model (linear, nonlinear, kinetics)

Linear adsorption. Dependency on environmental parameters (i.e. temperature, pH)
None

Degradation in sediment
Type of model (first order, power law, Menten)
Pseudo second order kinetics

Dependency on environmental parameters (i.e. pH, microbacterial activity, temperature)
pH, microbacterial activity, and temperature are all considered.

Mechanisms considered
Hydrolysis, oxidation, reduction, transformation, biolysis, are all considered.

Compartments considered
Sorbed and pore water degradation calculated separately.

Advection in sediment
Set by user

Diffusion in sediment
Set by user

Dispersion in sediment
Set by user

Bioturbation
Included.

Inhomogeneity of distribution (e.g. layer of pesticides at sediment surface)
None.

Exchange with surface water (diffusion, advection)
Diffusion and advection across interface.

4d. EXAMS

4d.1. General Information

Name of model
EXAMS II (Exposure Analysis Modeling System)

Name or number of most recent release
Version 2.95

Intended use of model
EXAMS was designed to evaluate the behavior of organic chemicals in aquatic systems. The system computes exposure, fate, and persistence, based on loadings, transport and transformations.

Model developer
Larry Burns, Ph.D.
Research Ecologist, Biology Branch
Environmental Research Laboratory
US Environmental Protection Agency
960 College Station Road
Athens, Georgia 30605-2700 USA
Phone +1 706 546 3511
BURNS.LAWRENCE@EPAMAIL.EPA.GOV

Sponsoring institution
US Environmental Protection Agency
Athens Environmental Research Laboratory
Center for Exposure Assessment ModeLling

Date of most recent release
October 1995

4d.2. Documentation and Systems considerations

4d.2.1. User manual

Availability
Both a user's technical manual and users guide are available. The User Manual contains conceptual and mathematical descriptions of the EXAMS (Version 1) model. The User's Guide contains short descriptions of how to use the system and the parameters used in version 2.94.

Exposure Analysis Modeling System (EXAMS) User Manual and System Documentation April 1982 456 pages Report No. EPA-600/3-82-023 Reproduction available from: US Department of Commerce National Technical Information ServiceSpringfield Virginia 22161 USA

User's Guide for EXAMS II Version 2.94 September 24, 1994 Approximately 90 pages Available from Model Author. The model is also available over the internet.

Language
English

Clarity
Good

Defines model limitations
Somewhat.

Includes conceptual model description
In User Manual.

Includes mathematical model description
In User Manual. Any modifications made between EXAMS and the newer EXAMS II are undocumented.

Includes sensitivity analysis
No.

Provides assistance in determining model parameters
The User Manual contains numerous literature references for parameters used in the model. The User Guide provides limited assistance on how various terms interact.

Provides test examples
Several test data sets are included and one complete example is generated as part of the installation procedure. A "Lake Zurich" example is available from the model author.

Provides references
Yes

4d.2.2. Other documentation considerations

Tightness of version control
Controlled by model author.

Availability of source code
Included in distribution of earlier versions, Now only available by special request.

4d.2.3. Systems considerations

Hardware requirements
IBM-PC compatible computer, 512K free memory, 5-10 MB hard-disk space, MS-DOS version 2.12 or higher. A VAX version is also available.

Run time for standard scenario

On a '486 50 MHz machine it requires approximately one minute per year to run the model.

Reliability

High

Clarity of error messages

Errors generated within the program to describe problems in data input and output are clear. Errors generated by the compiler (for example if your computer has insufficient memory) are generally unclear.

4d.2.4. Support

Method of support

US Environmental Protection Agency Center for Exposure Assessment Modelling continues to support this model.

Availability of information about bugs, corrections, and new versions

No information is systematically distributed

Training for users

No regularly scheduled training. Some training is occasionally available at short-courses at scientific meetings or other events.

4d.2.5. Input/Preprocessor

User friendliness

Good, will prompt for response.

Help utility

Included in system. On-line help is available for every parameter and command.

Data range checking

During run some out-of-range data are flagged/adjusted and user is warned.

Sample input files

Included.

Database included

Database contains some chemical and environmental data for limited selection of organic chemicals and environmental scenarios.

Availability of needed data

Data are generally available for simple assessments. Data may not be readily available for some parameters (for example indirect photolysis rates) used in some assessments.

Availability of standard scenarios

Some simple scenarios are included with model.

Flexibility

Very flexible, can represent flowing and static systems with various configurations, linkages, and loadings.

4d.2.6. Output/Postprocessor

Nature of output
Text (ASCII) report files. Some crude, text based based graphics

User friendliness
Moderate. Can ask for specific tables on screen. System will lead user through simple menus to obtain desired tables.

Help utility
None

Sample files
One sample file produced as part of model installation.

Flexibility
Inflexible.

Documents input parameters
Yes.

Clarity of output reports
Generally good. Some parameters are difficult to interpret without guidance from the manual.

4d.3. Model Science

4d.3.1. Compartments considered

Water, suspended solids, plankton, sediment pore water, sediment, benthos.

4d.3.2. Entry routes

Entry routes and application
Chemical loads can be applied to water and sediment segments.

Frequency of application
Loads can be either constant (length of time specified) or pulsed.

4d.3.3. Numerical technique

Adequacy of algorithm
Unknown

Definition of lower boundary condition of sediment
Solid - no seepage allowed. But multiple sediment segments can be simulated so seepage to a deeper sediment layer can be simulated.

Stability
Unknown.

Numerical dispersion

For simple scenarios numerical dispersion is not a problem. For more complicated scenarios (approx. 32 compartments) numerical dispersion migth be significant.

Time increments

Model automatically adjusts the integration interval (or it can be defined by user). Reporting interval for output can be specified in Mode 2.

Space increments (direction of flow for water, depth for sediment)

Size of model segment and communication between segments is defined by used.

Verification of numerical technique

Unknown.

4d.3.4. Surface water model (vertical and horizontal heterogeneity)

Model assumes instantaneous mixing and homogeneity within any given segment. Transfer of chemicals between segments can be described.

4d.3.5. Surface water hydrology model (static/dynamic)

Hydrology and transfer of compounds between segments are steady state.

4d.3.6. Surface water pesticide model

Metabolites

One parent and one metabolite/degradate can be modelled.

Adsorption to suspended solids
Type of model (linear, nonlinear, kinetics).

Linear sorption based on Koc.

Dependency on environmental parameters (i.e. temperature, pH)

None

Adsorption to water plants
Type of model (linear, nonlinear, kinetics)

Linear model of biosorption.

Dependency on environmental parameters (i.e. temperature, pH, plant characteristics)

None

Degradation in surface water
Type of model (first order, power law, Menten)

Pseudo second-order kinetics.

Dependency on environmental parameters (i.e. pH, light intensity, microbacterial activity, temperature)

pH, light intensity, temperature, microbial activity, are all considered.

Mechanisms considered

Hydrolysis, photolysis (direct and indirect), oxidation, reduction, transformation, volatilization, biolysis, are all considered.

Compartments considered

Dissolved and sorbed components calculated separately.

Advection in surface water

Set by user.

Dispersion in surface water

Set by user.

Volatilization

Liss-Slater method; across water-air interface

Inhomogeneity of distribution (e.g. layer of pesticides at water surface)

None

Exchange with sediment (diffusion, advection)

Diffusion and advection across interface

4d.3.7. Suspended solids model (static/dynamic)

Static (so constant concentration of suspended solids, but moving with water body)

4d.3.8. Aquatic vegetation model

Plant species
Not differentiated, only plankton are modelled.

Characterized by dry mass or surface area
Dry mass of "plankton" (mg/L) subjected to biosorption.

Type of model (static, dynamic: first order, power law, Menten)
Static

4d.3.9. Sediment model (horizontal and vertical heterogeneity)

Homogeneous sediment within any given segment.

4d.3.10. Sediment hydrology model (static/dynamic)

Seepage loads for both water and chemicals can be modelled.

4d.3.11. Sediment pesticide model

Metabolites
One parent and one metabolite/degradate can be modelled.

Adsorption to solid bottom material
Type of model (linear, nonlinear, kinetics)
Linear adsorption

Dependency on environmental parameters (i.e. temperature, pH)
None

Degradation in sediment
Type of model (first order, power law, Menten)
Pseudo second order kinetics

Dependency on environmental parameters (i.e. pH, microbacterial activity, temperature)
pH, microbacterial activity, and temperature are all considered.

Mechanisms considered
Hydrolysis, oxidation, reduction, transformation, biolysis, are all considered.

Compartments considered
Sorbed and pore water degradation calculated separately.

Advection in sediment
Set by user

Diffusion in sediment
Set by user

Dispersion in sediment
Set by user

Bioturbation
Included.

Inhomogeneity of distribution (e.g. layer of pesticides at sediment surface)
None.

Exchange with surface water (diffusion, advection)
Diffusion and advection across interface.

4e. ABIWAS

4e.1. General Information

Name of model

Simulation des abiotischen Abbaus im Wasser (Simulation of abiotic degradation in surface water)

Name or number of most recent release

Version 1.0

Intended use of model

Model simulates the abiotic degradation in surface water focussing on photodegradation in water.

Model developers

M. Klein, R. Frank, W. Klopffer

Sponsoring institution

Umweltbundesamt Berlin

Date of most recent release

March 1993 (English version)

4e.2. Documentation and Systems considerations

4e.2.1. User manual

Availability

User manual available at the Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, D-57392 Schmallenberg.

Language

Available languages: German and English

Clarity

Good

Model limitations

Model assumptions are described.

Includes conceptual model description

Yes

Includes mathematical model description

Yes, but not very detailed.

Includes sensitivity analysis

No.

Provides assistance in determining model parameters

No

Provides test examples
Yes

Provides references
Yes

4e.2.2. Other documentation considerations

Tightness of version control
Only one version exists, no further development planned

Availability of source code
Available on request

4e.2.3. System considerations

Hardware requirements
PC with MS-DOS

Run time for standard scenario
Not more than one minute (386 DX, 25 Mhz)

Reliability
No problems known

Clarity of error messages
No error messages

4e.2.4. Support

Method of support
Provided by M. Klein

Availability of information about bugs, corrections and new versions
No information is systematically distributed

Training for users
Available on request

4e.2.5. Input/Pre-processor

User friendliness
Very good (menu oriented shell)

Help utility
Information on function keys available

Data range checking
No

Availability of standard scenarios
Yes, standard data set for radiation data and surface water available (which is used by the German authorities involved in pesticide registration)

Availability of needed data
Data are readily available

Flexibility
Limited flexibility

4e.2.6. Output/Post-processor

Nature of output
Tables and graphic

User friendliness
Very good (menu oriented shell)

Help utility
Information on function keys available

Sample files
Provided together with the programme on floppy

Flexibility
No flexibility

Documents input parameters
Yes

Clarity of output reports
Good (but at present only in German language)

4e.3. Model Science

4e.3.1. Compartments considered

Single compartment model (Water)

4e.3.2. Entry routes

Entry routes and application
Model needs an initial concentration in the water body

Frequency of application
Not possible to consider

4e.3.3. Numerical technique

Adequacy of algorithm
Usually analytical solution of degradation. If numerical techniques necessary to calculate degradation, the runge-kutta method is used.

Stability
No problems known

4e.3.4. Surface water model

Single compartment

4e.3.5. Pesticide model

Metabolites

No metabolite considered

Adsorption to suspended solids

Sorption to suspended solids is calculated by the model (linear model without dependency on environmental parameters) but sorption has no influence on degradation

Degradation in surface water

Usually first order kinetics (if light intensity doesn't change during the simulation)

Dependency of degradation on environmental parameters

Program calculates the rate constant dependent on pH, water depth, temperature, radiation data, UV-spectrums of the water body and the pesticide. Based on the actual environmental and pesticide parameters an overall rate constant is calculated if the light intensity in the water body changes during the degradation process the time dependent rate constant is calculated numerically.

Advection

Concentration of the pesticide is simulated for static as well as for flowing water

Volatilization

The volatization rate is linearly interpolated based on the water depth.

Exchange with sediment

None.

4f. Other models considered but not assessed in detail

4f.1 GENEEC

GENEEC (the GENeric Expected Environmental Concentration) is a screening model developed by Parker and Rieder (1995) at the USEPA Office of Pesticide Programs. The purpose of the model was to screen out compounds which would obviously not have problems with runoff. Because of the intentionally conservative way that GENEEC estimates runoff, most compounds will be passed to the next modeling tier which consists of modeling using PRZM and several standard scenarios. GENEEC was designed to estimate acute and chronic PEC values under worst case conditions. It simulates runoff from a 10 hectare field into a one hectare pond that is two meters deep. In the field portion of the model application is made to bare soil. Factors that are considered in the field include: drift, single and multiple applications, incorporation, and degradation. Runoff from the field occurs two days after a single application or immediately after the final application when simulating multiple applications. Runoff is assumed to be equivalent to ten percent of the product remaining on the field. Factors considered within the pond include: sorption, sediment degradation, hydrolysis, and photolysis. The program runs quickly and the model output is very simple. Since GENEEC was not designed to provide accurate estimates of product runoff and cannot be adjusted for different cropping, soil, weather, or aquatic scenarios it was not included in the critical summary of models.

4f.2 AQUATOX

AQUATOX is a simulation model developed by Richard Park (Eco Modeling, 20302 Butterwick Way, Montgomery Village, Maryland, 20879, USA). It is used to simulate partitioning, volatilization, hydrolysis, and microbial degradation in aquatic systems. The partitioning algorithms are based on the fugacity concept (MacKay and Peterson 1981) and include partitioning to water, suspended sediment, and biota. Model predictions have been qualitatively compared with field results for atrazine, chlorpyrifos, and esfenvalerate with predicted behavior and concentrations were similar to that seen in the field studies (timing of events was good and concentrations were within approximately one order of magnitude for most events). The model is also able to predict potential biological effects on a wide range of aquatic species including plants, invertebrates, and fish based on laboratory toxicity data and ecological linkages within the aquatic ecosystem. The model is very user friendly. This model was not included in the critical summary of models for two reasons: it is not widely used and it is not available free of charge.

4f.3 RIVWQ

RIVWQ is an aquatic transport model developed by Williams and Cheplick (1993). It can accomodate tributary systems, non-uniform flow, and mass loadings anywhere along the model system. Hydraulic nodes throughout the system are linked so that any changes in one node are instantaneously reflected in other nodes. Dispersion processes are lumped into a single dispersion coefficient. A single lumped constant is used to represent all degradative processes (hydrolysis, biolysis, etc.). Dilution, advection, volatilization, water/sediment partitioning, sediment burial, and resuspension are all simulated. The model has been used with acceptable results in simulating pesticide contamination in low gradient streams. This model was not included in the critical summary of models because it is still in development and accessibility is limited.

4f.4 IMPAQT

IMPAQT is a simulation model developed by De Vries at Delft Hydraulics (1987). It is a dynamical, physico-chemical model, which simulates the total, dissolved and particulate concentrations in watercolumn and sediment. It was developed to calculate mid-term and long-term concentrations of organic micropoolutants and heavy metals in simple (e.g. well mixed lakes) and in complex aquatic systems (e.g. estuaries, network of channels). Next to micropollutants suspended matter may be simulated separately.

In IMPAQT micropollutants are subject to volatilization, biodegradation, photolysis, hydrolysis and instantaneous, reversible sorption to DOC, POC and phytoplankton. It is also possible to include lumped degradation constants. Forcing functions like temeperature or pH may be imposed on the system as a whole or on individual segments.

Loads of micropollutants and suspended matter can be specified for each segment. The model has been applied for heavy metals on a smaller (lake Ketel) and a larger lake (lake IJssel). For lake Ketel Cadmium contents were well simulated, for lake IJssel insufficient data were available for a good comparison between model output and measurements. The model was not included in this critical summary of models because IMPAQT is not freely available, it is the property of Delft Hydraulics, the Netherlands.

4f.5 SOM-3

SOM-3 is the steady state version of IMPAQT, developed in view of the sensitivity analysis of IMPAQT. Is a simple model estimating fluxes, concentrations and adaptation times of micropollutants in aquatic systems. The model is especially suited to make quick estimations of sediment concentrations in deposition areas influenced by constant loadings.

The model has not been included in this critical summary of models as it is more intended for regional scale calculations than calculations at field scale.

4f.6 SLOOT.BOX^{DMU}

SLOOT.BOX^{DMU} is a modified version of the Dutch SLOOT.BOX model, to be used in Denmark. The main differences between the two lie in the presence of macrophytes in the Danish version and another description of pesticide volatilisation. For Denmark three different types of surface waters (pond, lake and stream) have been characterised in summer and winter time, for which the model is then applied. Pesticides can enter the system by spray drift, advective flow, runoff, drainage and seepage. Erosion is not considered. Field studies will be carried out in 1995-1996 to compare model results with experimental data.

The SLOOT.BOX^{DMU} model was not included in this critical summary of models as it closely reflects the original SLOOT.BOX model.

4f.7 TOPFIT

TOPFIT is a general compartment model designed primarily for pharmacokinetics (Heinzel *et al.*, 1993). It has been utilised to evaluate data of the fate of plant protection products and their degradates in water and sediment from laboratory or outdoor ‘microcosm’ studies; and to subsequently predict concentrations in static bodies of water and sediment following a sequence of input events (both pulse and continuous) (Carlton & Allen, 1994). The program requires the user to define a compartment model describing degradation and sorption processes, and to input data sets describing the amount of parent compound and degradates (if appropriate) in the water and sediment phases. The program then iterates ‘best-fit’ values for the parameters which describe the fate processes in the compartment model. These parameters can either be used as pesticide fate inputs into models which contain a hydrology sub-model or can be used to predict environmental concentrations in the surface water and sediment of a static system following definition (by the user) of an application/contamination scenario.

4f.8 References:

Carlton, R.R. & Allen, R (1994) The use of a compartment model for evaluating the fate of pesticides in sediment/water systems. Proceedings of the Brighton Crop Protection Conference pp 1349-1354.

Heinzel, G, Woloszczak, R & Thomann, P (1993) TopFit 2.0 Pharmacokinetic and pharmacodynamic data analysis system for the PC. Gustav Fischer, Stuttgart, Germany. 647 pp ISBN 3-437-11486-7 US-ISBN 1-56081-386-7.

Mackay, D. and S. Peterson. 1981. Calculating Fugacity. Environmental Science and Technology 15(9):1006-1014.

Parker, R.D. and D.D. Rieder. 1995. The Generic Expected Environmental Concentration Program, GENEEC. Part B, Users Manual. Tier One Screening Model for Aquatic Pesticide Exposure. Environmental Fate and Effects Division, Office of Pesticide Programs, U.S. Environmental Protection Agency.

Rasmussen, D, 1995. surface water model for pesticides - SLOOT.BOX. Technical report V. National Environmental Research Institute, Denmark.

De Vries, D.J.. 1987. IMPAQT, a physico-chemical model for simulation of the fate and distribution of micropollutants in aquatic systems. TOW-IW T250, Delft Hydraulics.

De Vries, D.J. and M.P.J.M. Kroot. 1989. SOM-3, a simple model for estimating fluxes, concentrations and adaptation times of micropollutants in aquatic systems. User's manual, T0632, Delft Hydraulics.

Williams, W.M. and J.M. Cheplick. 1993. RIVWQ Users Manual. Waterborne Environmental, Inc. Waterborne Environmental (987-B Harrison Street, S.E. Leesburg, Virginia 22075, USA.

ANNEX 5 Report file from EXAMS simulation

This is a standard report from EXAMS using Mode 3. All of the chemical and environmental input values are listed as documentation. Tables 15 through 20 contain the results of the simulation. The PECsw and PECsed values were obtained from Table 20.

```
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Chemical: 1) FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 1.01.1  Chemical input data for neutral molecule (Sp.#1).
 *** Chemical-specific data: SET via "entry( 1)"
 MWT:   2.50E+02 VAPR:  1.00E-06 HENRY:          KOW:
 KVO:            EVPR:           EHEN:           KOC:   1.00E+02
 *** Ion-specific data: "entry(1, 1)"
 SOL:   5.00E+01 KPB:            KPS:
 ESOL:           KPDOC:
 *** Reactivity of dissolved species: SET via "entry(1, 1, 1)"
 KAH:            EAH:            KNH:   9.63E-04 ENH:
 KBH:            EBH:            KRED:           ERED:
 KBACW:          QTBAW:          KBACS: 5.78E-04 QTBAS:
 *** Reactivity of solids-sorbed species:     "entry(2, 1, 1)"
 KAH:            EAH:            KNH:            ENH:
 KBH:            EBH:            KRED:           ERED:
 KBACW:          QTBAW:          KBACS:          QTBAS:
 *** Reactivity of "DOC"-complexed species:   "entry(3, 1, 1)"
 KAH:            EAH:            KNH:            ENH:
 KBH:            EBH:            KRED:           ERED:
 KBACW:          QTBAW:          KBACS:          QTBAS:
 *** Reactivity of biosorbed species:         "entry(4, 1, 1)"
 KBACW:          QTBAW:          KBACS:          QTBAS:

 Photochemical process data;  Ion-specific data: "entry(1, 1)"
 KDP(1, 1):          RFLAT(1, 1):          LAMAX(1, 1):
 *** Reactivity of dissolved species: SET via "entry(1, 1, 1)"
 K1O2:           EK1O2:          KOX:            EOX:
 *** Reactivity of solids-sorbed species:     "entry(2, 1, 1)"
 K1O2:           EK1O2:          KOX:            EOX:
 *** Reactivity of "DOC"-complexed species:   "entry(3, 1, 1)"
 K1O2:           EK1O2:          KOX:            EOX:
  QUA(1,1, 1)          QUA(2,1, 1)          QUA(3,1, 1)
 Light ABSORption (n,1, 1):       (1)             (2)
  (3)             (4)             (5)             (6)
  (7)             (8)             (9)            (10)
 (11)            (12)            (13)            (14)
 (15)            (16)            (17)            (18)
```

```
 (19)            (20)            (21)            (22)
 (23)            (24)            (25)            (26)
 (27)            (28)            (29)            (30)
 (31)            (32)            (33)            (34)
 (35)            (36)            (37)            (38)
 (39)            (40)            (41)            (42)
 (43)            (44)            (45)            (46)
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Chemical: 1) FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 2.  Chemical input data: product chemistry.
 ---------------------------------------------------------------
 No product chemistry specified.
 ---------------------------------------------------------------
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical: 1) FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 3.  Chemical input data: pulse loadings.*
 ---------------------------------------------------------------

 IMONth         1         1         1         1         1
 IDAY           1         3         3         6         6
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         2         1         2
 IMASS (kg) 1.000E-03 2.630E-02 1.680E-04 7.530E-03 4.860E-05

 IMONth         1         1         1         1         1
 IDAY           8         8        11        11        14
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         2         1         2         1
 IMASS (kg) 1.010E-02 7.110E-05 9.010E-03 5.540E-05 3.950E-04

 IMONth         1         2         2         2         2
 IDAY          14        22        23        24        25
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       2         1         1         1         1
 IMASS (kg) 1.700E-06 1.940E-03 9.560E-04 3.980E-04 2.820E-04
 ---------------------------------------------------------------
 * N.B.: These values represent the input request stream only;
         they may be revised during simulation.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical: 1) FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 3.  Chemical input data: pulse loadings.*
 ---------------------------------------------------------------

 IMONth         2         3         3         3         3
 IDAY          26        18        19        20        23
```

```
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 1.910E-04 1.170E-04 1.390E-04 1.010E-04 1.030E-04

 IMONth         3         3         3         3         3
 IDAY          24        25        26        27        28
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 1.920E-04 3.390E-04 2.810E-04 2.750E-04 2.860E-04

 IMONth         3         3         3         4         4
 IDAY          29        30        31         1         2
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 4.160E-04 5.670E-04 4.240E-04 8.150E-04 7.920E-04
 ---------------------------------------------------------------
 * N.B.: These values represent the input request stream only;
         they may be revised during simulation.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical: 1) FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 3.  Chemical input data: pulse loadings.*
 ---------------------------------------------------------------

 IMONth         4         4         4         4         4
 IDAY           3         4         5         6         7
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 6.810E-04 4.530E-04 3.470E-04 2.280E-04 2.000E-04

 IMONth         4         4         4         4         4
 IDAY           8         9        10        11        12
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 2.400E-04 3.070E-04 1.980E-04 2.010E-04 1.350E-04

 IMONth         4         4         4         4         4
 IDAY          13        14        15        16        17
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 1.800E-04 3.670E-04 3.840E-04 2.170E-04 2.400E-04
 ---------------------------------------------------------------
 * N.B.: These values represent the input request stream only;
         they may be revised during simulation.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical: 1) FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 3.  Chemical input data: pulse loadings.*
```

```
 -------------------------------------------------------------- 

 IMONth         4         4         4         4         4
 IDAY          18        19        20        21        22
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 2.330E-04 2.140E-04 2.480E-04 2.250E-04 2.360E-04

 IMONth         4         4         4         4         4
 IDAY          23        24        25        26        27
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 3.600E-04 4.070E-04 2.720E-04 2.520E-04 2.650E-04

 IMONth         4         4         4         5         5
 IDAY          28        29        30         1         2
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 2.350E-04 1.590E-04 1.310E-04 1.540E-04 1.630E-04
 --------------------------------------------------------------
 * N.B.: These values represent the input request stream only;
         they may be revised during simulation.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical: 1) FOCUS EXAMPLE
 --------------------------------------------------------------
 Table 3.  Chemical input data: pulse loadings.*
 --------------------------------------------------------------

 IMONth         5         5         5         5         5
 IDAY           3         4         5         6         7
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 4.680E-04 6.880E-04 5.660E-04 4.670E-04 3.230E-04

 IMONth         5         5         5         5         5
 IDAY           8         9        10        11        13
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 3.210E-04 2.300E-04 1.420E-04 1.050E-04 1.030E-04

 IMONth         5         5         5         5         5
 IDAY          24        25        26        27        28
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 1.650E-04 1.060E-03 2.550E-03 1.580E-03 1.170E-03
 --------------------------------------------------------------
 * N.B.: These values represent the input request stream only;
         they may be revised during simulation.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
```

```
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical: 1) FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 3.  Chemical input data: pulse loadings.*
 ---------------------------------------------------------------

 IMONth         5         5         5         6         6
 IDAY          29        30        31         1         2
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 1.110E-03 1.030E-03 1.000E-03 1.190E-03 8.640E-04

 IMONth         6         6         6         6         6
 IDAY           3         4         5         6         7
 ICHEM-ADB#     1         1         1         1         1
 ISEGment       1         1         1         1         1
 IMASS (kg) 5.650E-04 4.280E-04 2.470E-04 1.510E-04 1.610E-04
 ---------------------------------------------------------------
 * N.B.: These values represent the input request stream only;
         they may be revised during simulation.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 4.13.  Mean environmental input data: biologicals.**
 ---------------------------------------------------------------
 Seg  T*    BACPL    BNBAC    PLMAS    BNMAS
  #   y    cfu/ml   cfu/100g  mg/L    dry g/m2
 ---------------------------------------------------------------
   1  L    1.00E+05          4.00E-01
   2  B             2.00E+07          1.00E-02
 ---------------------------------------------------------------
  * Segment types: Littoral, Epilimnetic, Hypolimnetic, Benthic.
 ** Average of 12 monthly mean values.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 5.13.  Mean environmental data: hydrologic parameters.**
 ---------------------------------------------------------------
 Seg  T*    STFLO    STSED    NPSFL    NPSED    SEEPS     EVAP
  #   y     m3/hr    kg/hr    m3/hr    kg/hr    m3/hr     mm/mon
 ---------------------------------------------------------------
   1  L    3.60     6.00E-01 5.00     4.00             9.00E+01
   2  B                                        1.50
 ---------------------------------------------------------------
  * Segment types: Littoral, Epilimnetic, Hypolimnetic, Benthic.
 ** Average of 12 monthly mean values.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 6.13.  Mean environmental inputs: sediment properties.**
```

```
 ---------------------------------------------------------------
 Seg  T*    SUSED    BULKD    PCTWA    FROC      CEC       AEC
  #   y     mg/L     g/cm3      %             meq/100g (dry)
 ---------------------------------------------------------------
   1  L    3.00E+01                   1.00E-01 2.50E+01 2.50E+01
   2  B             1.85     1.37E+02 1.00E-01 2.50E+01 2.50E+01
 ---------------------------------------------------------------
  * Segment types: Littoral, Epilimnetic, Hypolimnetic, Benthic.
 ** Average of 12 monthly mean values.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 7.  Environmental input data: physical geometry.
 ---------------------------------------------------------------
 Seg  T*   VOLume    AREA     DEPTH    XSA      LENGth   WIDTH
  #   y      m3       m2        m       m2        m        m
 ---------------------------------------------------------------
   1  L    1.00E+02 2.00E+02 5.00E-01
   2  B    1.00E+01 2.00E+02 5.00E-02
 ---------------------------------------------------------------
  * Segment types: Littoral, Epilimnetic, Hypolimnetic, Benthic.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 8.13.  Mean miscellaneous environmental input data.**
 ---------------------------------------------------------------
 Seg  T*    DFAC     DISO2     KO2     WIND     DOC     CHL pgmt
  #   y     m/m      mg/L    cm/hr@20 m/s@10cm  mg/L      mg/L
 ---------------------------------------------------------------
   1  L    1.19     3.20     8.00     7.00E-01 5.00E-01 2.00E-03
   2  B
 ---------------------------------------------------------------
  * Segment types: Littoral, Epilimnetic, Hypolimnetic, Benthic.
 ** Average of 12 monthly mean values.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 9.  Input specifications -- advective transport field.
 ---------------------------------------------------------------

 J FR AD        1         2
 I TO AD        0         1
 ADV PR      1.00      1.00
 ---------------------------------------------------------------
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 10.13.  Mean dispersive transport field.
 ---------------------------------------------------------------
```

```
 J TURB            1
 I TURB            2
 XS TUR m2      200.
 CHARL m        1.02
 DSP m2/hr*    2.847E-05
 ---------------------------------------------------------------
 * Average of 12 monthly mean values.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 11.13.  Mean environmental data:  global parameters.*
 ---------------------------------------------------------------
 OXRAD (M) 1.00E-09 RAIN(mm/mo) 100.0   CLOUD    4.00 LAT   34.0
 OZONE(cm) 0.315    ATURB(km) 2.00      RHUM(%)  50.0 LONG  83.0
 ELEV (m):  200.0    Air mass type(s): R
 WLAM, P/cm2/s/N nm:  1.272E-05 6.300E-02  48.0     2.696E+04
  4.208E+06 1.926E+08 3.529E+09 3.105E+10 1.743E+11 6.411E+11
  1.729E+12 3.875E+12 6.705E+12 1.111E+13 1.576E+13 1.993E+13
  2.451E+13 3.903E+13 1.819E+14 2.000E+14 2.334E+14 2.598E+14
  3.130E+14 3.279E+14 3.340E+14 4.967E+14 5.993E+14 6.426E+14
  6.220E+14 7.415E+14 8.507E+14 8.987E+14 9.039E+14 9.514E+14
  9.233E+14 9.792E+14 1.004E+15 1.059E+15 1.087E+15 1.098E+15
  1.130E+15 1.139E+15 1.145E+15 1.150E+15 1.127E+15 1.082E+15
 ---------------------------------------------------------------
 * Average of 12 monthly mean values.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical:  FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 12.01.13.  Mean kinetic profile of synthetic chemical,
 computed from chemical and environmental reactivity data. **
 ---------------------------------------------------------------
  Seg T*    Local pseudo-first-order process half-lives (hours)
   #  y    Biolysis  Photol   Oxidat   Hydrol   Reduct   Volatil
 ---------------------------------------------------------------
   1  L                              7.20E+02          5.71E+05
   2  B    6.22E-02                  2.02E+04
 ---------------------------------------------------------------
   * Segment types: Littoral, Epilimnetic, Hypolimnetic, Benthic
  ** Average of 12 monthly mean values.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 ---------------------------------------------------------------
 Table 13.13. Mean chemical reactivity profile of ecosystem. ***
 ---------------------------------------------------------------
 T* S   pH  pOH Temp Piston Mean  Bact.  Oxidant Singlet Reduct.
 y  e           Deg. Veloc. Light Popn.   Conc.  Oxygen  (REDAG)
 p  g            C.   m/hr    %   cfu/** Molar   Molar   Molar
 ---------------------------------------------------------------
 L  1  8.0  6.0 15.0 7.1E-02  14 1.0E+05 1.4E-10 8.1E-16
```

```
 B  2  6.0  8.0 15.0            2.0E+07
 ---------------------------------------------------------------
   * Segment types: Littoral, Epilimnetic, Hypolimnetic, Benthic
  ** Active bacterial populations as cfu/mL in water column, and
     as cfu/100 g (dry weight) of sediments in benthic segments.
 *** Average of 12 monthly mean values.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical:  FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 19.  Summary time-trace of spatially averaged, monthly
 mean chemical concentrations during 1987.
 ---------------------------------------------------------------
 Month   Average Chemical Concentrations     Total Chemical Mass
 -----   -------------------------------     -------------------
        Water Column      Benthic Sediments  Water Col  Benthic
    -------------------- ------------------- --------- ---------
    Free-mg/L Sorb-mg/kg Pore-mg/L Sed-mg/kg  Total kg  Total kg
 ---------------------------------------------------------------
 Jan 1.61E-02  0.16      6.66E-05  6.66E-04   1.61E-03  9.33E-06
 Feb 1.31E-03  1.31E-02  1.00E-08  1.00E-07   1.31E-04  1.40E-09
 Mar 8.59E-04  8.59E-03  6.20E-09  6.20E-08   8.60E-05  8.68E-10
 Apr 1.83E-03  1.83E-02  1.46E-08  1.46E-07   1.83E-04  2.04E-09
 May 3.09E-03  3.09E-02  2.33E-08  2.33E-07   3.09E-04  3.27E-09
 Jun 1.18E-03  1.18E-02  1.04E-08  1.04E-07   1.18E-04  1.45E-09
 Jul 1.24E-16  1.24E-15  6.25E-21  6.25E-20   1.24E-17  8.76E-22
 Aug 4.51E-24  4.51E-23  2.26E-28  2.26E-27   4.51E-25  3.17E-29
 Sep 1.96E-31  1.96E-30  9.84E-36  9.84E-35   1.96E-32  1.38E-36
 Oct 8.84E-39  8.84E-38  4.44E-43  4.44E-42   8.85E-40  6.17E-44
 Nov 0.00      0.00      0.00      0.00       0.00      0.00
 Dec 0.00      0.00      0.00      0.00       0.00      0.00
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical: 1) FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 14.01.13.  Total annual allochthonous chemical loads and
 pulses (kg) during year 1987.
 ---------------------------------------------------------------
 Seg  Streams  Rainfall    Seeps   NPS Loads   Drift    Pulse IC
 --- --------- --------- --------- --------- --------- ---------
   1                                                   8.757E-02
   2                                                   3.448E-04
 ---------------------------------------------------------------

1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3

 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical:  FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 15.01. Average distribution of chemical during 1987.
```

```
 ---------------------------------------------------------------
 Seg  Resident Mass   ******** Chemical Concentrations *********
  #                     Total    Dissolved  Sediments    Biota
     Kilos      %       mg/*     mg/L **     mg/kg       ug/g
 --- -------- ------  ---------  ---------  ---------  ---------
 In the Water Column:
   1 2.18E-04 100.00  2.181E-03  2.180E-03  2.180E-02  0.139
     ======== ======
     2.18E-04  99.65

  and in the Benthic Sediments:
   2 7.63E-07 100.00  5.650E-05  5.448E-06  5.448E-05  3.475E-04
     ======== ======
     7.63E-07   0.35
 Total Mass (kilograms) =    2.1885E-04
 ---------------------------------------------------------------
  * Units: mg/L in Water Column; mg/kg in Benthos.
 ** Includes complexes with "dissolved" organics.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical:  FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 16.01.1.  Distribution of average concentrations among
 aqueous chemical species.  All concentrations in ug/L (ppb).
 ---------------------------------------------------------------
 Seg T*   Total      DOC      - Chemical Species (by valency) -
  #  y   Aqueous  Complexed     (0)
 ---------------------------------------------------------------
   1 L   2.18     5.317E-06   2.2
   2 B  5.448E-03            5.45E-03
 ---------------------------------------------------------------
  * Segment types: Littoral, Epilimnetic, Hypolimnetic, Benthic.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical:  FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 17.01.  System-wide concentration means and extrema.
 Number in parens (Seg) indicates segment where value was found.
 ---------------------------------------------------------------
         Total         Dissolved     Sediments       Biota
     Seg   mg/*     Seg  mg/L **   Seg  mg/kg     Seg  ug/gram
     -------------  -------------  -------------  -------------
 Water Column:
 Mean     2.181E-03      2.180E-03      2.180E-02      0.139
 Max  (1) 0.263      (1) 0.263      (1)  2.63      (1)  16.8
 Min  (1) 0.000      (1) 0.000      (1) 0.000      (1) 0.000

 Benthic Sediments:
 Mean     5.650E-05      5.448E-06      5.448E-05      3.475E-04
 Max  (2) 1.244E-02  (2) 1.200E-03  (2) 1.200E-02  (2) 7.652E-02
```

```
 Min  (2) 0.000      (2) 0.000      (2) 0.000      (2) 0.000
 ---------------------------------------------------------------
  * Units: mg/L in Water Column; mg/kg in Benthos.
 ** Includes complexes with "dissolved" organics.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical:  FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 18.01.  Sensitivity analysis of chemical fate: 1987.
 ---------------------------------------------------------------
    Mean Values by           Mass Flux    % of Total  Half-Life*
        Process              Kg/ hour        Flux       hours
   ----------------          ----------   ----------  ----------
 Hydrolysis                  1.9528E-07      0.67      776.8
 Reduction
 Radical oxidation
 Direct photolysis
 Singlet oxygen oxidation
   All Chemical Processes    1.9528E-07      0.67      776.8
 Bacterioplankton
 Benthic Bacteria            8.6744E-06     29.54      17.49
   Total Biolysis            8.6744E-06     29.54      17.49
 Surface Water-borne Export  2.0490E-05     69.79      7.403
 Seepage export
 Volatilization              2.4636E-10      0.00     6.1576E+05
                             ==========
 Total mass flux:            2.9360E-05
 ---------------------------------------------------------------
 * Pseudo-first-order estimates based on flux/resident mass;
   assumes transport delays will not throttle fluxes.
1Exposure Analysis Modeling System -- EXAMS Version 2.95, Mode 3
 Ecosystem: FOCUS EXAMPLE DITCH
 Chemical:  FOCUS EXAMPLE
 ---------------------------------------------------------------
 Table 20.01.  Exposure analysis summary: 1987.
 ---------------------------------------------------------------
 Exposure Concentrations    96-h Acute  21-d Chronic   Long-Term
 ========================== ----------  ------------   ---------
 Water Column      Baseline  1.609E-04    0.000        0.000
  dissolved plus   Average   4.918E-02    1.533E-02    2.180E-03
  complexed mg/L   Peak      0.263        0.263        0.263
 Water Column      Baseline  1.026E-02    0.000        0.000
  plankton         Average    3.14        0.978        0.139
  ug/g dry weight  Peak       16.8         16.8         16.8

 Benthic Sediment  Baseline  8.083E-09    0.000        0.000
  dissolved in     Average   1.937E-04    5.875E-05    5.448E-06
  pore water mg/L  Peak      1.200E-03    1.200E-03    1.200E-03
 Benthic Sediment  Baseline  5.155E-07    0.000        0.000
  benthos          Average   1.235E-02    3.747E-03    3.475E-04
```

```
 ug/g dry weight  Peak      7.652E-02    7.652E-02    7.652E-02

Fate:  Average Resident Mass -- kg            2.188E-04
====      Water Column . . . . . . . . . . . .     99.65 %
          Benthic Sediments  . . . . . . . . .      0.35 %
       Total Flux of Chemical -- kg / hour     2.936E-05
          Chemical Transformations:  . . . . .      0.67 %
          Biological Transformations:  . . . .     29.54 %
          Volatilization:  . . . . . . . . . .      0.00 %
          Water-borne Export:  . . . . . . . .     69.79 %
```