SESSION 6B

HERBICIDES IN THE ENVIRONMENT: MODELLING APPROACHES

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Papers	6B-1 to 6B-5

FOrum for the Co-ordination of pesticide fate models and their USe (FOCUS): aims and objectives

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ABSTRACT

Risk assessment is essentially a predictive process that relies heavily on the estimation of exposure. When carrying out environmental risk assessments, there are many compartments to consider. The processes involved in the estimation of exposure levels will vary depending on these compartments and on the geographical or regional location. The FOCUS working groups were set up to identify the most appropriate mathematical models to use and to develop standard scenarios. It was intended that these should be an aid to both the industry and regulators in the initial assessment of risk from the use of plant protection products.

INTRODUCTION

Regulatory decisions rely on the ability to be able to estimate risk following the recommended uses of a Plant Protection Product. For new Plant Protection Products the process is entirely predictive. Monitoring data could provide more realistic exposure information for existing products although even in these cases, exposure for all conditions of usage will still need some predictive capability.

Risk is expressed as a function of the hazard and exposure. In the regulatory process, the estimation of risk is based on the determination of biological effects and the estimation of the likely exposure. Raising the quality of the regulatory decision will depend upon reducing the uncertainty of the biological effect occurring and the likely exposure levels reached. This uncertainty can be associated with the study itself or with the application of the results to real events. There is a need to reduce uncertainty before authorisations can be granted. This can be achieved in a number of ways. The simplest of which is to apply a large safety margin or Toxicity/Exposure Ratio (TER) which would clearly over-estimate risk.

The basic decision-making step can be simplified (Figure 1) showing that there are three components to consider. First, the test animal or the biological end-point should be relevant to the impact assessment. The figure used in this part of the assessment would normally be the No Observed Effect Level or NOEL. Secondly, the Predicted Environmental Concentration (PEC) or the estimate of the residue should be realistic in terms of the proposed rate and frequency of use otherwise an extreme worst case concentration will be applied. Thirdly, the margin used in the safety assessment (TER) should take the uncertainty into consideration, which could result in a large factor being used. For example, it is usual to apply factors to allow intra- and inter-species variation in consumer and operator risk assessments.

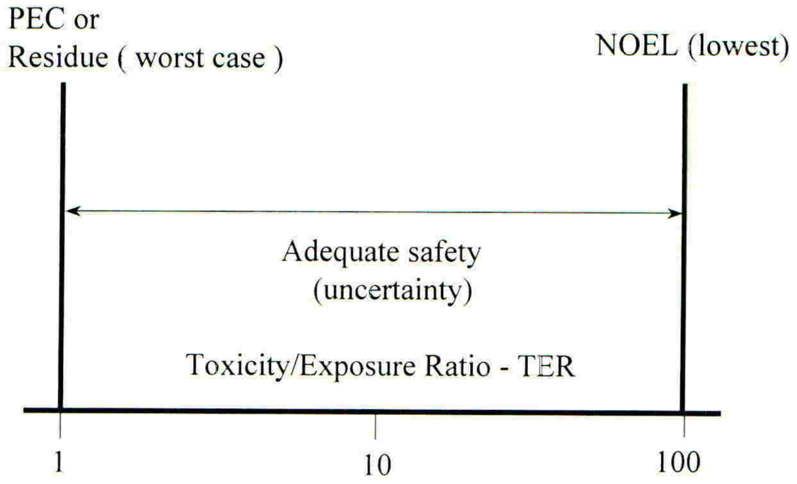

Figure 1. Simplified decision-making process.

In many regulatory situations, data do not exist in such quality to allow good estimates of exposure or biological effect. This results in so much uncertainty that the TERs have to be increased. Furthermore, there is a fully justified tendency for authorities to work with extreme worst case scenarios to overcome the effects of variability to establish PECs and to use the lowest known biological effect regardless of the relevance in the risk assessment (Tooby, 1996). The better the data generated by Agrochemical companies the less uncertain the PECs and biological end-points become, reducing the need for large TERs. For most risk assessments, it is the uncertainty over the exposure data, or PECs, that prompts the regulatory authority either to apply large safety factors (TERs) or to request additional costly field data.

PLANT PROTECTION PRODUCT DIRECTIVE

The harmonisation of the regulatory process across the EU through the Council Directive 91/414/EEC, and the various Annexes that followed, resulted in clear guidance on the data required for the risk assessment. The Annex III dossier had to contain exposure data relevant to operators, consumers and the environment. The “Uniform Principles” (Council Directive 97/57/EC) contained guidance on the evaluation procedure and decision-making process which made reference to the use of suitable calculation models to establish PECs. It went further and stated that no authorisations could be granted if TERs were not met or if certain environmental limits were exceeded. However, this was further qualified by the statement that authorisations could be granted if it was scientifically demonstrated that under relevant field conditions, the concentrations reached were not unacceptable. The estimation of robust PECs will be central to such assessments.

Exposure levels, or PECs, now play an enormously important part in the risk assessment and regulatory decisions can be affected by the quality of such data. It is commonplace now to use models in the assessment of consumer risk. Even the use of the various models for operator risk has been accepted in the first stage assessment. This particular area of risk assessment has progressed rapidly over the last few years due to support from the European Commission through specific working groups set up to develop EUROPOEM.

The use of models to predict the environmental concentrations likely to be found in soil within the treated area, on adjacent land and in ground- and surface-waters is more complex and has not been accepted yet within regulatory decision-making procedures. Nevertheless, the need to determine likely PECs in various compartments of the environment is clearly defined as a requirement under 91/414/EEC.

FORUM FOR THE CO-ORDINATION OF PESTICIDE FATE MODELS AND THEIR USE – FOCUS

It became clear during the development of the Directive and its Annexes that there was a need to define what models were accepted, for what purposes they were best used and to develop standard scenarios for regulatory purposes. In November 1992 an *ad hoc* group met in Brussels to set up what has become the FOrum for the Co-ordination of pesticide fate models and their USe – FOCUS. The working group is an informal grouping of regulators, industry representatives and experts from Government institutes.

A Steering Committee was set up to guide a number of working groups in the following fields.

1993	Leaching modelling working group
1994	Surface modelling working group
1995	Soil modelling working group

The leaching modelling working group was the first to prepare a report providing guidance on the prediction of the fate and behaviour of plant protection products in ground water. Much of the work of this group was used subsequently for the preparation of a report on soil persistence models. Alongside these working groups another group prepared a report on surface water models. Subsequently the following reports were accepted by the Standing Committee on Plant Heath as guidance documents.

1694/VI/95	Modelling environmental fate of PPPs in the context of their authorisation in the European Union
4952/VI/95	Leaching models and EU registration
6476/VI/96	Surface water models and EU registration of plant protection products
7617/VI/96	Soil persistence models and EU registration

The main aim of the working groups and the reports prepared by them were to provide industry and government regulators with expert advice on the current status of simulation modelling. In so doing it was also the intention to identify the deficiencies in the models when used in a regulatory capacity. The Steering Committee decided on a simple stepwise approach to be adopted by all of the working groups in developing the guidance notes. The following questions had to be considered.

- What was known about the existing models
- How to choose an appropriate model
- Was the model validated
- What was the availability of standard European scenarios
- How to evaluate the results

It should be noted that the Directive and the "Uniform Principles" refer to the need to establish PECs in air. An EPPO/CoE working group is currently developing suitable guidelines for the establishment of airborne concentrations under proposed conditions of use. An appropriate working group under FOCUS will consider this in due course.

SCENARIOS

Participants found the guidance on the use and selection of models very useful but they felt that a number of standard scenarios would provide a uniform approach to using the models and applying them to regulatory decision-making. It was agreed by the Steering Committee that ground water and surface water scenarios should be developed and two working groups were set up in 1997 to undertake this work. The three original working groups had discussed the need to develop scenarios across Europe so it was expedient to set up the new groups from the original membership but recognising the need to include representatives from all Member States (Figure 2).

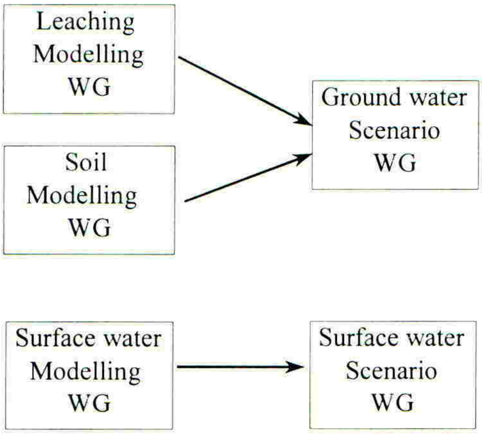

Figure 2 Relationship between FOCUS working groups (Nolting, 1998)

The Steering Committee set a very tight timetable to develop the scenarios. It was also agreed that representatives from Member States should be invited to a workshop, which was arranged in Bilthoven, to discuss the three reports already prepared and to be shown the provisional reports from the scenarios working groups. It was recognised that the problem of developing scenarios was very complex and not all scenarios would be available for the Bilthoven meeting. This workshop would also allow participants to gain practical experience of some of the models and proposed scenarios. It was important to involve experts and regulators from each of the Member States.

BILTHOVEN MEETING

The workshop took place on 3 and 4 September 1998 at the RIVM, Bilthoven, NL. Representatives of each Member State were given information about the aims of the FOCUS working groups; leaching, soil and surface water models; and soil/leaching and surface water scenarios. The scenarios were at a very early stage of development at that time but participants had the opportunity to hear about their development from the experts involved and subsequently to gain practical experience through a number of demonstrations.

Participants were encouraged with the work undertaken by the FOCUS groups and were impressed by the progress made since 1992. They recognised that although some models and scenarios could be used relatively easily for regulatory purposes, other scenarios would need to be used carefully until sufficient experience was gained. All participants looked forward to the development and refinement of further scenarios.

FUTURE PROGRAMME

The Steering Committee was keen to ensure that the final phases of the programme were completed on time and a very ambitious timetable was proposed (Table 1).

It was recognised that training was necessary for the use of the models and scenarios. So it was proposed to run a technical workshop, or a series of workshops in various regions of the European Community, sometime in the second quarter of 2000. A further workshop should be arranged for the Working Group on Pesticides – Legislation, Member State experts and ECPA to discuss the use of scenarios in the regulatory process.

USE OF MODELS AND SCENARIOS IN DECISION-MAKING

Two factors have to be considered when using the models and proposed standard scenarios. Firstly it has to be recognised that they have not been validated. Clearly the more site specific the intended decision, the more uncertainty will be associated with the estimation and the more likely that field or lysimeter data will be necessary to augment the findings. Secondly, the regulatory process is itself carried out in stages with a standard assessment conducted initially, for Annex I listing, followed by Member State authorisations for products. These latter authorisations will almost certainly require some data on specific scenarios relevant to that region or climate.

All of the FOCUS working groups recognised that the use of models and scenarios needed to follow a simple stepwise procedure. The leaching model working group set out clear instructions in their guidance document 4952/VI/95 which has been followed in principle by the other groups. Three steps were proposed: utilising standard scenarios for a first classification; specific scenarios for the identification of vulnerable situations; and site-specific data used alongside lysimeter or field data. In most cases for Annex I listing, only steps 1 and 2 should be needed. Step 3 would be used in a more refined assessment to support product authorisations.

Table 1 Future timetable

DATE	ACTIVITY
December 1999	- Focus working group reports and computer files made available to FOCUS Steering Committee; Member States; and ECPA for comment.
	- Working group chairmen to present reports to the Working Group on Pesticides – Legislation.
	- Comments to be sent by end February 2000 to the Commission and FOCUS working group chairmen.
March 2000	- FOCUS working groups to meet to modify reports and files according to comments received.
Mid-April 2000	- FOCUS Steering Committee to meet to discuss and approve reports and files.
End-April 2000	- Finalised reports and files to be made available.
May 2000	- Working Group on Pesticides – Legislation to adopt reports and files as a guidance document.
	- Reports and files to be made available to OECD.
May 2002	- Exchange of experiences between Member States after two years of use. Also to include experience from OECD members.

The use of models should not be confined simply to the final regulatory assessment at the end of the process. They should be used by the industry to develop scientific arguments and to identify the most appropriate higher tier testing and the most relevant sites to generate the best data for a risk assessment. Modelling does offer the ability to produce results from a number of conditions (climate or usage pattern) that can be used in a more informed regulatory decision. However, there now needs to be a period when models are used in the regulatory process to gain the necessary experience at all levels from Annex I listing to product authorisation.

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The development of FOCUS scenarios for assessing pesticide leaching to groundwater in EU registration

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ABSTRACT

A workgroup established under FOCUS (FOrum for Co-ordination of pesticide fate models and their USe) has chosen nine scenarios as representative of the range of climatic and soil conditions in agriculture regions in the EU where groundwater recharge occurs. These scenarios, to be used in initial evaluations for Annex 1 listing under the Directive 91/414/EEC, are considered to be reasonable worst cases (approximately 90th percentile) with the vulnerability split evenly between soil and weather properties. The workgroup has identified 26 crops as representative of EU agriculture, and agronomic parameters for those crops appropriate to each scenario have been obtained. The MARS database has been used to provide 20 years of weather data for each scenario. Computer shells containing the weather data, soil properties, crop parameters, and irrigation schedules have been developed for three models (PELMO, PESTLA, and PRZM) and for one of the nine scenarios also for the MACRO model. User input is limited to providing information on pesticide properties and application. All model shells provide pesticide concentrations leaching below 1 m depth averaged over periods of one, two or three calendar years. Some models also provide averages at greater depths when appropriate soil and

pesticide information are available. The scenarios will become available during the course of 2000.

INTRODUCTION

The Registration Directive 91/414/EEC, concerning the placing of plant protection products on the EU market came into force in 1993. According to this Directive, active substances are registered at the EU level (via placing compounds on Annex I of the Directive) whereas Member States are responsible for the registration of formulated products. Annex VI of the Directive gives the uniform principles for the registration process and implies that first estimates of predicted environmental concentrations (PECs) in the environmental compartments should be obtained via mathematical modelling. So modelling plays an important role in the decision-making process for the environmental aspects.

In 1993, the EU Commission and the European Crop Protection Association jointly established FOCUS (acronym for the FOrum for the Co-ordination of pesticide fate models and their USe) to provide guidance to the Member States, the European commission, and industry on the appropriate role of modelling in the EU registration process. The FOCUS organisation consists of a steering committee and working groups. The working groups consist of experts both from industry and from governmental or private institutes of Member States. Guidance was firstly developed for leaching to groundwater (FOCUS Leaching Modelling Workgroup, 1995) and later for soil persistence and surface water (FOCUS Soil Persistence Modelling Workgroup, 1997; FOCUS Surface Water Modelling Workgroup, 1997). The guidance developed by the workgroups included a description of the relevant models and their strengths and weaknesses. Any PEC model calculation assumes a scenario which is therefore an important element of the guidance. Several Member States have developed national scenarios for the registration of formulated products. However, no standard scenarios are currently available for the assessment of active substances at the EU level. Although the previous FOCUS workgroups developed recommendations for scenarios, they could not develop actual standard scenarios within their limited time frame.

Standard scenarios are needed because they increase the uniformity of the regulatory evaluation process by minimising the influence of the person that performs the PEC calculation and because they make PEC calculations and their interpretation much easier for both regulators and industry. Therefore the FOCUS Workgroup for Groundwater Scenarios was charged in 1997 by the FOCUS Steering Committee with developing a set of standard scenarios which can be used to assess potential movement of plant protection products and their relevant metabolites to groundwater as part of the EU process for placing active substances on Annex 1. Since this process proceeds at the community level, the standard scenarios have to apply to the whole EU. As a result, their selection criteria necessarily differ from those of the national scenarios used by individual Member States for decision-making on formulated products: any similarity with previously existing national scenarios will therefore be purely coincidental. The FOCUS Steering Committee prescribed that about 10 realistic worst case scenarios should be developed within a time frame of about 2 years. The product of the workgroup should consist of a report and a diskette containing input data for the scenarios covering at least the input needs of the models PELMO, PRZM and PESTLA.

GENERAL APPROACH FOR SCENARIO SELECTION

The aim of the FOCUS Workgroup for Groundwater Scenarios was therefore to develop about 10 realistic worst-case scenarios for pesticide leaching for the registration process of active substances at the EU level. The realistic worst case was implemented via the concept that scenarios should correspond with 90th percentile vulnerability situations. In general, the vulnerability of a scenario is a function of all system properties, which include pesticide properties: for instance, sensitivity of leaching to weather may be larger for weakly sorbing pesticides than for strongly sorbing pesticides. So a correct theoretical approach would imply development of hundreds of scenarios at the EU level which should all be run for the specified pesticide: a 90th percentile vulnerable scenario could then be identified from the resulting frequency distribution. However, the development of hundreds of scenarios was beyond the scope of the workgroup.

So a more pragmatic approach was followed: the vulnerability was assumed to be independent of pesticide properties and it was split evenly between soil properties and weather. Furthermore, the effects of soil properties and weather on pesticide leaching were assumed to be independent. Even then, the exact percentile for the soil properties and weather which will provide an overall vulnerability of the 90th percentile cannot be determined precisely without extensive simulations of the various combinations present in a specific region. Initially it was considered that the value for a 70th percentile soil and a 70th percentile weather would be a good representation of an overall 90th percentile. However, after performing some exploratory statistical analysis, it was decided that the overall 90th percentile could be better approximated by using an 80th percentile soil and an 80th percentile weather. The 80th percentile for weather was determined by performing simulations using multi-year weather data while the selection of the 80th percentile soil by expert judgement could only be approximate due to the lack of available soil databases. The actual percentiles of the soils selected thus probably lie between 60 and 95.

The locations were selected by an iterative procedure based on expert judgement with the following objectives: (i) be representative of major agricultural regions (as much as possible), (ii) span the range of temperature and rainfall occurring in EU arable agriculture and (iii) be distributed geographically across the EU with no more than one scenario per country. The selection process involved an initial proposal of about ten regions derived from examining information from a number of sources (FAO climatic regions, recharge map of Europe, temperature and rainfall tables, land use information, etc.). This proposal was refined by dropping similar climatic regions and adding regions in climatic areas not covered by the original proposal. Although some of these added scenarios are not located in major agricultural regions, they represent areas with a significant percentage of arable agriculture in the EU, albeit diffuse. The long-term average rainfall was obtained for a representative location in each region (Heyer, 1984). The end result was the selection of the nine locations shown in Figure 1 with target values of annual rainfall given in Table 1.

This approach contrasts with that of initially dividing Europe into 5-15 climatic zones and picking a representative location from each climatic zone. The latter approach could lead to criticism that the location selected in the climatic zone was not representative of some of the areas in the climatic zone. The selected locations should also not be viewed as sites representative of agriculture in the countries in which they are located. Instead the locations viewed collectively should be considered only as representative of agricultural areas in the EU.

SELECTION OF SOIL PROFILES

An important criterion was that the selected soil really exists (so properties of a soil profile of at least 1 m depth should be available). The selection of the soil was based on the properties of soils present in the specific agricultural region represented by a location. Thus unrealistic combinations of climatic and soil properties were avoided. The intent was to choose a soil that was significantly more vulnerable than the median soil in the specific agricultural region but not so extreme as to represent a worst case (thus approximating an 80th percentile vulnerability). Vulnerability of a soil profile was assumed to be determined by its texture and organic matter content. This is justifiable because sensitivity analyses have shown that PELMO, PRZM, PESTLA and MACRO are all very sensitive to organic matter content (see Boesten, 1991, for PESTLA) and that the capacity-flow models PELMO and PRZM are additionally very sensitive to texture. For these capacity-flow models, leaching is greater in sandy soils than in loams.

Due to a lack of available databases on soil properties, the selection of the appropriate soils generally had to be performed by expert judgement rather than a systematic selection procedure. An exception was the Okehampton location where SEISMIC, an environmental modelling database for England and Wales (Hallet *et al.*, 1995), was used to select a suitable soil. The FAO soil maps were used to obtain information on the average sand and clay fractions and the organic matter in a region. Based on these average values, target values for soil texture and organic matter were developed for each location. Then various members of the workgroup, usually in consultation with local experts, picked soils meeting these target values (values for topsoil parameters are provided in Tables 1 and 2). Soils which did not drain to groundwater were excluded where possible. In some cases, special consideration was given to soils at research locations where measurements of soil properties were readily available. In a few cases, the target values had to be re-examined during the process of picking specific soils.

The soil profile data were available as a function of the soil horizons and contained the following measurements as a function of depth: (i) organic matter or organic carbon, (ii) percentages sand, silt and clay, (iii) pH and (iv) dry bulk density.

There is evidence that the transformation rate of pesticides decreases with increasing soil depth. In general this depth dependency will be a function of both soil and pesticide. However, given the limited data available in the literature, it was decided to assume the same depth dependency for all soil profiles irrespective of the pesticide properties. So the following multiplication factor for the transformation rate is assumed: 1 for the 0-30 cm layer, 0.5 for the 30-60 cm layer and 0.3 for the 60-100 cm layer. Below 100 cm, the factor is set to zero (no transformation). This is the default option for the scenarios. If more information is available for the pesticide considered, the user may adjust the depth dependency accordingly.

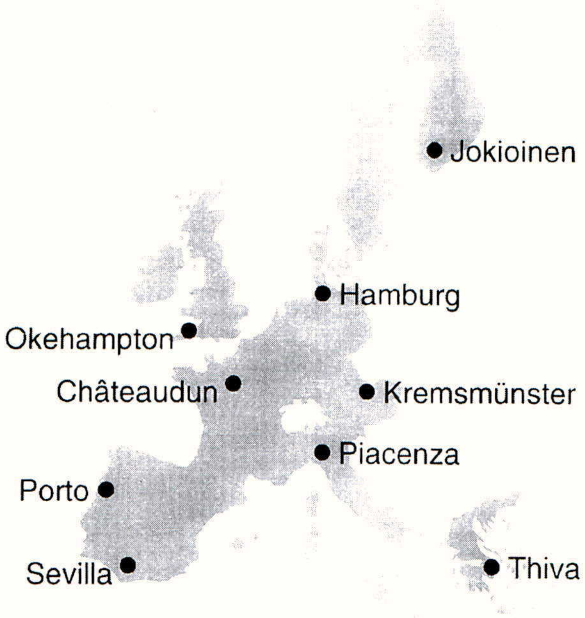

Figure 1. Map indicating the locations of the nine FOCUS groundwater scenarios.

Table 1. Soil and climatological properties for selecting the nine FOCUS groundwater scenarios.

Location	Code	Texture of surface soil layer (USDA classification)	Target annual rainfall (mm)
Châteaudun	C	silty clay loam	600
Hamburg	H	sandy loam	700
Jokioinen	J	loamy sand	600
Kremsmünster	K	loam / silt loam	900
Okehampton	N	loam	>1000
Piacenza	P	loam	750
Porto	O	loam	1150
Sevilla	S	silt loam	550
Thiva	T	loam	500

Table 2 shows that the organic matter contents in the top 30 cm range between 1 and 4% for all scenarios except those for Jokioinen and Porto which are above 6%. The large organic matter content for Porto is the result of the fluvial origin of the soil. Table 2 also shows that the decrease in organic matter with depth varies strongly between the locations: for instance, Jokioinen shows a strong decrease with depth whereas organic matter in Porto decreases only moderately with depth. Table 2 shows that the average volume fraction of water at field capacity (pF = 2) for the 0-100 cm layer ranges between 20 and 40%. The sandy loam from Hamburg and the loamy sand from Jokioinen have values that are lower than the seven other soils. The table shows that seven out of the nine scenarios have 30-38% water at field capacity: so most of the scenarios consist of soils with comparatively high field capacities. Additionally, Table 2 shows that the average groundwater levels for four of the nine scenarios are close to 1.5 m depth. Two scenarios (Hamburg and Sevilla) have levels of about 2 m depth and the remaining three (Châteaudun, Okehampton and Thiva) have levels deeper than 5 m.

SELECTION OF CROPS

The scenarios were made as realistic as possible by including most major European crops (except rice which was excluded since rice scenarios are being developed elsewhere and the regulatory models being used are not suitable for predicting leaching under these flooded conditions). Scenarios were developed for five crops grown in all nine locations (apples, winter cereals, grass including alfalfa, summer potatoes and sugar beet) and for 21 crops grown in at least one but not all nine locations. These 21 crop scenarios are in alphabetical order: beans (field), beans (vegetable), berries (bush), cabbage, carrots, cereals (spring), citrus, cotton, linseed, maize, oilseed rape (summer), oilseed rape (winter), onions, peas (animals), potatoes (winter), soybean, strawberries, sunflower, tobacco, tomatoes, vines. Sometimes a crop not typically grown in a specific area (for example, sugar beet in Okehampton) was included because it might be grown in similar soils and climates within the EU.

Theoretically, the crop also plays a role in the definition of the vulnerability of a scenario. However, as described above, the assumption was made that the vulnerability of the scenario was based on soil and weather only. Therefore, in general, average or median values were chosen for crop parameters. For all soil-crop-weather combinations, the consistency of the crop data was checked and, if necessary, crop data were modified. The following parameters were used to characterise a crop in a scenario: (i) dates of planting/sowing, emergence and harvest, (ii) maxima in time of the leaf area index, of soil cover and of the effective rooting depth together with the corresponding date (same date for all three maxima). Mostly, crop parameters were obtained from local experts who also checked the relevant crops for each location. The data on effective rooting depth were checked against possible soil restrictions.

SELECTION OF METEOROLOGICAL AND IRRIGATION DATA

The leaching models need daily meteorological data. These were derived from the MARS database (Terres, 1997). This database is based on a 50 x 50 km grid for the whole EU (plus Turkey and part of North Africa). For each grid cell meteorological properties were available on a daily basis for periods from 15-30 years. The grid cells in which the nine soil profiles

Table 2. Characteristics of the nine FOCUS groundwater scenarios (see Table 1 for explanation of location code). The irrigation amounts are the maxima of the six crop groups.

	Location code								
Property	C	H	J	K	N	P	O	S	T
Organic matter content (%)									
0-30 cm layer	2.3	2.6	7.0	3.6	3.4	1.7	6.6	1.6	1.3
30-60 cm layer	1.5	1.7	1.5	0.8	1.1	1.0	4.0	1.2	1.1
60-100 cm layer	0.5	0.1	0.6	0.5	0.5	0.3	3.7	1.0	0.4
Average volume fraction of water in 0-100 cm layer assuming pF=2 anywhere	0.38	0.25	0.20	0.35	0.31	0.30	0.38	0.36	0.35
Average depth of groundwater table (m)	12	2	1.5	1.6	20	1.5	1.5	2.4	>5
Average annual rainfall (mm)	650	790	640	900	1040	860	1150	490	500
Average annual irrigation (mm)	360	0	0	0	0	400	0	870	670
Average annual air temperature (°C)	11	9	4	9	10	13	15	18	16

were located, were selected and meteorological data for the 20-year period from 1975 to 1994 (which seems a defensible minimum period for deriving an 80th percentile) was obtained. If annual rainfall differed too much from the target values in Table 1, the daily rainfall of the scenario was scaled (i.e. multiplied with a constant factor) to obtain acceptable values for annual rainfall. This is justifiable because annual rainfall may vary strongly within distances as short as 50 km (e.g. from effects of mountains), which is not relevant for EU scenarios. The scaling procedure was applied for four of the nine scenarios (Kremsmünster, Okehampton, Porto and Thiva).

Irrigation was included for scenarios where this would be necessary for normal agriculture (Châteaudun, Piacenza, Sevilla, Thiva). Irrigation scenarios were based on the IRSIS irrigation scheduling software (Raes *et al*., 1988) and were developed for six crops (potatoes, maize, apple trees, alfalfa, tomatoes and sugar beet). It is assumed that the irrigation scenario of any crop is equal to one of these six. It is also possible that a crop is not irrigated (e.g. because winter wheat may grow on all locations without irrigation, it was assumed that winter wheat is not irrigated anywhere).

Table 2 shows that average annual rainfall ranges from about 500 mm to 1100 mm. For the locations where rainfall was not scaled, the annual rainfall differed by less than 10% from the target values. Table 2 also shows that the annual irrigation amounts can be considerable for the irrigated locations. As it is assumed that winter wheat is not irrigated, the actual irrigation minimum for all four irrigated scenarios is zero. For Châteaudun and Piacenza, the maximum annual irrigation is 360-400 mm, whereas it is much larger for Sevilla and Thiva (670-870 mm). Sevilla and Thiva have the smallest amounts of annual rainfall (490-500 mm). However, if a crop with the maximum irrigation is grown, the sum of rainfall plus irrigation is 1170-1360 mm (and Sevilla has the largest sum of all locations). So irrigation may have an enormous impact on the water balance in Sevilla and Thiva. Table 2 shows that average annual air temperature ranges from about 4 to 18°C. Jokioinen is by far the coldest scenario with about 4°C whereas Châteaudun, Hamburg, Kremsmünster and Okehampton are about 10°C. The four scenarios in the right part of the table are the southern scenarios with the highest temperatures.

IMPLEMENTATION OF SCENARIOS INTO MODELS

Models

The aim was to develop scenarios generally suitable for evaluating potential movement to groundwater. The intent was not to produce scenarios for e.g. one specific version of a model, but rather to describe a set of conditions that can continue to be used as existing models are improved and better models developed. However, simulating any of these scenarios with an existing model also requires the selection of many model-specific input parameters. Therefore, for uniform implementation of these standard scenarios, the workgroup generated input files needed to describe the scenarios with a relevant computer model. As required by the FOCUS Steering Committee, the scenarios were developed for three widely used regulatory models: PELMO 3.0, PESTLA 3.4 and PRZM 3.12 (Jene, 1998; Van Den Berg & Boesten, 1999; Carsel *et al.*, 1998). These models are based on the chromatographic transport theory and thus do not account for preferential flow through structured soils. One scenario was additionally developed with the MACRO 4.1 model (Jarvis & Larsson, 1998) to demonstrate to the Member States the effect of preferential flow. Within the EU, MACRO is the most widely used model that considers macropore flow of pesticides. The Châteaudun location was chosen for the MACRO scenario because the Châteaudun soil is heavier than at most of the other locations and because experimental data were available for calibrating MACRO soil parameters.

Procedure for crop rotation

Including realistic crop rotations in the scenarios appeared to become too complex to be justifiable for the workgroup. Therefore it is assumed that any crop is grown each year, so any model run will assume the same crop in all years. Some crops (such as potatoes) are rarely grown year after year in most agricultural regions. Therefore, an option was added to allow applications every year, every other year, or every third year. In order to conduct comparable evaluations, the simulation period was extended to 40 and 60 years for applications made every other year and every third year, respectively (by repeating the years of the 20 year data set in an appropriate order).

Simulation period

As follows from the previous section, the models need to be run for 20-, 40- or 60-year periods. In order to appropriately set soil moisture in the soil profile prior to the simulation period and because leaching may not always be largest in the first year of application (especially for persistent compounds with moderate to strong adsorption to soil), a six year "warm-up" period has been added prior to the simulation period (six years was chosen because it is divisible by 1, 2, and 3 so the warm-up period does not depend on application frequency). So all models need to be run for 26, 46 or 66 years. Simulation results during the warm-up period are ignored in the assessment of leaching potential.

Simulation depth

All simulations need to be conducted to a sufficient depth in order to achieve an accurate water balance. For capacity models such as PRZM and PELMO, this means that simulations need to be conducted at least to the maximum depth of the root zone. For models based on Richards equation such as PESTLA and MACRO, the simulations should be conducted up to greater depths (e.g. below the deepest groundwater level). With respect to concentrations of active substances and metabolites, the EU Uniform Principles (Annex VI of Directive 91/414/EEC) refers to concentrations in groundwater. However, a number of factors make simulations of chemical transport in subsoils difficult. This includes lack of information on subsoil properties, lack of information of chemical-specific properties of crop protection products and their metabolites (especially degradation), model limitations, and sometimes presence of fractured rock or other substrates which cannot be properly modelled using existing models. Therefore, at this time, output from all model shells report integrated fluxes of water and relevant compounds at a depth of one meter. When technically appropriate, models may report integrated fluxes at deeper depths such as at the hydrologic boundary or water table. As more information becomes available and improvements to models occur, the goal is to be able to simulate actual concentrations in groundwater.

Model output

The leaching of a compound is characterised by the mean concentration moving past a specified depth (currently 1 m as described above). This is defined as the integral of the solute flux over the period (total amount of active substance or metabolite moving past this depth) divided by the integral of the water flux over the period (total water recharge past this depth). In periods when the net recharge past 1 m depth is zero or negative, the mean concentration should be set to zero. The period is one calendar year for simulations for 26 years, two calendar years for simulations for 46 years and three calendar years for simulations of 66 years. So a model run always produces mean concentrations for 20 periods. All models have implemented this procedure and rank these 20 values from lowest to highest and select the 17th value representing the 80th percentile value for this weather series to get the overall 90th percentile as described before.

Input parameters for pesticides and their metabolites

Information on the properties of pesticides and their metabolites, application rates, and application timing must be left to the users to provide. However, the report of the workgroup (to be published in 2000) will contain detailed guidance to assist them in selecting the relevant properties of the pesticide. As the vulnerability of the scenarios is to be reflected in the soil properties and climatic data rather than in the properties chosen for the pesticides and their metabolites, mean or median values are recommended for parameters such as the degradation rate and the sorption coefficient.

CONCLUSION

Based on a simplified concept for assessing scenario vulnerability, nine groundwater scenarios for use in EU registration are being developed for the PELMO, PESTLA and PRZM models and one scenario for the MACRO model. They will become available during the course of 2000.

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FOCUS scenarios for assessing pesticide movement to surface water in EU registration

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ABSTRACT

Some years ago the European Commission established the FOCUS-organisation, in which governmental agencies, academia and industry worked together on the role of mathematical models in the registration process of plant protection products to estimate the predicted environmental concentration in the environmental compartments soil, groundwater and surface water. After having developed guidance on the use of specific models required for the estimation of surface water concentrations as the next step the development of European scenarios to be used in the models was considered a logical follow-up.

The process of developing the scenarios is dealt with including the reasoning to come to the choices made. In addition, some conclusions and recommendations of the working group are presented. Finally, some ideas are presented on the way the scenarios could be used in the EU-registration process for plant protection products in the future. An important condition for the use of models and scenarios is the availability of models and data including the expertise to interpret the results at the national authorities. Proposals will be presented to overcome these current gaps.

INTRODUCTION

In 1994 the European Commission established the FOCUS organisation. FOCUS stands for Forum for the Co-ordination of pesticide fate models and their Use. The European Directive 91/414/EEC deals with the process for putting plant production products on the market. In accompanying Annexes the data requirements (Annex II for the active substances and Annex III for the products) and the final Uniform Principles (Annex VI, 97/57/EEC) are mentioned. The Uniform Principles describe the criteria that must be fulfilled by the products to be put on the market in the Member States and also the way the registration authorities have to determine the concentrations to be expected in the environment after the application of the products. It is stated that "a suitable and at Community level validated calculation model" should be used for the environmental compartment soil, groundwater and surface water. For this reason three FOCUS Working Groups were established: 1) leaching to ground water, 2) surface water and 3) soil. All three groups gave an overview of the existing and useful models at the area of concern. Three reports (DOCs 4952/VI/95, 6476/VI/96 and 7617/VI/96) were adopted as guidance documents by the Standing Committee on Plant Health (SCPH) in Brussels to be used by all the Member States in performing risk assessments for registration purposes of plant protection products. As a follow-up of this activity and also based on the conclusions of the different groups the FOCUS Steering Group thought it useful to establish two new Working Groups on the development of European scenarios, one for groundwater/soil scenarios and one for surface water scenarios. The current paper describes the process the Working Group on Surface Water Scenarios has followed to develop these scenarios. The underlying reasoning for the choices and some preliminary conclusions and recommendations are mentioned.

GENERAL APPROACH FOR SCENARIO SELECTION

To develop a scenario for a calculation method for a concentration of an active substance in surface water several items are relevant. In the dossier package a registration company (or registrant) has to deliver to the governmental authorities, there are a lot of data on compound specific information relevant for the environmental compartments of the ecosystem, like:

- application data, i.e. dosage, frequency, interval;
- physico-chemical data, i.e. melting and boiling point solubility, vapour pressure, octanol-water partitioning coefficient K_{ow}, dissociation constant pKa;
- fate data, i.e. degradation in water/sediment systems, degradation in soil, hydrolysis, photolysis, sorption characteristics;
- ecotoxicological data, i.e. toxicity for water organisms, for birds, for earthworms, for micro- and macro-organisms, etc.

Some of these data is needed for the calculation of the Predicted Environmental Concentration (PEC) in surface water. There are, however, also other data a model may need before it is used for this purpose, the scenario data. To this type of data belong, e.g. crop, agronomic parameters like tillage, environmental parameters like hydrogeology, meteorology and soil data.

The following definitions are used in the context of development of EU-scenarios:

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

scenario data: freely chooseable information required to run the model applied in a specific situation and related to agricultural (crop, agronomic parameters like tillage), environmental (hydrogeology, surface water characteristics), climatic (meteorology), and soil (pH, % organic matter) characteristics.

The scenario definition calls for information on crops, soils, climate (precipitation and temperature), land use and steepness data. Several data based were consulted to find the relevant data to determine the areas in Europe that could be examples for the intended purposes. Table 1 shows the final selection and nomenclature of the scenarios to be used in the calculation models as determined by the working group.

Table 1. Defined scenarios.

Code	**Climate**	**Soil**	**Temperature**	**Precipitation**	**Slope**	**Type**	**Weather station**
D1	Scandi-navia	Clay	Cold	Moderate	Gentle	Drainage	Lanna
D2	North-west Europe	Clay	Temperate	Moderate	Gentle	Drainage	Brimstone
D3	Northern maritime	Sand	Temperate	Moderate	Flat	Drainage	Vredepeel
D4	Northern maritime	Loam	Temperate	Moderate	Gentle	Drainage	Skousbo
D5	Western maritime	Heavy loam	Temperate	Wet	Moderate	Drainage	La Jaillière
D6	Eastern Mediterranean	Heavy loam	Warm	Moderate	Gentle	Drainage	Thebes
R1	Middle European land	Silty	Temperate	Wet	Gentle	Run-off	Weiherbach
R2	Atlantic southern maritime	Loamy	Temperate	Very wet	Very steep	Run-off	Porto
R3	Middle European Mediterranean	Sandy loam	Warm	Wet	Steep	Run-off	Bologna
R4	Southern European Mediterranean	Loamy	Warm	Moderate	Moderate	Run-off	Roujan

In addition to the data summarised in Table 1, data on crops and types of surface waters (water bodies) are needed. In identifying the most relevant crops in Europe a list of crops was prepared taking into account the importance of the crop in aerial terms and distribution over Europe. The following crops were selected: cereals (not maize), maize, potatoes, sugar beet, oil seed rape, sunflower, Soya bean, tobacco, hops, vegetables, pome/stone fruit, citrus, vines and olives. For these crops specific data needed to be collected, some being scenario independent, like leaf area index, etc., others being scenario dependent, like emergence time, harvest date, etc. Using 1:25.000 maps of the areas a choice was made on the water bodies present in the locations, like ditches, small streams or ponds. Also the dimensions of the water bodies were determined. In Table 2 an overview is given of the different water bodies. It is assumed that the dimensions do not differ for the locations.

Table 2. Parameterisation for water bodies.

Variable	Ditch	Stream	Pond
Depth (m)	0.3	0.5	1.0
Replacement time (days)	50	0.1	50
Distance from field to water's edge (m)	0.5	0.5	3.0

WEATHER DATA

The weather data of the selected locations were analysed statistically for the mean weather year in the time period available. The MARS-project of the EU Joint Research Centre in Ispra, Italy, provided the meteorological data used. An additional requirement for the selection of the mean year was the presence of relevant storm events during the spring period especially for the run-off locations. To be able to run all the models a period of 16-month starting with the mean year was used to perform the calculations.

WATER BODIES

Three water types have been selected for the application of the scenarios: a small ditch, a stream and a pond. The determined default values for these water bodies are given in Table 2. The indicated values are not intended to be definitive but should be seen as an expert judgement's view on the intended reasonably worst-case situation.

MODELS

The inputs to water bodies after application of plant protection products are drift, drainage, run-off and atmospheric deposition. Atmospheric deposition is still not taken into account because of missing mathematical instrumentation. Drift will be described by interpolating the drift data as presented by Ganselmeier *et al.* (1995), drainage is calculated by the model MACRO (Jarvis and Larsson, 1998), run-off by the model PRZM (Carsel *et al.*, 1998) and finally, the fate of the substance in surface water by the model TOXSWA (Adriaanse, 1996). The way the models are connected to each other in the calculation sequence is given in Figure 1.

CURRENT WORK

The working group will present the final report at the end of the year 1999, including the description of the work done, the final input data for the different scenarios, using some example data of existing active substances and the results of the calculations following the sequence of Figure 1. Input files are being prepared for crops, weather, soil and other parameterisations required for the models, like dimensions of the area under consideration, the amount of surface water, the dimensions of the water bodies, etc.

The scenarios are intended to be used in the EU for the registration of plant protection products. It is of vital importance that the approaches proposed are understood and agreed in the Member states and that there is a willingness to use the models and the scenarios. Therefore, an intensive training and familiarisation programme will be started to introduce the scenarios in the Member States and industry. It is the intention to prepare a CD-ROM containing the models, the scenarios and the necessary documentation.

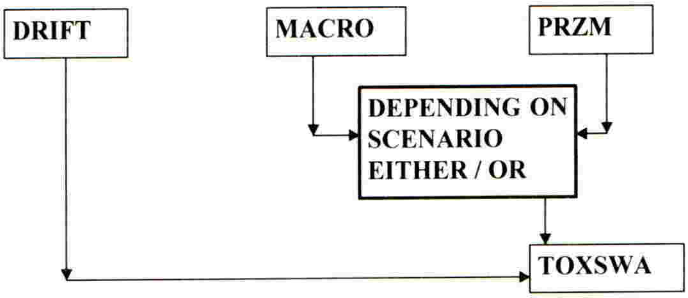

Figure 1. Calculation sequence of models.

The final report will also contain information on the Geographical User Interfaces of the different models to help the user in getting started with the models in the process of the evaluation of data concerning the determination of the Predicted Environmental Concentration (PECs) as described in Directive 91/414/EEC.

CONCLUSIONS

At the moment of the presentation of this paper a lot of work has been done or is carried out in the near future. Therefore it should be clear that nothing has been finalised yet and the results obtained should be considered as draft and treated with care. Currently, ten scenarios have been developed for use in PEC calculations for surface water, intended for the decision making within the framework of 91/414/EEC. The scenarios take into account several parts of Europe, with specific properties concerning soil, weather, crops and surface water bodies. The approach taken is a stepwise or tiered method in which the results of the PEC estimation may be compared to acute and chronic toxicity data for different species of aquatic organisms. If at a low tier the relevant trigger values are exceeded the next tier comes into operation. The working group believes that a useful tool has been reached to bring the process of risk assessment of plant protection products to a higher level of sophistication in which risk assessors and risk managers of different interests can have faith. More work needs to be done on the validation of the models, although the models use the current state-of-the-science in the mathematical description of processes occurring in the environment and in this case the aquatic compartment. Experts in fate and behaviour of plant protection products and experts on ecotoxicology have to work close together to further develop the comparison of modelling results and results of ecotoxicological testing. If agreement may be reached in this comparison the risk assessment process for regulatory use in the framework of 91/414/EEC can make a great step forward.

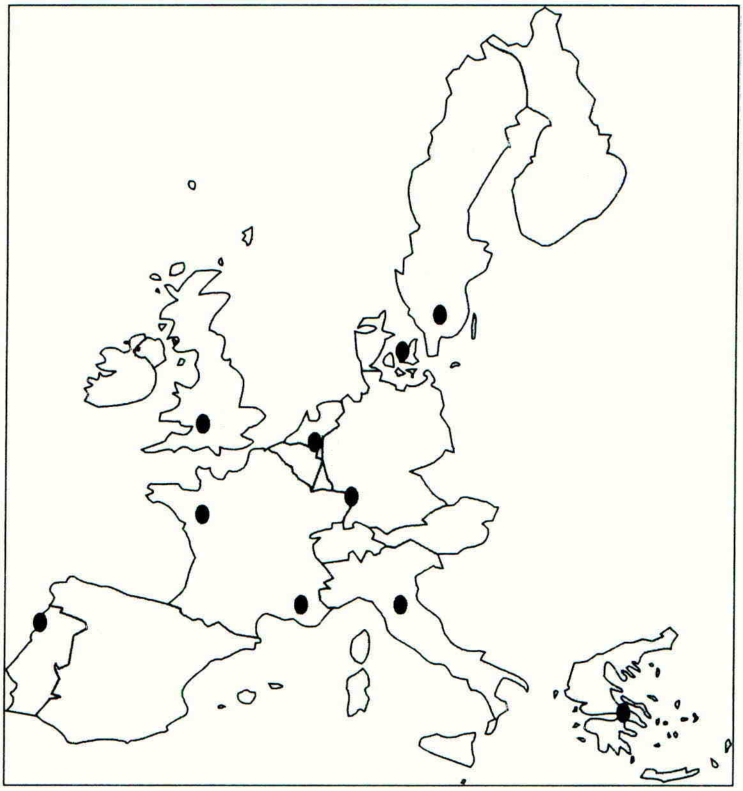

Figure 2. Areas/locations of the European Scenarios.

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Sensitivity analyses for the FOCUS leaching models

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ABSTRACT

Systematic sensitivity analyses using two different approaches (one-at-a-time and Monte Carlo techniques) were carried out for all four FOCUS leaching models (PELMO, PESTLA, PRZM and MACRO). Four scenarios were used comprising two hypothetical pesticides and either a sandy soil or a more structured medium loam soil. This paper presents results for PELMO 3.00 and the preferential flow model MACRO 4.1. Predictions of percolation by the two models were only slightly affected by a few input parameters. In comparison, pesticide losses were affected by numerous parameters and extremely large sensitivities were noted. In most scenarios, pesticide losses predicted by the two models were most affected by sorption and degradation parameters. However, investigations for one scenario involving a structured clay loam with MACRO revealed that, under specific circumstances, pesticide losses can be more affected by changes in hydrological properties of the soil.

INTRODUCTION

Pesticide fate models have played an increasing role in the registration of crop protection products in the last decade and this has been reinforced by EU directive EEC/91/414. Although pesticide fate models are widely used, little is known about the influence of the variation of input parameters on model results (the "sensitivity" of a model) or the implications of inaccuracies and approximations in the determination of parameters or in the modelling process itself on model predictions (the "uncertainty" of a model).

Sensitivity analysis provides the modeller with a list of parameters classified according to their influence on model results. Combined with information about the uncertainty of parameters, it can help differentiate between the parameters which require the most time and financial investment in their determination (those which are uncertain and that have a large influence on model output) and those which are less important in modelling terms. Also, it helps improve modelling in that it gives a list of parameters that will improve the modelling dramatically when changed. From a regulatory point of view, information on the sensitivity of models helps identify the parameters that should be looked at when reviewing modelling studies submitted for pesticide registration. It provides a means to assess the uncertainty in pesticide fate modelling and thus the confidence that should be attributed to modelling results. For all these reasons, sensitivity and uncertainty analyses provide valuable information to the whole modelling community, from the model developer, through to the non-expert or expert user and to the regulators.

Information on the sensitivity of pesticide fate models is scarce and where available, is usually limited to a few parameters, typically sorption and degradation parameters (Boesten

& van der Linden, 1991), or to one scenario (Jarvis, 1991). Although one would expect these specific parameters to significantly influence model results in most cases, they may not be the most sensitive parameters in all pesticide-soil-crop-climate scenarios.

This paper presents the results from one-at-a-time and Monte Carlo sensitivity analyses for the two pesticide fate models MACRO 4.1 and PELMO 3.00 using four scenarios with contrasting pesticide and soil properties. The number of input parameters considered was maximised.

METHODOLOGY

Models

The sensitivity of the four leaching models recommended by the FOCUS working group (MACRO, PELMO, PESTLA, PRZM) has been investigated. The latest versions of all models were used and this paper presents some results for MACRO 4.1 (July 1998 release) and PELMO 3.00 (July 1998 release). Models were combined with SENSAN, a sensitivity analysis tool which enables a model to be run repeatedly (Doherty *et al.*, 1994). Input parameters were automatically changed in the relevant input files before each run and values for selected model outputs were recorded. Furthermore, all model runs were documented and archived to allow further investigations.

Scenarios used

Sensitivity analysis results are usually dependent on the scenarios considered (Ferreira *et al.*, 1995). In order to represent a significant range of variation in environmental conditions, four scenarios were compiled by integrating two hypothetical pesticides with two soils of contrasting properties. Pesticide 1 has a Koc of 20 ml g^{-1}, a laboratory half-life in soil of 7.8 days at 20°C and is slightly volatile [Henry's constant=5×10^{-7} (-)]. Pesticide 2 has a Koc of 100 ml g^{-1}, a laboratory half-life in soil of 23.3 days at 20°C and is non-volatile. The two pesticides were considered to be applied to soils from the Wick and Hodnet series (Table 1) on 1 November. Weather data were selected from long-term records data for Silsoe (Bedfordshire, UK). The year 1979 was chosen from the 30-year dataset as being a wet year, especially during the winter and the spring periods. This choice was made to ensure that the weather scenario would be relevant to a large portion of the country and Europe, and that the pesticides which were chosen would leach to at least 1-m depth. The data for 1979 were repeated as many times as required to allow complete disappearance of the two molecules from the water moving to 1-m depth.

Derivation of sensitivity

One-at-a-time sensitivity analysis

One-at-a-time sensitivity analysis is one of the simplest ways of investigating the sensitivity of a model (Hamby, 1994). It consists in varying one parameter at a time while holding the others fixed. It provides the advantage of being easy to conduct and of producing results that

Table 1. Selected physico-chemical properties for the two soils used in the scenarios

	Wick soil				Hodnet soil			
Horizon no.	1	2	3	4	1	2	3	4
Organic carbon (%)	1.70	0.80	0.30	0.20	1.15	0.48	0.40	0.30
Sand (%)	57	70	73	77	33	42	29	26
Silt (%)	33	20	16	9	48	42	48	55
Clay (%)	10	10	11	14	19	16	23	19
Texture [a]	ZL	ZL	ZL	ZL	CL	ZCL	CL	CL
Bulk density	1.35	1.45	1.41	1.53	1.39	1.62	1.55	1.48
pH H_2O	6.5	7.0	7.0	6.9	6.7	6.8	6.8	6.8

[a] ZL: silty loam, CL: clay loam, ZCL: silty clay loam

can be readily presented in a graphical form. On the other hand, the sensitivity is assessed on individual parameters without regard to the combined variability resulting from considering all input parameters simultaneously. In the current study, the sensitivity of the model was assessed via an index representing the influence of the change of a particular parameter as compared to the base-scenario (*i.e.* the results from the run which was carried out with all input parameters at their nominal values). The Maximum Absolute Ratio of Variation (MAROV) for each model input parameter was calculated as follows:

$$MAROV = MAX_i\left(\frac{Percentage\ \ of\ \ variation\ \ in\ output}{Percentage\ \ of\ \ variation\ \ in\ \ input}\right)$$

where *i* represents the number of different values taken by a parameter.

The larger this index, the more influence a parameter has. MAROV can be visualised as the maximum slope of the line joining the origin and the different data points in a chart representing the percentage of variation in output *vs.* the percentage of variation in input.

Monte Carlo sensitivity analysis

The principle here is to run the model many times with values for input parameters sampled randomly in probability distribution functions. In contrast to the one-at-a-time approach, all selected parameters are varied at the same time. The Latin Hypercube Sampling scheme was used as it helps to reduce the number of runs required to achieve significance in the results. A total of 250 model runs was carried out for each scenario for each model combination as it is sufficient to achieve satisfactory results given the number of parameters. Each model input parameter included in the analysis was assigned a probability distribution function using expert judgement. Standardised multiple linear regressions on ranked data were performed to assess the contribution of each input parameter to the overall variability of the model results. The use of a rank transformation was made necessary by the non-linearity of pesticide leaching models.

RESULTS AND DISCUSSION

A total of *ca.* 4,500 runs were carried out to derive the sensitivity of PELMO and MACRO. The following discussion mainly concentrates on results from the one-at-a-time sensitivity analysis. Monte Carlo results can be found elsewhere (Dubus & Brown, 1999).

Sensitivity of results for percolation to changes in input parameters

Results related to percolation ('recharge' in PELMO) were far less sensitive to changes in inputs for both models than results for pesticide losses. Although meteorological inputs were not included in this investigation, these data (and especially the potential evapotranspiration) are known to significantly influence results for percolation. For all parameters considered, MAROV values for percolation were generally <1, which means that a variation of a parameter by 10% would affect percolation results by less than 10%. The hydrology in MACRO was dominated by a specific parameter (XMPOR) which represents the water content at the boundary between the two flow domains that are defined in this model. The initial soil moisture in the profile and some crop parameters, such as the maximum rooting depth and a parameter which describes the root distribution within the profile, were also near the top of the list of parameters affecting percolation results. As for MACRO, the PELMO model was mostly affected by a set of parameters related to the water contents in the different horizons (*i.e.* the field capacity and the initial soil moisture content).

Sensitivity of results for pesticide losses to changes in input parameters

Pesticide losses were affected by a much larger number of parameters compared to percolation and to a greater extent relative to percolation.

For the capacity model PELMO, total pesticide losses were mostly affected by parameters related to sorption (Freundlich coefficient and exponent) and degradation (degradation rates, increase in degradation with temperature) as outlined in Figure 1. A large number of parameters were classified as extremely sensitive or very sensitive. Extremely sensitive parameters have a MAROV >10, which means that a variation of 10% in the input parameter (e.g. by increasing the input parameter from 1 to 1.1) will at least double pesticide losses. For the fourth scenario (leaching of pesticide 2 in the Hodnet soil), extremely large MAROV values (>10,000) were found. This can be partly attributed to the use of a <u>maximum</u> ratio of variation as opposed to a mean or a range. The MAROV indicator is nevertheless relevant for classification purposes. Another factor which may explain extremely large MAROV values is that pesticide losses for the fourth scenario were predicted to be very low (*ca.* 1×10^{-4} g/ha) and calculations may be close to the model error. Extreme sensitivities for extremely low concentrations have also been observed by Klein (1997). When ranking parameters according to their influence on pesticide losses, the classification was found to be different for the different scenarios. For instance, although the first five most influential parameters were similar for three scenarios, their detailed ranking was different (Figure 1).

For the preferential flow model MACRO, the sensitivity of pesticide losses to changes in individual parameters was much smaller than for PELMO (six parameters with a MAROV >10 for MACRO for two scenarios compared to 17 for PELMO for the four different scenarios). Although individual parameters were less sensitive in most scenarios, the total number of influential parameters was greater for MACRO than for PELMO.

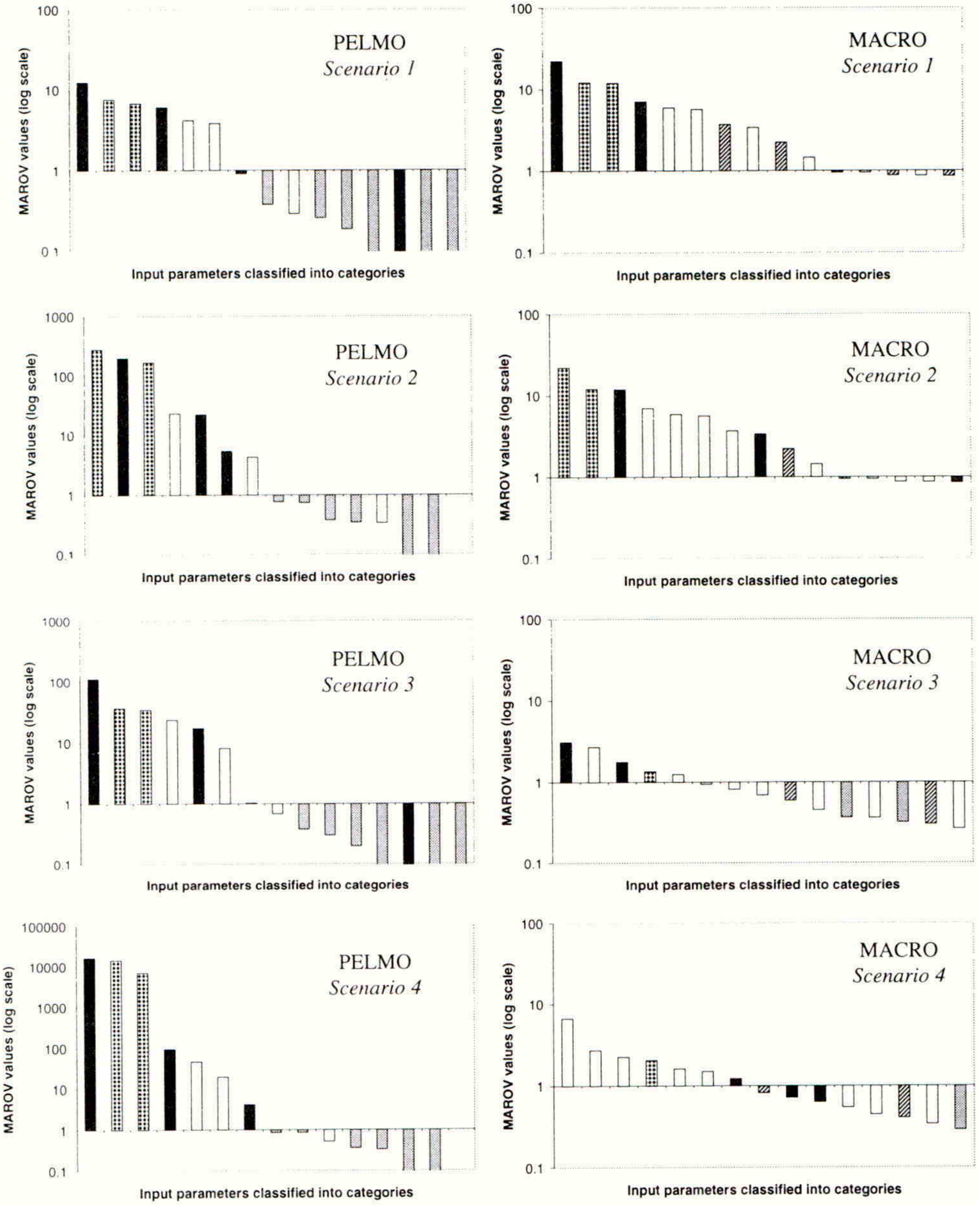

Figure 1. Sensitivity results of pesticide losses in PELMO 3.00 and MACRO 4.1. The larger the MAROV value, the more influence on pesticide losses the parameter has.

The 15 most sensitive parameters have been classified into five categories as follows:

■ Degradation parameters
▩ Sorption parameters
☐ Hydrological & soil parameters
▒ Crop-related parameters
▨ Miscellaneous

The relative dominance of Freundlich coefficient and exponent, and that of degradation rates was noted for the two scenarios involving the sandy loam, especially for Pesticide 1. However, this was not the case for the two scenarios involving the more structured Hodnet soil where parameters which describe the hydrology of the soil had a significant influence on pesticide losses (MAROV > 1). This was exemplified by the fourth scenario (Pesticide 2 on Hodnet soil) for which the top three parameters were TPORV (the saturated water content), ZN (the pore size distribution factor for macropores) and XMPOR (the boundary soil water content). Sorption parameters appeared fourth and tenth in the list of most sensitive parameters for this scenario, whereas parameters related to degradation ranked seventh (degradation rates), ninth and thirty-third.

CONCLUSIONS

Results from a sensitivity analysis conducted on the two registration models PELMO 3.00 and MACRO 4.1 showed that model predictions for percolation are only slightly affected by changes in input parameters considered here. In contrast, pesticide losses were influenced by more model inputs and to a greater extent. Prediction of pesticide losses by the two models were most affected by parameters related to degradation and sorption phenomena. In scenarios involving a medium structured soil, hydrological parameters were the main inputs determining the extent of pesticide losses. Detailed information on the sensitivity of the models to individual parameters has been prepared (Dubus & Brown, 1999).

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Predicting herbicide losses from hard surfaces: scenario characterisation and model concepts

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ABSTRACT

The environmental impact of non-agricultural pesticides is currently assessed by comparing available toxicological data with predicted environmental concentrations (PECs) assuming that 100 % of the applied compound is washed off the surface by a 25mm rainfall event. Studies sponsored by a consortium of government and industrial bodies have provided data, which is being used to develop an exposure model for herbicide losses from hard surfaces. Two scenarios are modelled: A 10 ha urban catchment draining to a small stream; a major road in a rural setting draining via gully pots to a small stream. Fixed parameters have been set for rainfall amounts, characteristics of the receiving body, 'hard' and non-hard surface type and run-off characteristics and herbicide application factors. A sub-model to predict the percentage of applied herbicide washed off each target surface has been developed based on results from 'field studies'. The only user inputs to the model are herbicide application rate, Koc and solubility.

INTRODUCTION

Herbicides are commonly used for total weed control on non-agricultural surfaces such as footpaths, road edges and railway track beds. In contrast to the fate of pesticides applied in the agricultural environment, there is almost no information on the dissipation and re-distribution of herbicides used in 'hard surface' environments and any associated contamination of receiving surface waters. In the absence of such information, the UK Pesticides Safety Directorate use a crude exposure assessment that assumes all of the herbicide applied on hard surfaces 'not intended to bear vegetation' is lost to surface waters in a volume equivalent to 25mm of rainfall. To redress this lack of information, a series of projects have been carried out to investigate and model the losses of herbicides from a variety of relevant man-made surfaces. This paper reports on the development of a set of 'hard surface' scenarios and an associated first-tier model for predicting surface water exposure resulting from herbicides applied to land not intended to bear vegetation.

DEVELOPMENT OF SCENARIOS

Herbicide is applied to hard surfaces in both urban and rural locations but the amounts of herbicide applied and methods of application differ depending on the surface type involved. To allow for these differences, two hard surface scenarios defined:

1. A small urban catchment with hard surfaces draining via gully pots to a small stream.
2. A major road in a rural setting with hard surfaces draining via gully pots to a small stream. The stream also receives drainage from an adjacent 1ha agricultural field.

Initially, it was proposed that an additional rural railway scenario would be included, but when a pilot field study established that wash-off losses from a railway formation were an order of magnitude lower than from a major road, the proposed railway scenario was rejected.

For both selected scenarios, a number of worst-case assumptions are made:

- Herbicides are applied in the early spring (March or April).
- Herbicides are applied in a continuous swath, rather than spot-applied.
- A significant rainfall event occurs 24 hours after herbicide application.
- Rainfall amounts are representative of a 'wet quartile' year.
- There is no degradation of herbicides before or during wash-off or during transport in the stream.
- There is no retention or dissipation of herbicide within the gully pots.

Derivation of rainfall patterns and amounts

Two rainfall parameters are required by the model in order to estimate concentrations relevant to 'acute' and 'chronic' exposure: First, the amount of rain falling in the 24 hour period 24 hours after application. Secondly, the time taken to accumulate the amount of rainfall that generates maximum herbicide wash-off from hard surfaces.

Values for a 'wet quartile' year are derived from detailed analysis of daily rainfall data measured over a period greater than 20 years (1959 – 1981), at six weather stations in the UK.

Table 1. 75th percentile daily rainfall at each of the representative weather stations based on cumulative frequency analysis for a 22 year period from 1959 – 1981.

Site	Climatic region	75th percentile daily rain (mm)	75th percentile number of days for 15mm rainfall
Lowestoft	Dry	3.75	7
Cambridge	Dry	4.0	7
Keele	Average	4.75	5
Brighton	Average	5.5	6
Newton Rigg (nr Penrith)	Wet	4.75	5
Swansea	Wet	7.0	4
Mean Value		**4.96**	**6**

The selected stations (see Table 1) are representative of parts of the country termed dry, wet and average depending on their long-term average annual rainfall. The two relevant rainfall parameters were calculated for each of the six weather stations and an average of these six values was used as the model parameter. The amount of rain falling in the 24 hour period, 24 hours after herbicide application was calculated from the cumulative frequency distribution of daily rainfall during the months of March, April and May for each site. 75th percentile values for daily rainfall are given in Table 1 and indicate that a realistic average for England and Wales is 5mm. Results from one of the hard surface 'field' studies suggested that a total of 15 mm of rainfall was required to produce maximum herbicide wash-off from a major road catchment comprising 100% hard surfaces. Using this as an indicator, the 75th percentile number of days required to accumulate 15mm of rainfall within the months of March, April and May at each of the representative stations was calculated. Results of these calculations are also given in Table 1 and show that a realistic England and Wales average for this model parameter is six days.

The derived critical rainfall parameters within the model are thus 5mm for the size of the first rainfall event after pesticide application and a total period of 6 days to accumulate 15mm of rainfall. To complete the rainfall pattern for the scenarios, the 10mm of rainfall remaining after the first rain event is divided equally over the remaining 5 days, giving 2mm per day.

Characteristics of the receiving water body

The characteristics of the receiving water body in each scenario are based as closely as possible on those proposed by the EC FOCUS working group on the development of surface water scenarios for calculating PECs in surface waters (Linders, 1999). This group has identified three types of surface water body, a ditch, a pond and a small stream. The first two each have a water residence time of 50 days and, given that the volumes of runoff entering the water body from the hard surfaces scenarios will be relatively large, neither of these water bodies is considered relevant. The receiving water body for all three hard surface scenarios is thus a small stream defined as being 2m wide with a water depth of 0.5m, a sediment depth of 0.3m, a sediment organic carbon content of 5% and a sediment bulk density of 0.8 g cm^3.

The length of the stream is dependent on the type of scenario. For the major rural road, stream length is 100 m, as in the similar FOCUS surface water scenario. For the urban scenario however, where the size of the catchment is 10ha, 100m is unrealistically short and a length of 316m is used. This represents one side of a 10ha square.

The stream contains no suspended solids and there is no uptake of herbicide by stream vegetation, thus reinforcing the overall 'worst-case' condition assumptions for the scenarios. It is assumed to have a 'steady state' and a daily turnover so that the depth and volume of water do not change. For each day, whatever volume of water drains into the stream, an equivalent volume drains out. This mechanism gives a relatively rapid water movement and is very simple to model.

Scenario Surface Characteristics

Each of the three scenarios has a fixed set of relevant surface characteristics that defines the nature and area of each different type of surface present.

The urban scenario has an arbitrarily defined total catchment area of 10 ha. Surface characteristics within this area are based on the available land cover statistics for Milton Keynes. Three broad types of surface are present. First, asphalt and concrete (roads, kerbs, and pavements), a proportion of which are sprayed with herbicide. In total asphalt and concrete cover 22.5% of the catchment. Concrete is present only as kerbs and pavements and the ratio of asphalt to concrete is 2:1. Secondly, buildings with storm drainage, which generate large amounts of runoff but do not get sprayed with herbicide. These cover 45% of the catchment. Finally, non-hard surfaces (parks, gardens *etc*) that generate some runoff but do not get sprayed with herbicide. These cover 32.5% of the catchment. Runoff from all three areas goes directly to the 316m long stream that drains the catchment.

The rural major road scenario comprises of a 100m stretch of road edged with concrete kerb stones along both sides. Surface characteristics are based on the study site for roadside wash-off, a stretch of the A6 trunk road running through the village of Shardlow in Derbyshire. The road surface, which is all asphalt, is 7m wide and drained via gully pots on both sides directly to an adjacent stream. Kerbstones are 12cm wide and 10cm high. On the stream side of the road, a 3m wide grass verge also drains directly to the stream. This verge includes a 20m length of 1m wide asphalt path, which directly adjoins the concrete kerb and drains into the gully pots. On the other side of the stream is a 1ha agricultural field that runs along its entire 100m length and drains directly into it.

The exact dimensions of each surface type in each scenario are given in Table 2.

Table 2. Surface characteristics for the scenarios

Surface type	**Area (ha) Urban scenario**	**Area (ha) Major road scenario**
Asphalt	1.5	0.072
Concrete	0.75	0.0024
Buildings	4.5	0
Non-hard surfaces	3.25	1.038
Total	**10**	**1.1124**

Rainfall-Run-off characteristics for the different surfaces

Research by Van de Ven *et al.* (1992) has shown that < 0.5mm of rainfall is needed to 'wet' a road surface before runoff occurs. It is therefore assumed that, prior to the first rainfall event the road surface is dry and the amount of rainfall needed to wet the surface is 0.4mm.

The rainfall-run-off characteristics used for the different hard surfaces in the defined scenarios are based on Ellis *et al.* (1986) who studied run-off from a 0.05 ha road surface catchment on the north west fringes of metropolitan London. Total surface run-off accounted for between 34 and 83% of measured total rainfall input. Losses were attributed to surface depression storage capacity and subsequent evaporation, pervious surface areas, infiltration losses down surface joints and cracks, vehicular-induced spray losses and instrumentation error. Bearing in mind the first-tier model requirement for a realistic worst-case scenario, a run-off value of 80% of incident rainfall was selected for all the hard surfaces within each scenario. This represents a value at the uppermost end of the range measured by Ellis *et al.* (1986).

Rainfall run-off for the non-hard surface areas in each scenario is 40% of incident rainfall, a value derived for slowly permeable soils in the HOST project (Boorman *et al.*, 1995). It is assumed that most soils in the defined scenarios will be compacted and disturbed.

Herbicide application

The only fixed scenario parameters relating to the herbicide are the application method as it affects the proportion of hard surface sprayed and the amount of interception by plants. These parameters vary according to the scenario type.

Within the urban catchment, the area sprayed is calculated assuming that herbicide is applied to a 30cm swath that includes road edges, kerbs and the adjacent pavement. The 30cm wide swath comprises 15cm on asphalt and 15cm on concrete. In addition, herbicide is 'spot sprayed' to weeds growing in cracks and joints of the paved areas. The total area that is spot sprayed represents 2% of the paved area not covered by the strip spray. According to CIRIA (1994), the average area for a gully pot catchment is 200 m^2. Based on this area, an urban road width of 7m and an adjacent paved area of 2m, the calculated area of concrete and asphalt that receives herbicide spray is 6.8 and 5.45 m^2 respectively. These represent 3.4% and 2.73% of the total concrete and asphalt surfaces in the catchment. The worst-case scenario assumes herbicide application to a heavy weed infestation and, because of this, 10% of the applied herbicide is intercepted by vegetation.

The most common application method for applying herbicide to a rural major road is by continuous strip spraying. The area of hard surface sprayed for this scenario is therefore taken to be two continuous 30cm wide swaths, one each side of the road. Kerb stones are 12cm wide and thus it is assumed that 15cm of the 30cm wide swath falls on asphalt, 12cm on concrete and 3cm is lost to non-hard surface adjacent to the kerb stones. Any herbicide falling on the non-hard surface areas is not taken into account in the model. In addition, a 20cm strip along the grass side of the asphalt path adjacent to one of the road kerbs receives herbicide spray. This application pattern covers 24 m^2 of concrete and 34.2 m^2 of asphalt, representing 100% and 4.75% of the total area of each surface type respectively. As with the urban scenario, 10% of the applied herbicide is intercepted by vegetation.

MODEL CONCEPTS

The only direct user-inputs to the model are herbicide application rate (g/ha), Koc in soil (ml/g) and solubility (mg/l). During application 10% of the herbicide is intercepted by plants and lost to the system. This proportion together with the herbicide application rate and the area of each type of hard surface that receives pesticide is used to calculate the herbicide load reaching each type of hard surface area within each defined scenario.

The calculated load reaching the hard surface area is then used as input to a sub-model that calculates the mass of herbicide washed-off the different hard surfaces for each day of the six-day simulation period. The sub-model is based mainly on results of a 'controlled' wash-off study carried out to investigate losses from different types of hard surfaces (Shepherd *et al.*, 1999). For each surface type, masses lost are calculated for each 0.5mm increment of rain. Herbicide is lost in both soluble and non-soluble form, the amounts depending upon solubility of the compound in relation to run-off volumes and mass applied. Empirically derived 'retention factors' retain a fraction of the applied herbicide upon individual surfaces, preventing complete wash-off of compound in the first few rainfall increments. During wash-off, some herbicide is adsorbed to individual surfaces, depending upon the compound's Koc and an empirically derived, surface-specific 'adsorption fraction' which is applied to the

Koc. The calculated mass of herbicide lost to the stream each day is further reduced by instantaneous partitioning to the upper 1cm of sediment in the stream. Partition coefficients are calculated from the compound Koc in soil and the organic carbon content of the sediment.

Runoff volumes (l) for each rainfall event are calculated from the surface area of each surface type present in the scenario multiplied by the total rainfall in the event (mm) minus the amount needed to wet the surface (mm) multiplied by the percentage run-off for each surface type. These calculated run-off volumes are added to the initial volume of water in the scenario stream to give the daily volumes of water moving through the stream.

Finally, daily average concentrations of herbicide in the stream are calculated from the mass in solution and the total volume of water moving through the stream. Studies are currently being performed to evaluate the model at the urban and major road catchment scales.

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