TERRACE

Terrestrial Runoff modelling for Risk Assessment of Chemical Exposure

YEAR THREE REPORT
Version 1.0

Final report on the TERRACE project

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EXECUTIVE SUMMARY

This report outlines the work carried out throughout the CEFIC-LRI funded project TERRACE (TErrestrial Runoff modelling for Risk Assessment of Chemical Exposure), and gives details of work carried out in Year 3.

In the first year of the project, a review of the state of the art in contaminant transport modelling for application at the catchment scale was undertaken. A shortlist of three preferred options that provide very different approaches to catchment scale modelling was presented:

- ANSWERS-2000; a physically based distributed model.
- SWAT-2000; a conceptual semi-distributed model.
- SWATCATCH; an empirical semi-distributed model.

Of these 3 models, SWAT-2000 was selected for further development for the 2nd and 3rd year of the project. The selection of SWAT-2000 was justified on a number of grounds:

- It was designed for assessment of land management practices in large catchments.
- It is spatially distributed.
- It has an extensive parameter database and a GIS-based graphical user interface.
- It incorporates sub-models for the processes operating in agricultural catchments (i.e. soil erosion, nutrient & pesticide transport, crop growth, etc,)
- Some validation work has been carried out.

The second year of the study focussed on two main aspects:

- Investigating and obtaining pan-European databases to facilitate application of a diffuse source pollutant computer modelling package.
- The development of our preferred modelling option, SWAT-2000, for use in Europe.

In Year 3 SWAT has been applied to the Exe catchment in south-west England, and outputs, in the form of contaminant load-duration curves have been produced for transfer to the GREAT-ER river modelling package. This allows diffuse source contaminants to be input to GREAT-ER as quasi point sources along the river network. A linkage between load-duration and flow-duration curves is used to sample the load-duration curve at an appropriate percentile point.

Finally a validation and implementation plan for the derived diffuse source pollution modelling approach is given.

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1. Introduction

This document is a final report on work carried out at Cranfield University and the University of Durham under the auspices of the CEFIC-LRI funded project ‘Terrestrial Runoff Modelling for Risk Assessment of Chemical Exposure (TERRACE).

1.1 Rationale

The overall aim of the TERRACE project was to develop a simulation model for evaluation of diffuse-source chemical runoff at the regional scale across Europe. The TERRACE model should be capable of integration with the GREAT-ER system (Boeije *et al.*, 1997; Boeije *et al.*, 2000; Feijtel *et al.*, 1997; Feijtel *et al.*, 1998). The ultimate aim for development of GREAT-ER and its constituent sub-models is to provide a comprehensive modelling tool for use in environmental risk assessment at the regional level throughout Europe. GREAT-ER and its components are spatially distributed, thereby allowing more accurate prediction of regional-scale Predicted Environmental Concentrations (PECs) than the lumped models presently used in environmental risk assessment for new compounds (Knopfler, 1994). The requirement for more accurate prediction of PECs is especially pressing given the more restrictive licensing environment which stems from the European Commission’s proposed Water Framework Directive[1] and the White Paper setting out a future ‘Community Policy for Chemicals’[2].

1.2 Objectives of the TERRACE project

Given the above rationale, the four objectives of the TERRACE project are:

1. To review the current state-of-the-art in runoff and contaminant transport modelling. This includes an assessment of the validation status of models examined, and of their compatibility with commonly used risk assessment strategies.
2. To integrate selected runoff and contaminant transport models with a geo-referenced database of model parameters within a geographical information system (GIS).
3. To carry out a preliminary application of this system to an example river basin, in order to demonstrate its utility to potential end-users.
4. To specify a plan for validation of the modelling system.

A work plan for the project (Fig. 1.1) shows how these objectives were distributed over the three years of the project.

1. In Year 1 suitable modelling approaches were reviewed and data sources for models were investigated. This resulted in short-listing of three possible models, ANSWERS-2000, SWAT and SWATCATCH in order of decreasing complexity. Of these the United States Department of Agriculture (USDA) Soil Water Assessment Tool (SWAT) was judged to be the most appropriate tool.

[1] http://www.wwffreshwater.org/pdf/wfd.pdf
[2] http://www.europa.eu.int/comm/environment/chemicals/index.htm

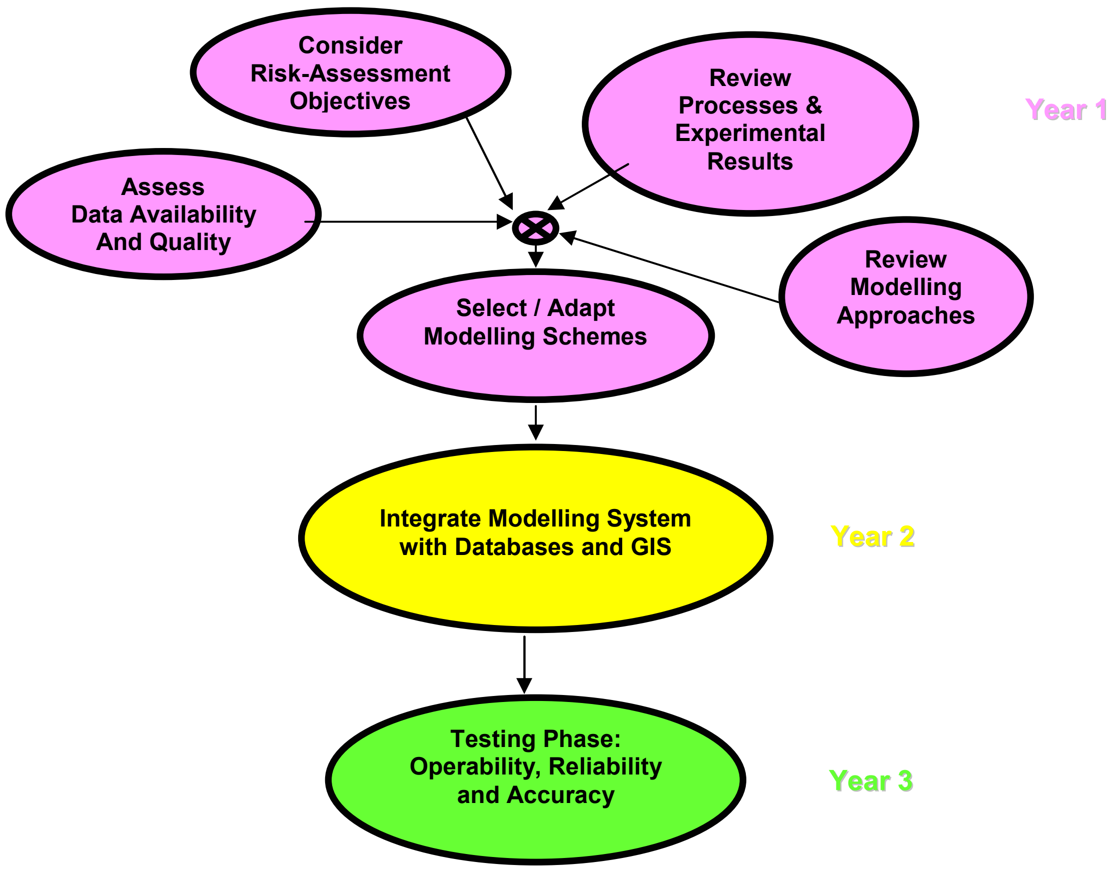

Fig. 1.1 Work plan for the TERRACE project

2. In Year 2 the databases required to apply SWAT at the European level were constructed. SWAT runs from a series of default databases giving information about climate, soils, plants, land management and chemicals. However, some of these data sets are specifically for US conditions and a European SWAT database was therefore required. Some of the data for these databases are not directly available at the European level and so a number of model parameter estimation routines (MPERs) were developed to estimate parameter values.

3. In Year 3 a UK specific database was developed for application of the SWAT model to a trial catchment, with subsequent transfer of data to GREAT-ER. The selected catchment was the Exe in south-west England (Fig. 1.2), which was chosen because it was a focus site for development of LowFlows2000. LowFlows was the hydrological engine at the heart of the original GREAT-ER point source pollution project. However, for diffuse pollution it was felt necessary to define flow and pollutant curves at monthly rather than annual level. The new LowFlows2000 package works at monthly level and a catchment where it had been tested was an obvious choice for this study.

Fig. 1.2 The Exe catchment

This report summarises the work done in Years 1 and 2 and details work done in Year 3. Further details of work in Years 1 and 2 can be found in White *et al*, 2001 and White *et al*, 2002.

In addition, a validation and implementation plan for the TERRACE software is outlined.

2. Model selection

2.1 Model overview

In Year 1 of the project an extensive review of the state of the art in contaminant transport modelling for application at the catchment scale was carried out (White *et al.*, 2001). The study examined the background, structure and applicability of a wide variety of contaminant transport modelling approaches. Models were grouped into three classes, which essentially represent their three spatial scales of application: soil profile, field and catchment. At an early stage, the first of these three scales was excluded from further consideration. Some models from the other groups were also excluded, because of their lack of recent development, their complexity or their empirical nature. This left a long list of nine models for further consideration. These were:

Field scale:	EPIC, GLEAMS, Opus, PRZM, PELMO & RZWQM
Catchment scale:	ANSWERS-2000, SWAT-2000 & SWATCATCH

These models provided us with a range of modelling strategies, from empirical to physically-based at spatial scales which are relevant to TERRACE.

An assessment of the validation status of these nine models, with detailed descriptions of validation results, was then carried out, and important issues arising from this review were discussed and reported.

The report then proceeded to a consideration of model data requirements and data availability within Europe and at a national level. Again issues arising from this review were highlighted.

Finally a model shortlist for further evaluation and development in TERRACE was presented. This shortlist included three models - ANSWERS-2000, SWAT-2000 and SWATCATCH - which provide examples of three very different approaches to catchment scale modelling. Of these, SWAT-2000 is the preferred option for the TERRACE project. The other two models would enable assessment of Predicted Environmental Concentrations in very different ways. Details of the SWAT model can be found in the second year report (White *et al*, 2002).

With this model shortlist in mind compatibility of the TERRACE models with GREAT-ER was considered, and the options for development environments were considered.

None of the evaluated models explicitly includes the capability to model organic compounds or dioxins resulting from atmospheric deposition or sewage sludge application to land. However, the basic structure of the models means that modification of existing model components was not an unrealistic prospect.

2.2 Data requirements and availability

SWAT-2000 requires a wide range of temporal and spatial data inputs, together with characteristic data for contaminants, soils and plants. The second year report (White et al, 2002) details data requirements and identifies European and national datasets which satisfy these requirements. In many cases the data are not available directly but have to be transformed into the format required by the model. A number of model parameter estimation routines were defined in the second year report. This report includes information on other data transformations necessary for the UK application of SWAT-2000.

3. The Exe application of SWAT-2000

3.1 Outline of modelling work

The aim of the Exe catchment modelling in TERRACE was to run an example application of the diffuse source model and to demonstrate how the SWAT software could be used to provide contaminant inputs to the GREAT-ER model.

In order that the TERRACE and GREAT-ER models should be compatible it was necessary first to link the flow components of the two models. TERRACE does not deliver water to the GREAT-ER model but should be able to deliver the contaminant loads associated with each percentile flow in each reach in the GREAT-ER set-up for a catchment. It was decided early in the project that the diffuse source contaminant-flow relationships would be better defined at the monthly, rather than the annual level. This is because similar rainfall events cause different runoff profiles carrying different levels of contaminant at different times of the year, dependent on a complex mixture of antecedent soil moisture conditions, evaporative demand and vegetative cover. The existing GREAT-ER model at the start of this project used LowFlows to provide hydrological data for each reach. This was provided at the reach level and was on an annual basis, as annual flow duration curves. However, an upgrade of the LowFlows software, LowFlows2000, provides flow-duration curves at the monthly level and is currently being incorporated into an updated version of GREAT-ER. LowFlows2000 has been developed and tested on the Exe catchment, making this an obvious choice for an application of TERRACE.

The modelling procedure for the Exe therefore included various principal steps:

1. Obtaining, checking and processing all input data required by the SWAT model.
2. Setting up the model databases and spatial data inputs.
3. Calibration and validation of the model for a recent period, for which better quality validation data were available Flow data were naturalised (i.e. adjusted for abstraction from and discharge to the river) by the EA. Spatially the model was discretised into 11 sub-basins based on gauging station locations (Fig. 1.2).
4. Comparison of flows and concentrations of contaminants at monitoring stations in the catchment.
5. Discretisation of the catchment by GREAT-ER reach definitions, giving 63 sub-basins. This is not every river reach defined in LowFlows2000, but a subset which will be produced for future inputs to the GREAT-ERII package.
6. Setting up the model for a 30-year run for the period concurrent with Low-Flows2000.
7. Calibration/validation of the 30-year model run against flow-duration curves per reach provided by LowFlows2000.
8. Production of contaminant load duration curves linked to the flow duration curves for input to GREAT-ER.

This outline procedure provides a highly simplified overview of the work carried out. Details of each stage in the process are given below.

3.2 *Data availability and data modification*

In order to model fluxes of water and contaminants throughout a catchment at daily time scale SWAT requires a large number of data inputs. Some of these are specific to a certain catchment, whilst others are more generic. The catchment specific data can be divided into spatial and temporal data, whilst the generic, or characteristic, data are relevant to particular plants, soils or contaminants and will apply wherever they are found/used.

3.2.1 Spatial data

The Exe catchment has a total area of 1530 km^2. It extends from almost the north Devon coast to the south coast, reaching its tidal limit (the downstream end of hydrological catchment models) at Trews Weir in Exeter. The catchment is characterised by moorland and rough grazing in the far north, with increasing amounts of pasture to the south, finally merging to an area of arable crops in the south and west of the catchment. Soils vary from peat in the north to a mixture of poorly to well drained soils in the south. Many of the soils have a high surface stone content. The climate of the area is best described as warm and wet. Annual rainfall for the catchment as a whole is 1097mm. There are few frost days during the year, but agricultural activity is constrained by the wetness of soils which can remain at field capacity well into the spring.

Topography

Due to the size of the catchment and its topographic variability the European 1km topography identified as a potential topographic data source was not sufficiently detailed to resolve the location of the river network in the Exe. Therefore a much more detailed, 50m grid, digital elevation model (DEM) was used (Fig. 3.1). This was supplied by CEH-Wallingford as part of the LowFlows2000 package.

River network/gauging stations

The river network for the Exe was taken from the EA and LowFlows2000 definition of rivers. This was necessary in order to ensure compatibility between node locations when the link between TERRACE and GREAT-ER is made. The locations of gauging stations are used to define one set of nodes within LowFlows2000 and GREAT-ER and were therefore supplied as part of the LowFlows2000 linkage. The location of gauging sites is shown in Fig. 1.2.

Meteorological sites

Meteorological data was acquired from the Environment Agency (EA) (36 raingauges, Fig 3.2) and British Atmospheric Data Centre (BADC) (131 raingauges (Fig 3.3), 14 temperature gauges (Fig 3.4)). BADC data are available only for bona fide research studies and can therefore not be passed to third parties. Rainfall and temperature data were acquired for the period 1960-1999, or subsets thereof.

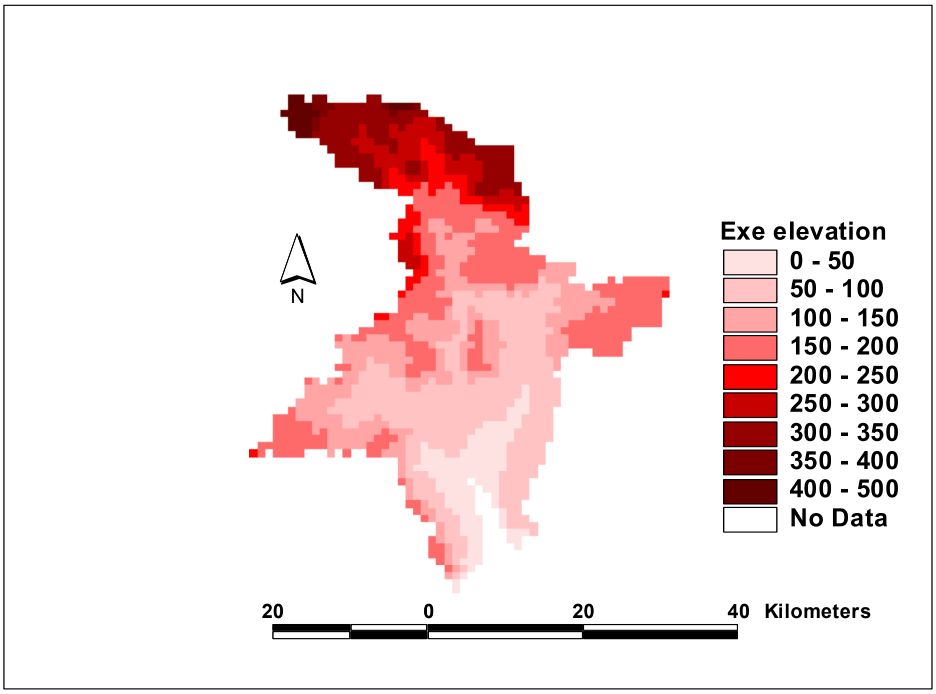

Fig 3.1 Topography of the Exe catchment

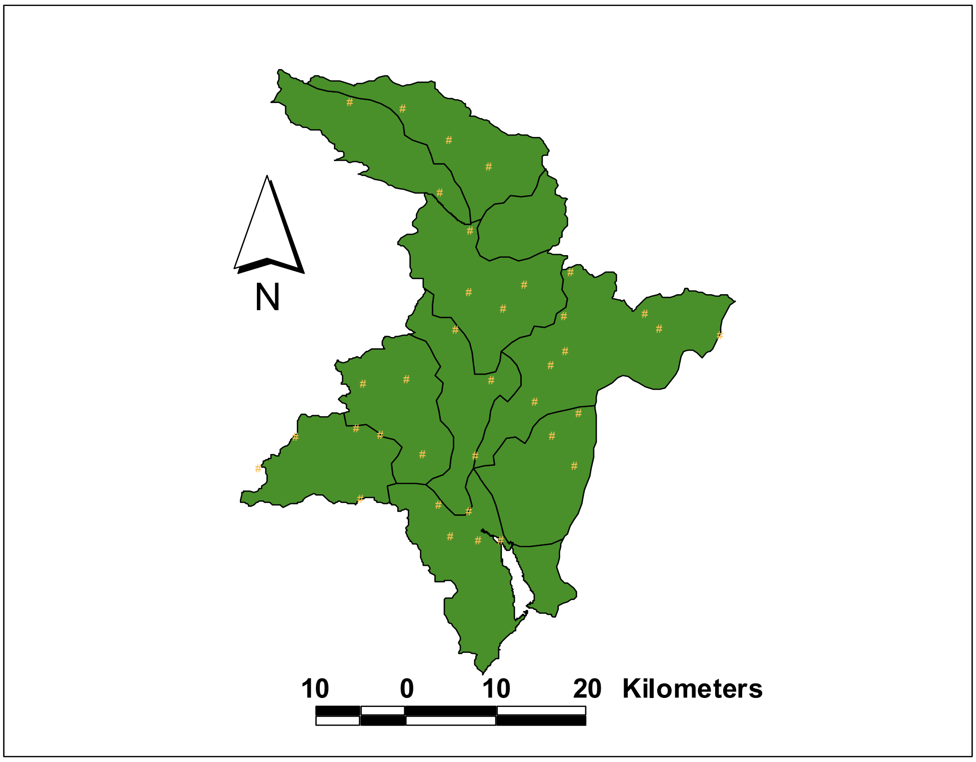

Fig 3.2 EA raingauge sites

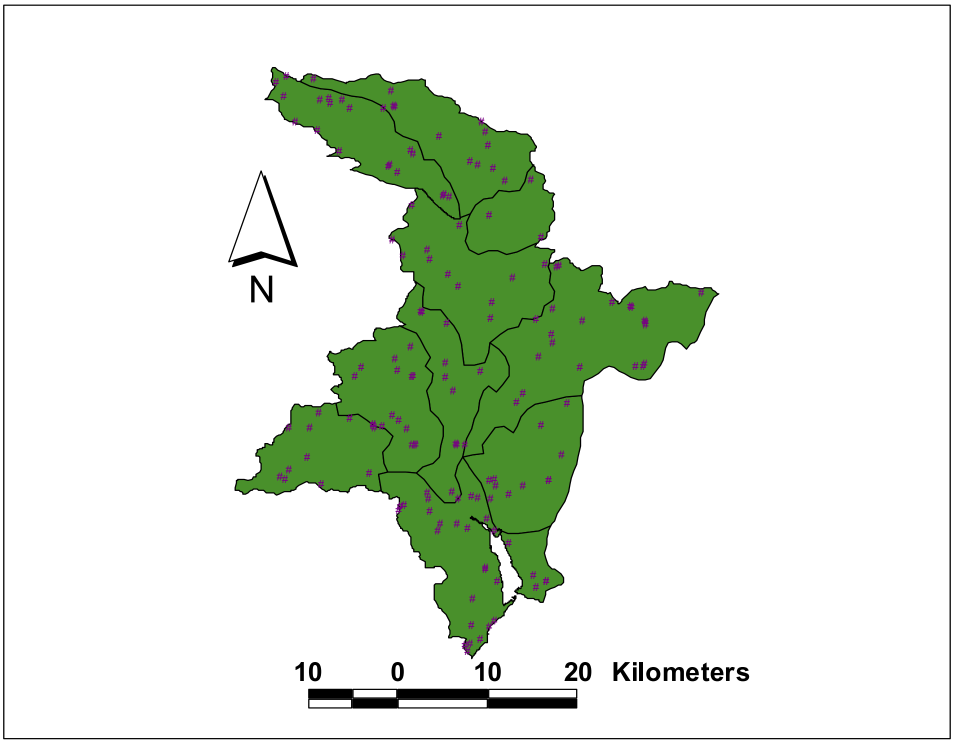

Fig 3.3 BADC raingauge sites

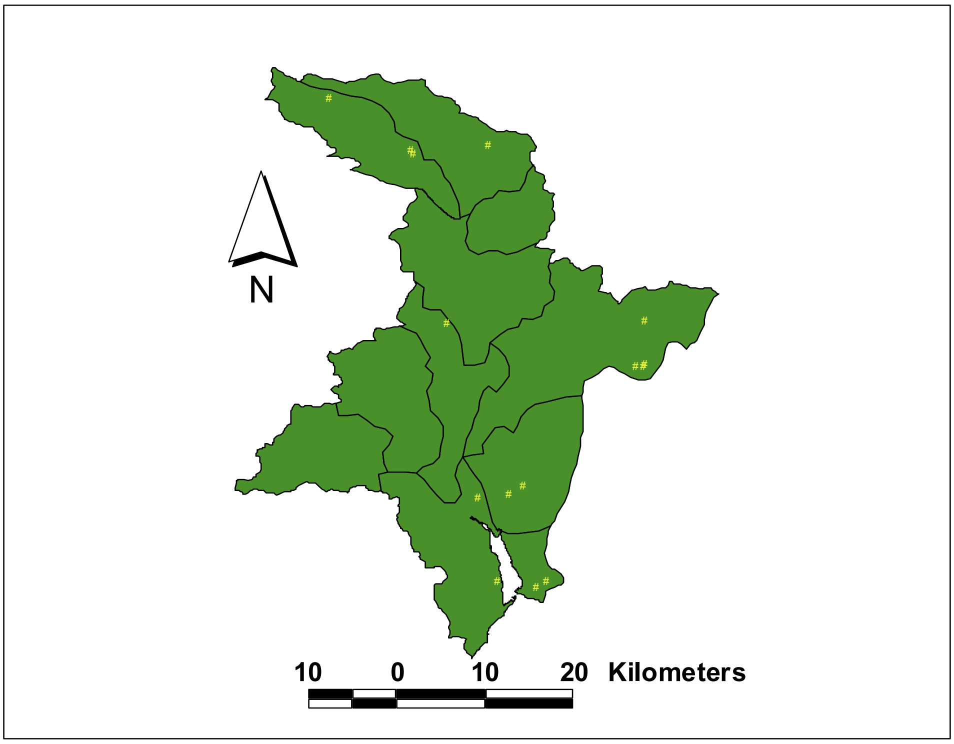

Fig 3.4 BADC temperature sites

Water quality monitoring locations

The Environment Agency (EA) monitors water quality at a greater number of sites than their flow gauging sites. However many parameters are below detection level for most, if not all, of the sampling dates. The location of all water quality monitoring sites was supplied by the EA. In addition we used one site which is monitored by South West Water, Pynes Water Treatment Works intake, as their monitoring of pesticides, whilst intermittent is more frequent than that carried out by the EA. Fig. 3.5 shows the location of all water quality monitoring sites where Mecoprop has been recorded.

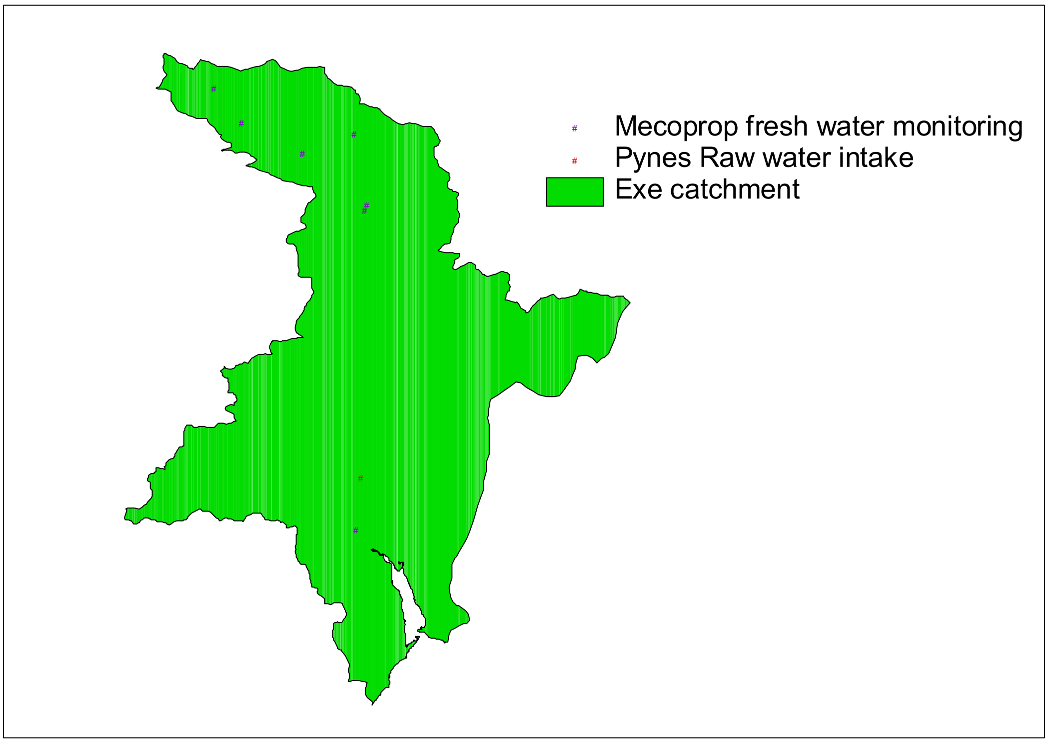

Fig 3.5 EA Water Quality monitoring sites

Soils

The UK National Soils map was used to provide information on the spatial distribution of soil series in the Exe. This was simplified to give dominant soil associations in order to restrict the number of hydrological response units (unique soil-land use combinations) defined by the SWAT software (Fig. 3.6).

Land cover

The spatial distribution of major land cover classes was provided by the CORINE map (Fig. 3.7). This defines all arable land within one class.

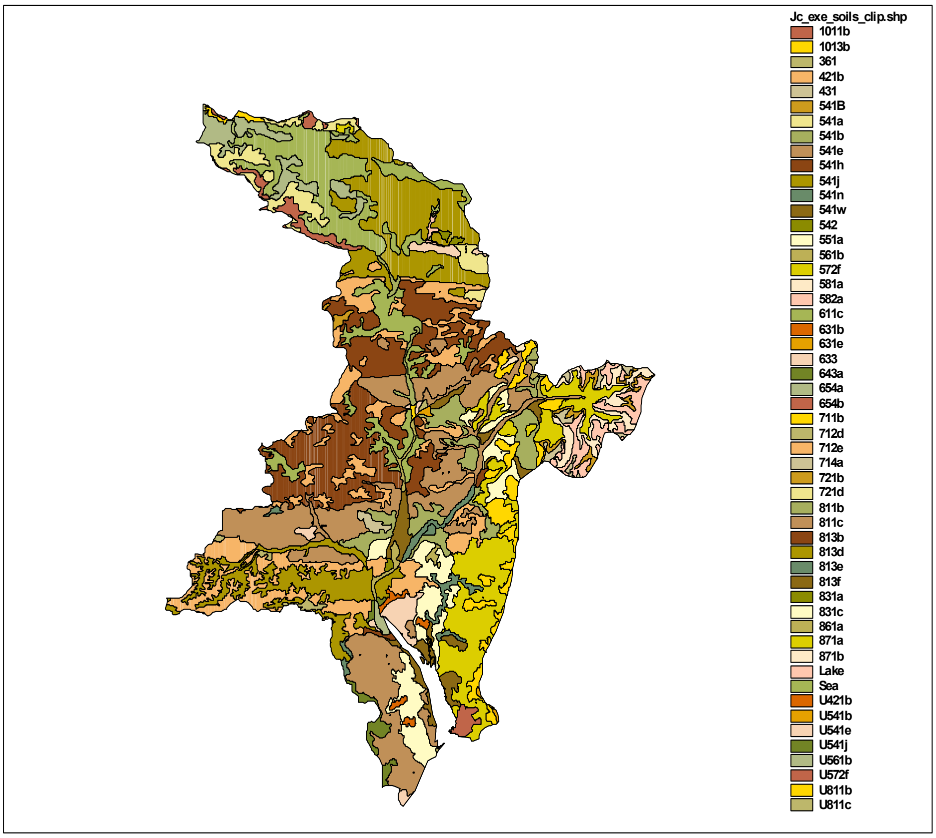

Fig 3.6 Major soil associations in the Exe catchment

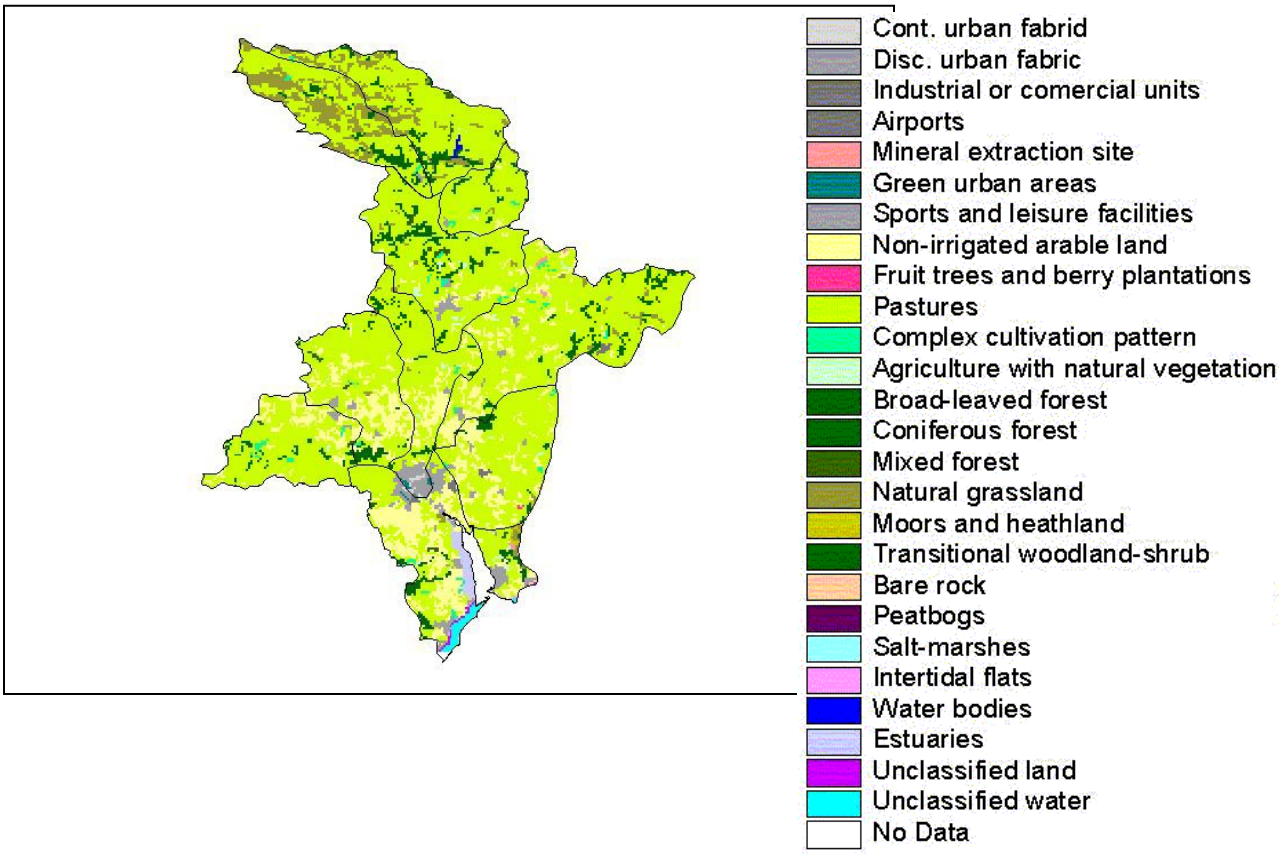

Fig 3.7 Corine land cover map for the Exe

3.2.2 Temporal data

River discharge

Time series of river discharges at daily resolution were supplied by the EA in Exeter as detailed in Table 3.1.

Data are available from the Flood Estimation Handbook (NERC, 1999) based on monitored data and the Hydrology of Soil Types (HOST) classification (Boorman et al, 1995) about the response that can be expected at each of these stations in terms of Specific Percentage Runoff (SPR, a measure of the rapid surface and near-surface response of the catchment) and Baseflow Index (BFI, a measure of the groundwater contribution to total river flow at a catchment outlet). Table 3.2 gives the available SPR and BFI data for gauging stations in the Exe catchment.

Table 3.1 Data availability for gauging stations in the Exe

Gauging station	Period of record	Naturalised or raw data
Trews Weir	1979-1980	Raw
Cowley	1965, 1967-1994,1996-2001	Raw
Broomhill	1989, 1992, 1996-2000	Raw
Coleford	1994-1998	Raw
Thorverton	1957-2000	Naturalised
Stoodleigh	1957-2000	Naturalised
Pixton	1967-2000	Raw
Brushford	1968, 1976-80, 1999-2000	Raw
Woodmill	1963-2001	Raw
Upton	1994-1995, 1997	Raw
Upton-tributary	1994-2001	Raw
Bessom Bridge	1994-1999	Raw
Wimbleball	1981-2001	Raw

Table 3.2 Expected SPR and BFI indices for the Exe sub-catchments

Gauging station	SPR (%)	BFI (%)
Cowley	-	45
Thorverton	-	51.3
Stoodleigh	33.07	51.8
Pixton	19.65	50.1
Brushford	35.99	56.5
Woodmill	43.38	52.4

In addition, various techniques area available for analysis of flow time series which allow extraction of a baseflow, or groundwater contribution, time series from the total flow record. Such information is valuable when assessing the process representation of a model as opposed to simply the goodness of fit between an observed and predicted flow time series. Fig. 3.8 gives an example of such a time series for Upton together with the total monitored flow for the same period. Two methods of baseflow separation were tested for the Exe, the IH turning points method (Institute of Hydrology, 1980) and the USDA-SCS baseflow filter (Arnold et al, 1995). The former method was used for model evaluation as results were, visually, more convincing.

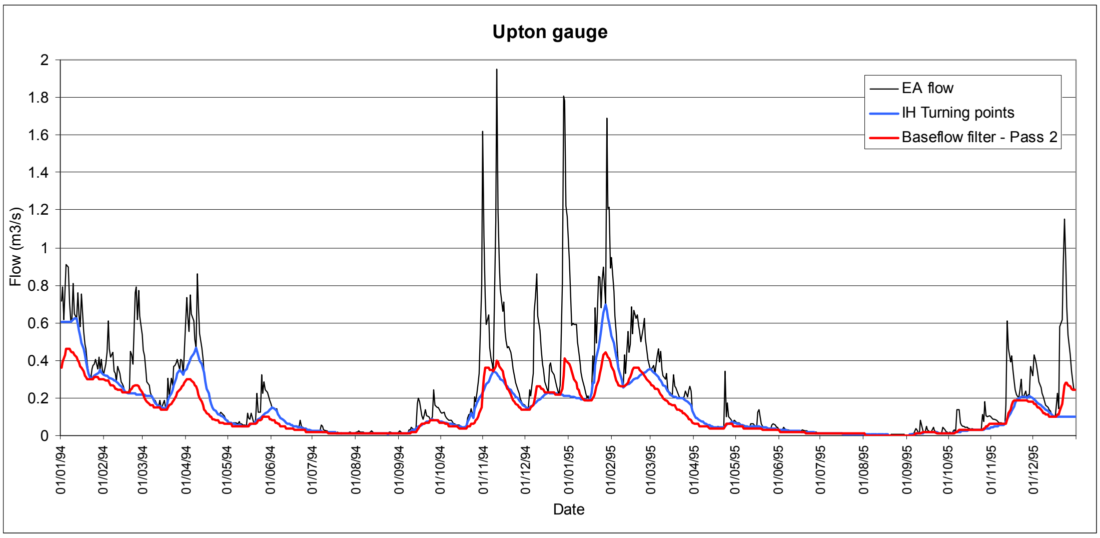

Fig 3.8 Monitored outflow at Upton and baseflow estimated from IH turning points method and USDA-SCS Baseflow filter

Precipitation and temperature

The daily precipitation and temperature data from BADC have various shortcomings:

- There are often gaps in the data set ranging in length from one day to several months.
- Data are sometimes not collected or reported every day and then an aggregate total for the period with no data is given. This means that apparently very high rainfall occurs on a day after several dry days. The rainfall amounts can be substantial.
- Sometimes dates are missed or repeated in the database, so even where 365 or 366 data points exist for a year all dates may not be represented.

A programme was therefore written to check the data sets, infilling missing dates and flagging spuriously high daily rainfall values. Where there were substantial gaps in data these need to be infilled. This was done by deriving relationships between rainfall at one gauge and its neighbours. The best correlated site was then used to infill data values, moving successively to less well correlated sites in the case of consecutive data gaps at two gauges. Where no local data were available to infill data gaps a mean value for the day (at monthly level) was used to infill.

Evapotranspiration

Originally SWAT was allowed to estimate potential evapotranspiration using the Hargreaves method which requires daily maximum and minimum temperature and radiation inputs (dependent on latitude). However, this gave very high potential ET values and resulted in high actual evapotranspiration and an inability of the model to correctly model flow volumes leaving any part of the catchment. Monthly PET values were therefore compared with those given by Smith, 1976 for the region. Summer PET in particular was over-estimated in comparison with local data. Therefore PET values were calculated using Hargreaves outside the SWAT model and were then scaled at a monthly level to better match those recorded by Smith, 1976. Fig. 3.9

shows an example of the scaled data. There is the possibility that climate change since 1970 has resulted in a shift in PET for the area. However, the values scaled in accordance with Smith meant that outflows from the catchment, and its various sub-catchments could be well modelled. Therefore for all model runs, PET has been calculated outside the SWAT package and fed into the model as an "observed" PET data set.

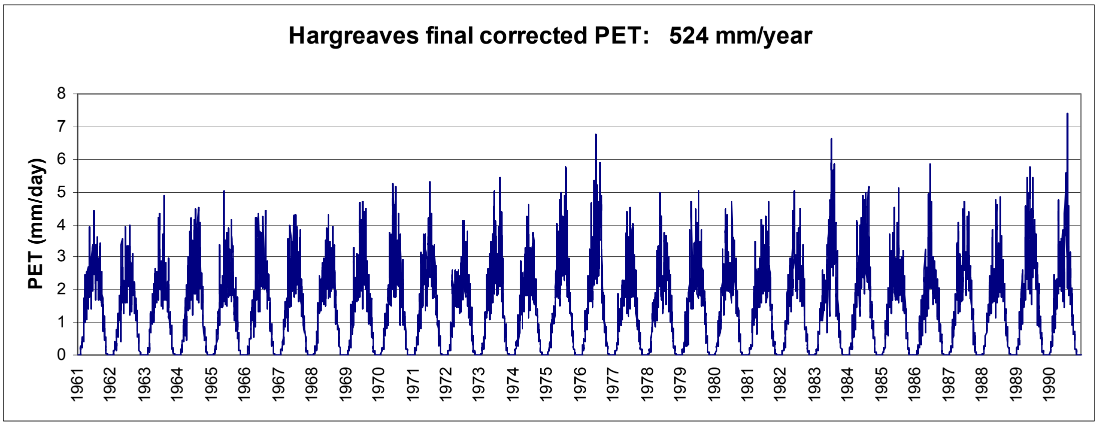

Fig. 3.9 Scaled potential evapotranspiration data for the years 1961-1990

Reservoir outflows

Where there are reservoirs in a catchment SWAT gives two options for modelling:

a. model the catchment upstream and the reservoir within the main catchment model
b. use a time series of releases from the reservoir as a boundary condition input to the main catchment model

The first approach requires information about the stage-volume curve and operational procedures for the reservoir which were not available for Wimbleball. Therefore the second approach was used. A time series of release data was provided by South West Water and the EA. However, Wimbleball reservoir was only impounded in 1982. No gauging station was located at the dam site pre-construction, and therefore flows form this part of the catchment pre-impoundment were estimated by modelling the Wimbeball catchment for the period 1961-1982. Further details are given in Section 3.4.

Water quality

The EA collect a standard suite of water quality data at approximately four-weekly intervals for a number of sites in the Exe. Data were obtained for all of these sites for the period 1997-2000. However, analysis of these data sets showed that pesticide detections were recorded as being at the detection limit (i.e. may or may not have been present) for almost all sites and monitoring dates. At the same time it was known that South West Water (SWW) did at various times have a problem with pesticides in water abstracted at their water treatment plants. The apparent inconsistency between these statements is believed to be largely due to differences in the sampling frequency and flow conditions at the time of sampling. EA sample at regular but infrequent intervals regardless of flow condition, whereas SWW sample in response to anticipated high concentration events and thus have more detailed but intermittent data records.

The data record supplied by SWW for their Pynes Water Treatment plant at Exeter has been used to validate pesticide outputs for the 1997-99 period (Fig. 3.10).

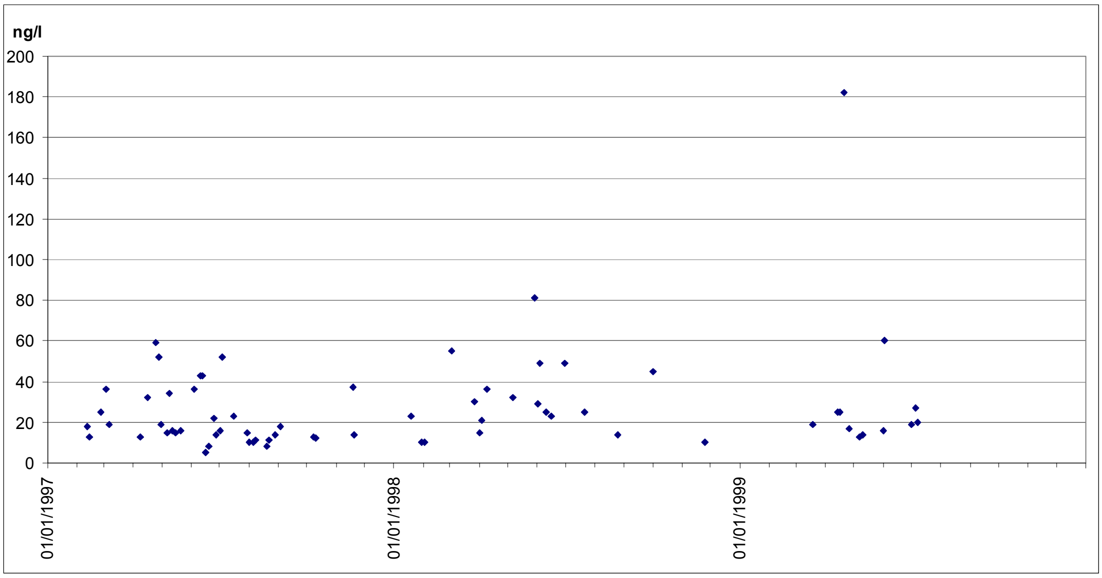

Fig 3.10 Mecoprop concentrations recorded at Pynes Water Treatment Works

Cropping patterns

In order to refine the CORINE “arable “ class to particular cropping patterns, the land use statistics available from the Edinburgh Data Library (EDL), based on Defra Parish Census statistics were used. EDL data provide a probabilistic 2km grid resolution data set, where probable proportions of crops within the 2km grid cell are given. There were again a number of problems with this data set, with for example a mismatch between what was defined as arable land by CORINE and the arable land total from EDL. Therefore, the two map layers were overlain and for every intersection of EDL and CORINE areas defined as arable, the dominant crop from the EDL layer was used. A typical rotation for the south-west region (Table 3.3) was then used to vary the crops grown from year to year. Fig. 3.11 shows a typical land use distribution for the Exe catchment as used in SWAT.

Table 3.3 Typical crop rotations for the Exe

Year 1				Year 2				Year 3				Year 4			
W	S	S	A	W	S	S	A	W	S	S	A	W	S	S	A
Spring barley			Winter barley				Winter barley				Oilseed rape				
Spring wheat			Winter wheat				Winter wheat				Oilseed rape				
Spring barley			Winter barley				Winter barley				Oilseed rape				

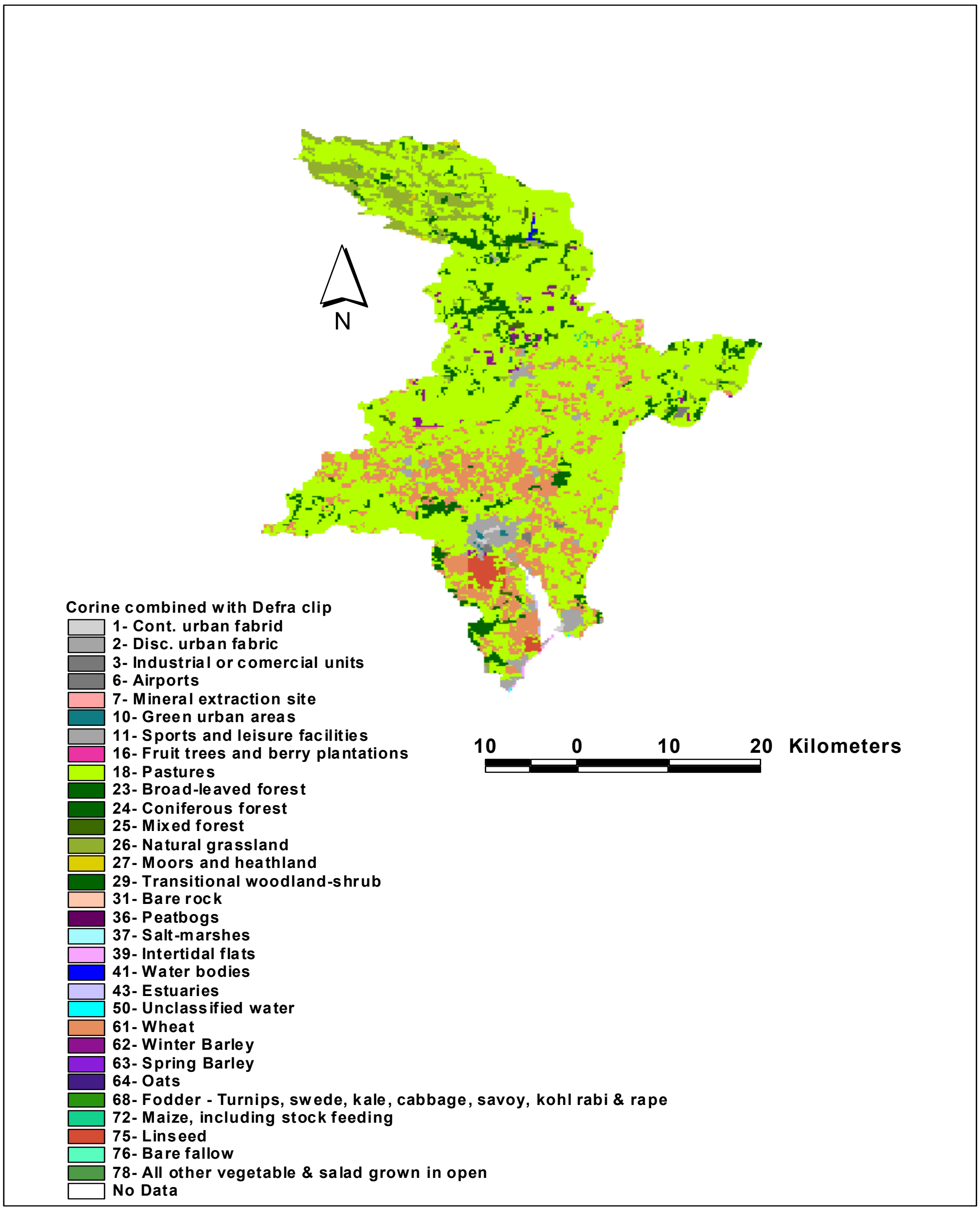

Fig. 3.11 SWAT basic land use –rotation patterns were superimposed in arable areas

Management operations

In addition to the rotation of crops grown at a particular location, SWAT requires information on planting, harvest and tillage dates as well as application dates and rates for nutrients and pesticides. Such data are not available on a field by field basis for the Exe. We therefore started from information on typical ploughing, planting and harvest dates for the arable crops in the standard south-west region rotations (Hough, 1990) (Table 3.4) and wrote software to calculate the dates of other operations. For all management operations the processing software checks for an available "access" period to the fields based on rainfall occurrence. This is a simplified version of limiting operations based on soil moisture status and is aimed at replicating the way a farmer might decide when to access his land to carry out a farming operation.

Table 3.4 Optimum times for ploughing, planting and harvest

Crop	Ploughing	Planting	Harvest
Oilseed rape	Aug	III Aug – I Sept	Aug
Spring barley	Sept – Oct	II Feb – II Mar	I Aug – I Sept
Spring wheat	I Sept – III Oct	II Feb – II Mar	I Aug – I Sept
Winter barley	II Aug – II Sept	II Sept – II Oct	II Jul – II Aug
Winter wheat	III Aug – II Sept	III Sept – II Oct	II Aug – I Sept

Tillage

Takes place in the interval between harvesting one crop and planting another, or in the case of perennials, may occur at any time of year. Tillage both alters the way a soil behaves hydrologically and mixes crop residues and possible pollutants within the plough layer. The tillage method and depth to which tillage is effective must therefore be defined.

Planting

Crops are planted according to date by first checking the optimum planting date window (Table 3.4).

Harvesting

Crops are grown and harvested by heat unit accumulation. Temperature above a base temperature and below an optimum means plant growth is controlled only by a curve defining the rate of increase in leaf area index and hence in biomass. Over the optimum temperature the plant experiences temperature stress which reduces the growth rate. Once planted crops follow a growth pattern determined by the accumulation of heat units and a leaf area accumulation curve unless stressed. The shape of this curve, and the total required heat units for a plant to reach maturity determines when the plant reaches maturity, senesces and is harvested. Stresses can also be caused because of lack of nutrients or lack of water. The maximum of these stresses is the one that limits plant growth at any given time.

There are two options for plant harvesting:

- Harvest - for plants where you are just removing some biomass (e.g. fruit or silage).
- Harvest and Kill – for plants which are removed in their entirety or where residues are left on the land and may subsequently be ploughed in.

Grazing

Grazing – removes biomass from the vegetation at a rate defined by the stocking density of animals. Grazing also provides an input of nutrients to the soil, again at a rate defined by stocking density.

Fertiliser application

Once again we do not know when, where or at what rate nutrients are added to the fields. We know the range of application rates for different crops in this region from MAFF publications (MAF, 2000a; MAFF, 2000b) and the Fertiliser Manufacturer's Association annual handbooks and can use best practice to identify at what application rate and when, during the crop growth cycle a particular input should be made. A computer program has been written to do this.

Sewage sludge application

Sewage sludge application is considered as one means of applying nutrients to the soil. Within the Exe sewage sludge is supplied to farms within a 15km radius of major sewage treatment works (Fig. 3.12). This means that all of the catchment (except the moorland in the north) may be receiving sewage sludge. Sewage sludge, unlike animal slurries, is applied through drilling rather than on the soil surface. Thus contaminants within the sludge which can be considered to behave in a way similar to pesticides should be added as a "pesticide" dose at the same time as sludge application but should be mixed in the soil profile in a way similar to that seen for tillage operations.

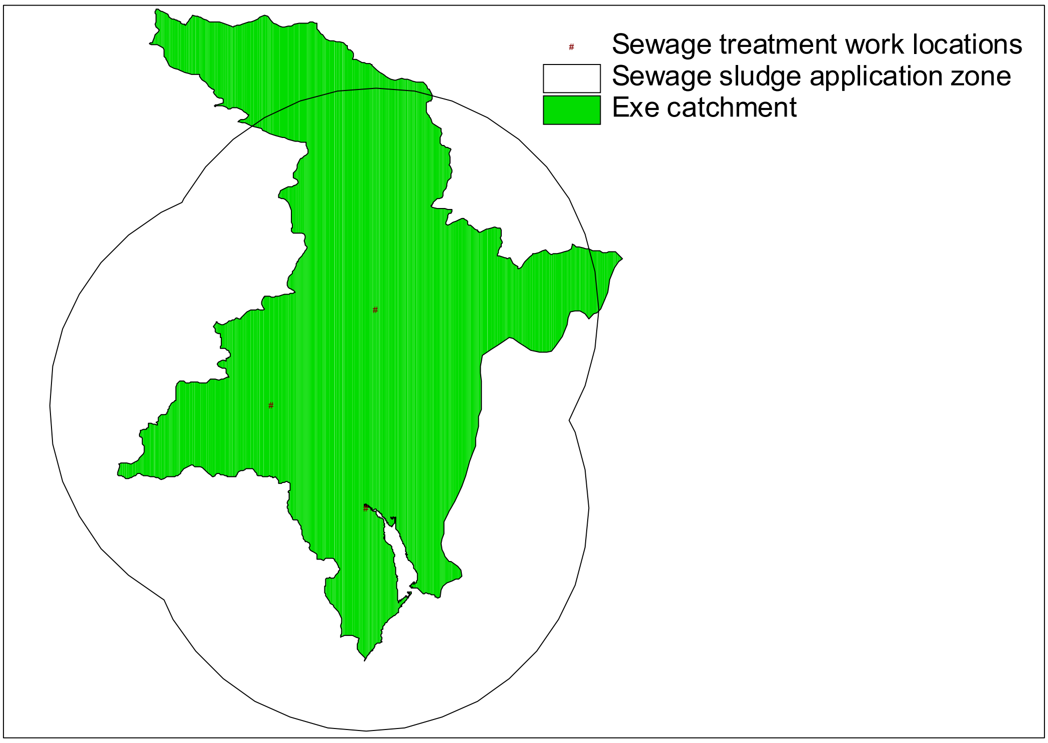

Fig 3.12 15km radii from sewage treatment works superimposed on the Exe catchment

Pesticide application

Again we do not know where and when pesticides are applied, and we can only assume that pesticides are applied at the rate advised. As an example we have selected Mecoprop for the Exe as it is a pesticide that is found in surface waters at levels above the detection limit. Defra pesticide usage statistics are given as an average application rate in kilograms per hectare of a particular land use per month. It should be noted that the Defra statistics do not distinguish between winter and spring sown varieties of the same crop. These data are provided as a rate relative to the TOTAL area under that particular crop regardless of whether it receives a pesticide application in a particular month. Stated usage rates are therefore very low (Table 3.5).

Table 3.5 Defra pesticide usage statistics for wheat in the south-western region of England, 1996

Region	Crop	Pesticide	Month	Application rate (kg/ha)
South Western	Wheat	Mecoprop	3	0.0006711
South Western	Wheat	Mecoprop	4	0.1152899
South Western	Wheat	Mecoprop	5	0.0005904
South Western	Wheat	Mecoprop	6	0.0007139
South Western	Wheat	Mecoprop	10	0.0184028
South Western	Wheat	Mecoprop	11	0.0141901
South Western	Wheat	Mecoprop-P	3	0.0018549
South Western	Wheat	Mecoprop-P	4	0.0600639
South Western	Wheat	Mecoprop-P	5	0.0213817
South Western	Wheat	Mecoprop-P	10	0.0093714
South Western	Wheat	Mecoprop-P	11	0.0056231
South Western	Wheat	Mecoprop-P	12	0.0018556

In the south west of the UK Defra statistics show that Mecoprop and Mecoprop-p are applied to a total of 11 land use classes (Appendix A) only a sub-set of which are represented in the Exe and in our model. Two principal methods have been used to time and allocate pesticide applications.

The Defra data can be used to look at the percentage of pesticide application in a particular month (Fig. 3.13). A pesticide can then be applied at the recommended rate for that crop type to a percentage of the total area of that crop commensurate with the Defra statistics. Thus for Mecoprop application to grass in the Exe catchment in a particular month the proportionate percentage of the HRU's with grass will receive an application of Mecoprop or Mecoprop-p (proportions determined from Defra usage statistics) at an average recommended dosage. These HRU's are currently selected for dosage in a random way across the catchment, although more sophisticated algorithms, perhaps related to stage of crop growth or silage cutting, could be considered. In calculating the percentage of area for pesticide application per month it has been assumed that Mecoprop-p is applied at half the dosage rate of Mecoprop.

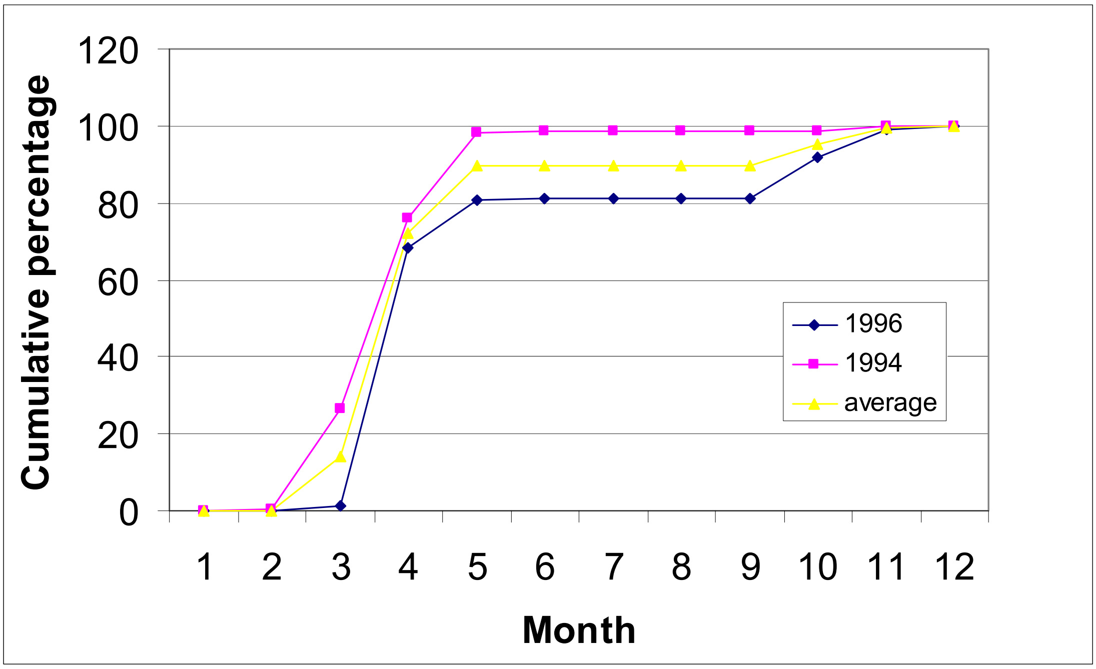

Fig. 3.13 Cumulative percentage application of Mecoprop and Mecoprop-p to spring and winter wheat from Defra pesticide usage statistics for the south-west of England

Pesticide applications are made to cereal crops at a certain growth stage as per recommendations for use of Mecoprop and Mecoprop-p contained in EU documents (Appendix B). Applications are made at the recommended dosage rate as kg ha^{-1} of active substance. In our case the dominant arable crop is wheat. Clearly application in October, November or December can only be made to areas under winter wheat, whilst applications in May and June are most likely to be to spring wheat. Also, from Defra statistics it can be seen that applications in autumn will be of Mecoprop-p rather than Mecoprop. It should however be noted that Mecoprop-p was not available until the early 1990's and therefore applications for the 30-year model run use Mecoprop alone.

Atmospheric inputs

Atmospheric deposition – can be considered in the same way as a pesticide input. Contaminants can be input as monthly loads and can be distributed spatially according to an overlay of the atmospheric modelling grid and the SWAT HRU distribution map. Problems arise because the input concentrations at a mean monthly level are too low to input to SWAT. One solution to this may be to input atmospheric contaminants with major rainfall events. No atmospheric input data (beyond a pre LRI data set) have been supplied to the TERRACE team.

3.2.3 Characteristic data

Soils

A range of information is needed in SWAT to characterise the way a soil will store and release water and contaminants. Soils are defined as a series of layers above a permanently saturated or impermeable zone. For each layer SWAT requires information about the layer thickness, soil texture (% silt, sand and clay), organic matter content, stone content, hydraulic conductivity, soil hydrological group (in the context of the USDA-SCS Curve number approach), barriers to root growth and soil erodibility (although this is only used in the context of the currently exposed top soil layer). Details of Model Parameter Estimation Routines (MPERs) were given in the second year report and will not be reported here.

The majority of these parameters can be taken directly from the UK Natmap soils database, although soil erodibility was calculated from other data values. Soil hydrological group was defined by producing an association between soil HOST class and USDA hydrological group, although at the soil association level this sometimes required adjustment to account for local variation in the association. For example, Halstow and Fladbury soil associations are nationally classified as Hydrologic Group C, but in the Exe these associations are dominated by higher clay content and therefore higher runoff potential soils series. In such cases the soils Hydrologic Group was increased by one value, in these examples to Class D.

Plants

The crop database linked to SWAT contains parameters related to crop grown in the USA. Although most of these crops are also found in the UK, some plants such as Heather (*Calluna vulgaris*), are not found in the database. In other cases, such as winter wheat, the crop parameters are slightly different for British crop varieties. The SWAT-2000 crop database was therefore modified to allow the simulation of crops found in Britain.

Parameter values found in the literature were collected and entered in the database. In all, three crops were modified or added: Heather (Calluna vulgaris) was added whilst winter wheat and pastures (Perennial ryegrass) were modified.

The main parameters required by SWAT-2000 to simulate plant growth include: the Biomass / Energy Ratio, the maximum leaf area index, parameters related to the leaf area development and the biomass development, the maximum canopy height and the maximum rooting depth as well as the base and optimal growth temperatures.

Fertilisers

No changes were made to the database.

Pesticides

Data were taken from the website of the Institut National de la Recherche Agronomique (NRA) – “Agritox” (http://www.inra.fr/agritox/).

3.3 Exe catchment modelling 1997-1999

An initial model run for the Exe was made for the period 1997-1999 because for this period we have better quality data for model set-up (land use, pesticide and nutrient usage statistics, climate inputs), calibration (flow, water quality) and validation (flow and water quality). The idea is to determine parameter values for the model in order to obtain the best possible results at HRU, sub-catchment and catchment level so that we have confidence in the way the model reproduces the important phases of the hydrological cycle which act as transport modes for various contaminants. Once set these parameters will be used for a longer model run for a period compatible with the LowFlows2000 application to the Exe catchment (1961-1990).

3.3.1 Catchment discretisation

The catchment was discretised for this exercise into 11 sub-catchments, defined by the gauging stations shown in Fig. 1.1. In addition to the 9 gauging stations defined in Table 3.1, some data were also available for two gauging stations upstream of Brushford (shown as red dots on Fig. 1.1) and these were also used for discretisation to allow output at these points if necessary.

The outlet of a sub-catchment in SWAT is the first geographically located point at which time series and summary information can be extracted from the model. Data output is also possible for each HRU, but unless HRU's are explicitly defined as individual fields (as in the application for Colworth) the HRU's are not geographically located in space and may consist of a number of non-contiguous areas with the same soil and land use combination within a sub-catchment. Therefore the number of HRUs always exceeds the number of sub-catchments, and the same HRU land use-soil combination may occur within every sub-catchment and will be assigned a separate HRU identifier.

Data output at the sub-catchment level allows comparison of the observed and predicted time series of flow and water quality at the catchment outlet as well as allowing the expected and actual hydrological process response to be compared. Thus a baseflow time series extracted from the observed flow series can be compared with the SWAT groundwater component of flow output from the sub-catchment. Flow through drains can be compared with any information on drain flow from the catchment (e.g. at what time of year drain flow occurs, how long it persists). Surface response largely controls the rapid rises and falls in flow hydrographs and can therefore be checked against the occurrence of such peaks.

At HRU level, it is again possible to look at the contribution to sub-catchment flow from a particular soil-land use combination via surface, groundwater, through-flow or drainage routes , as well as to look in a more detailed way at plant growth (leaf area and biomass accumulation, senescence, harvesting), stresses on plant growth during the year, periods of plant dormancy, soil moisture variation through the year, contaminant transfers across the surface and through the soil profile, and so on.

By using the full range of outputs from SWAT at HRU, sub-catchment and catchment level to check against expected or observed behaviour patterns it is possible to build confidence in the way the model represents process rather than how good it is at matching final output. This is important for TERRACE and for CEFIC because a model that predicted the right outputs at a large scale, but with the wrong process mechanisms at any or all levels within the model, would risk rejection of the proposed methodology by the responsible European authorities.

SWAT has another major advantage for LRI. The model is sensitive to changes in land management practices and crop rotations. Although this demands a high level of data input and hydrological competence in setting up and running the model, it also means that more confidence can be placed in the model outputs. There will always be uncertainty in many of the data inputs. Our knowledge of the spatial variation in soils and their hydrological behaviour, for example, is incomplete. We will never know exactly what is happening (or worse what did happen) on every day of the year in every field in a large catchment. These uncertainties will be with us for a long time to come. By having a model which can be shown to robustly reproduce the hydrological behaviour at HRU, sub-catchment and catchment level we can restrict the level of uncertainty in the model predictions.

3.3.2 Model inputs

Model inputs were as defined by the descriptions of spatial and temporal data above.

A number of initial model parameter values need to be set in order for the model to start its run with a logical set of hydrological conditions and to minimise the warm-up period needed for the model. For a model start date in January the important initial values were found to be:

- Water content in the shallow aquifer – should be high
- Water content in the soil profile – should be high

3.3.3 Model calibration

A number of model parameters were then defined for adjustment in the model calibration process, following SWAT User Guidelines and sensitivity analysis for other set-ups. After each model run an analysis of model behaviour at HRU, sub-catchment and catchment level was made.

The main actions taken were:

- Moved soils Halstow and Fladbury from Hydrologic Class C to Class D to allow for wetter conditions found locally in the Exe. This helped in improving prediction of flow peaks.
- Amended potential evapotranspiration to give monthly totals comparable with Smith, 1976 data for the region. This helped in obtaining a correct division of water between components in the catchment water balance.
- Ensure that water content of the shallow aquifer starts at a reasonable level for winter conditions

- Adjust the baseflow recession constant (α_{bf}) to a value seen in outflow hydrographs

3.3.3 Results

The model performance was checked at each stage of model calibration at the HRU sub-catchment and catchment level. Indicative results are given here for:

- Thorverton, Woodmill and Cowley sub-catchments
- Winter wheat and pasture land uses

In each case results are compared with observed or indicative data or expected behaviour patterns. Details are given with each example.

Model calibration at Cowley

The aim of the 1997-1999 model calibration run was to ensure that the SWAT model was behaving as well as possible in terms of the outflow predicted from the catchment and the contributions to that outflow from different flow components (surface flow, throughflow, drain flow and baseflow). It will never be possible to completely match the observed outflow hydrograph at a point as we do not know what crops were grown where within the catchment during the period of model run. Land use definitions and the timing of operations have therefore been based on regional information and data. The result of this is that the Nash-Sutcliffe model efficiency, the standard hydrological method of model evaluation, will not be high. In addition, SWAT does have a problem in correctly responding to high daily rainfall events. This is not unique to the Exe application. Fig. 3.1 shows the best time series prediction for the Cowley outlet.

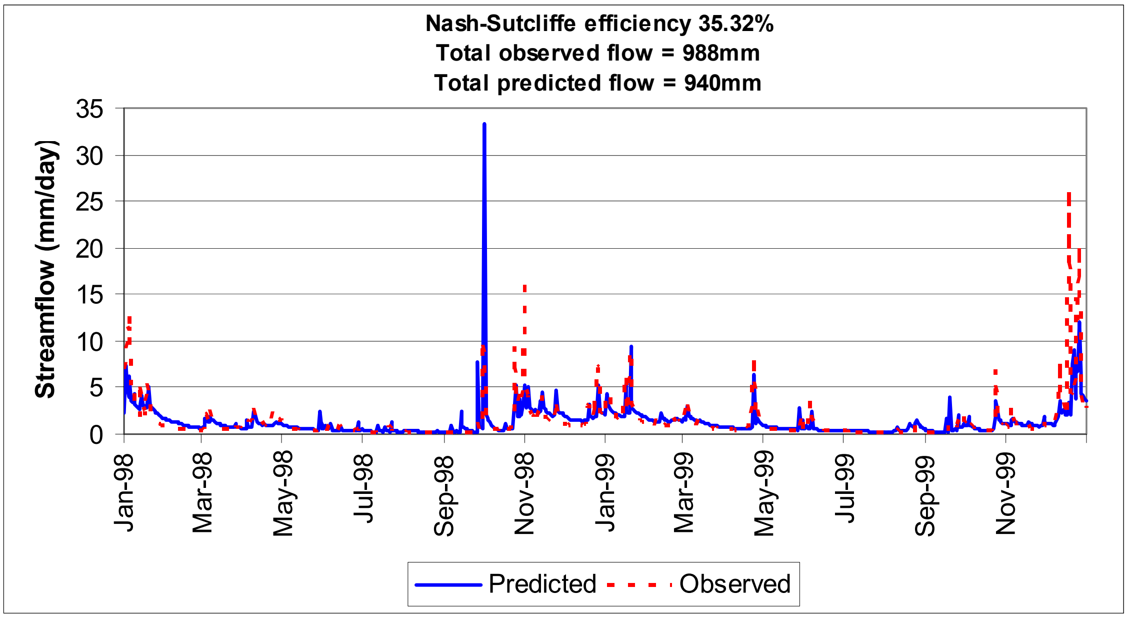

Fig 3.1 Observed and predicted river discharge at Cowley, 1998-1999

However, ultimately we are interested in flow duration curves for linkage to the GREAT-ER model. Fig. 3.2 shows such a curve for the Cowley time series shown above.

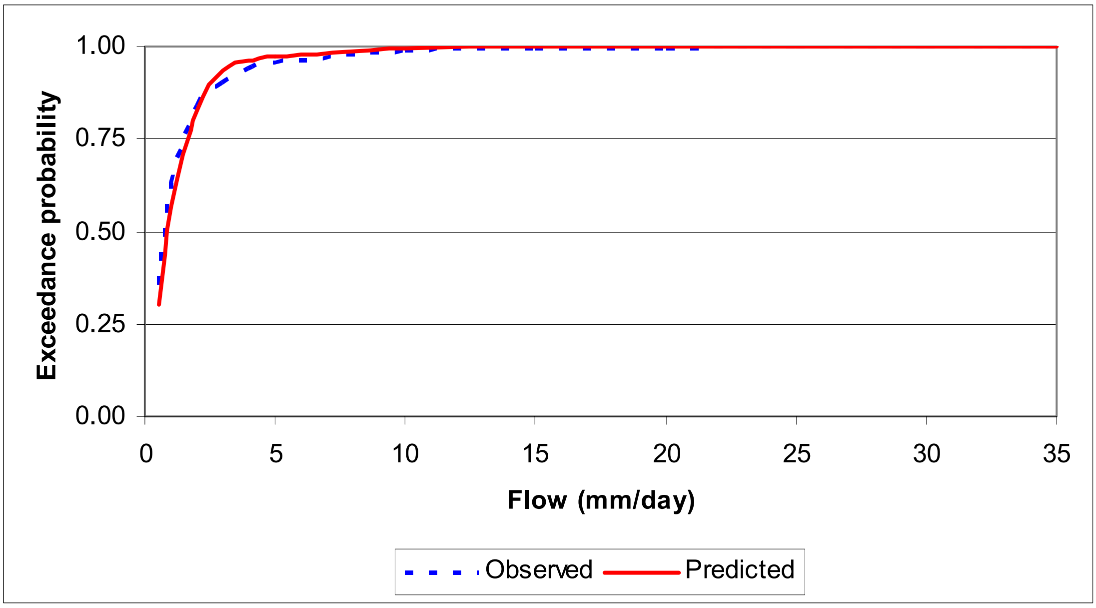

Fig. 3.2 Flow exceedance curve for Cowley 1998-1999

The final check on hydrological behaviour is to check the size and proportion of different components of the water balance. Table 3.6 gives average annual values for the 1997-1999 model run.

Table 3.6 Average annual water balance components for Cowley sub-catchment 1998-99

	Rainfall	Potential ET	Actual ET	Surface flow	Baseflow	Total water yield
mm	923.7	468.6	425.5	85.8	323.1	469.5
as % of rainfall		50.7	46.1	9.3	35.0	50.8
as % of flow				18.3	69.0	
Comparison	1449mm[1] 865mm[2]	467mm[1] 523mm[2]	415mm[1] 398mm[2]	- SPR soils 12-60%	45% BFI BFI soils 31-90%	494 mm observed EA data

1. From Smith, 1976 Zone 43 North
2. From Smith, 1976 Zone 35

Several conclusions can be drawn from Table 3.1. Rainfall for the period was average for the region. Potential evapotranspiration was scaled to match data from Smith (1976) but actual evapotranspiration has been calculated within SWAT and is well estimated. Around half of the rainfall leaves the catchment as river flow at Cowley. Of this, some 69% comes from baseflow and 18.3% from surface flow. The remainder will be from throughflow. The baseflow component appears a little high compared with the Baseflow Index for this catchment (Boorman et al, 1995). However, the range of BFI values for soils in this catchment show that such a response is still credible. Similar agreement can be seen for the standard percentage runoff figures from the same source.

The next stage is to check that plants within the Cowley catchment are growing properly and are reaching maturity and being harvested correctly. The following figures (Figs 3.3-3.6) give crop growth and associated soil moisture profiles for two hydrological response units (HRUs) in the Cowley catchment. HRU14 is a pasture growing on Neath soil (0541hPG) whilst HRU16 is a wheat HRU growing on Crediton soil.

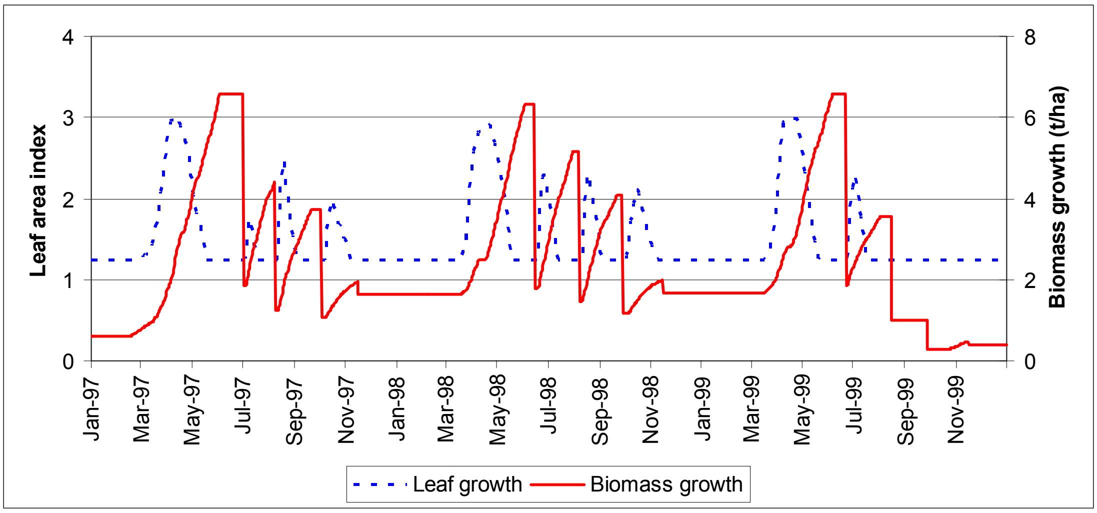

Fig 3.3 Growth of pasture in HRU14, Cowley catchment

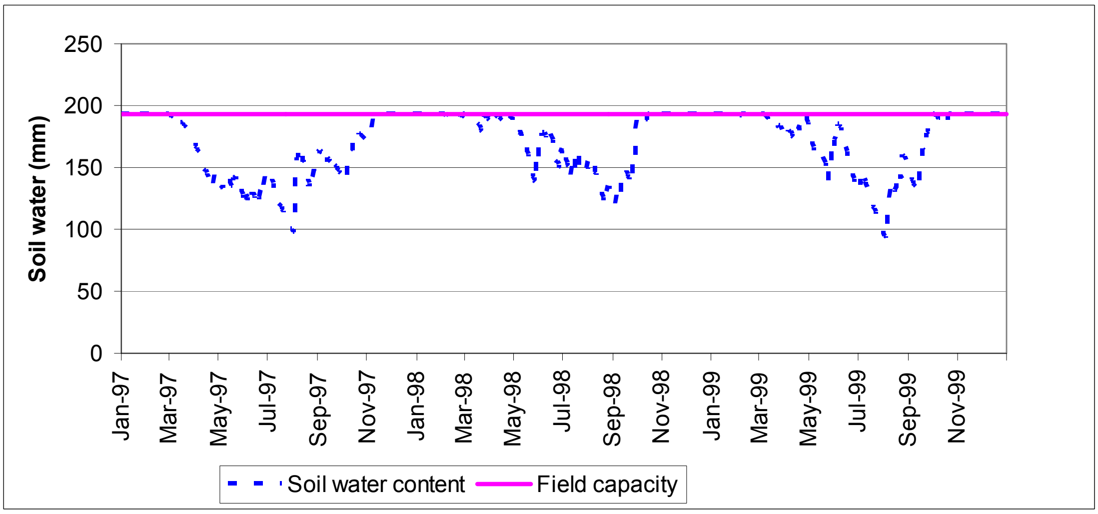

Fig 3.4 Soil moisture profile for HRU14, Cowley catchment

For HRU14 pasture is harvested three times per year for silage, which is why leaf area index and biomass drop three times and then resume growth. The amount of biomass removed with each harvest operation is specified. Other pasture areas in the Exe are grazed resulting in an on-going control on LAI and biomass. The flat area on the LAI and biomass curves between November and February is when vegetation in this area is dormant. The impact of silage cutting can be seen on the soil moisture curve. Soils in this area are at field capacity for much of the autumn and this extends through winter until late spring. The end of field capacity conditions for this area is expected between 20 April and late May and a return to capacity is expected between late August and October, maximum soil moisture deficit is expected to be around 100mm (Smith, 1976). The model is reproducing all these aspects of soil moisture well.

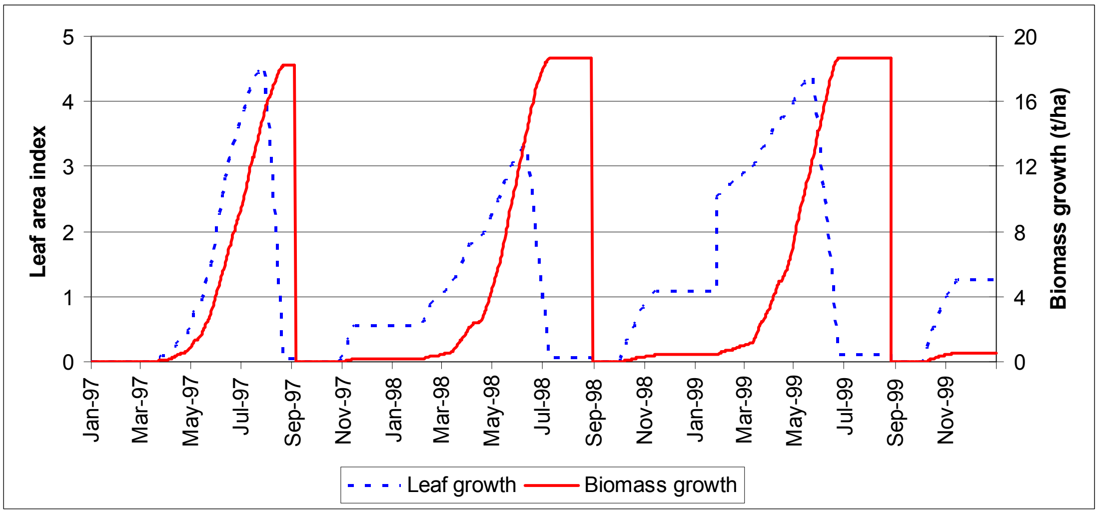

Fig 3.5 Growth of winter wheat rotation in HRU16, Cowley catchment

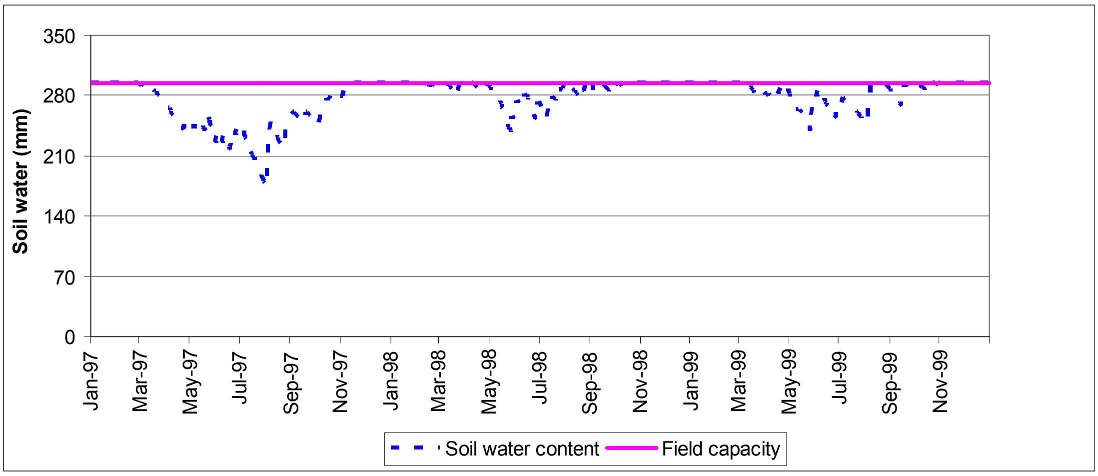

Fig 3.6 Soil moisture profile for HRU16, Cowley catchment

For HRU16 the crop rotation is spring wheat in year 1 followed by two years of winter wheat. Thus the latter two crops show an initial growth followed by a period of dormancy and then re-initiation of growth in the spring. LAI reaches a maximum and then decreases during senescence whilst biomass remains at a high constant level before being removed in one day at harvest. For this soil, field capacity is much higher and actual soil moisture deficits are much lower for the second two years than for year 1.

Model calibration at Thorverton

Predictions for the catchment to Thorverton show the best values of Nash-Sutcliffe model efficiency, in part because of the greater certainty about land use in this part of the catchment, which includes less arable land. Fig. 3.7 shows the 1998-1999 time series, whilst Fig. 3.8 gives the corresponding flow exceedance curve.

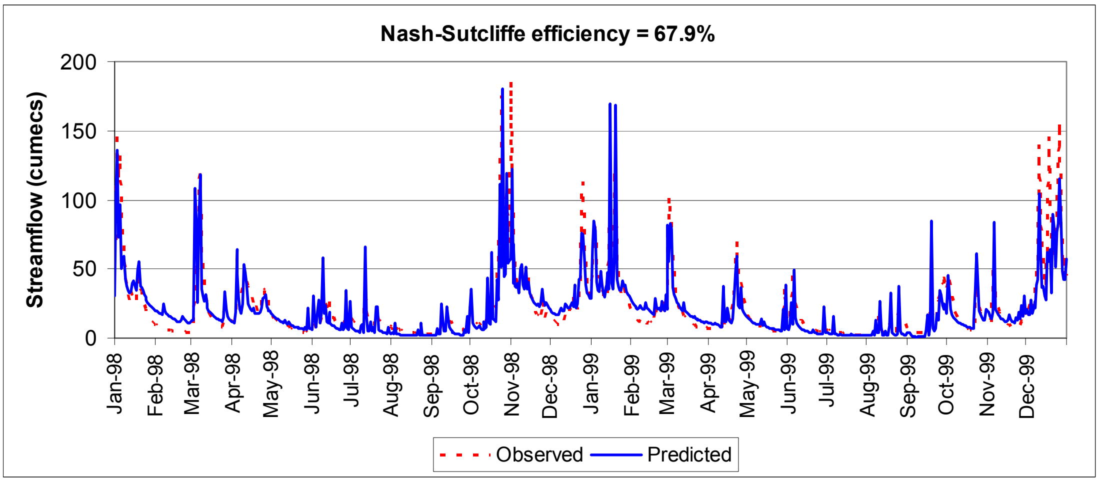

Fig 3.7 Observed and predicted river discharge at Thorverton, 1998-1999

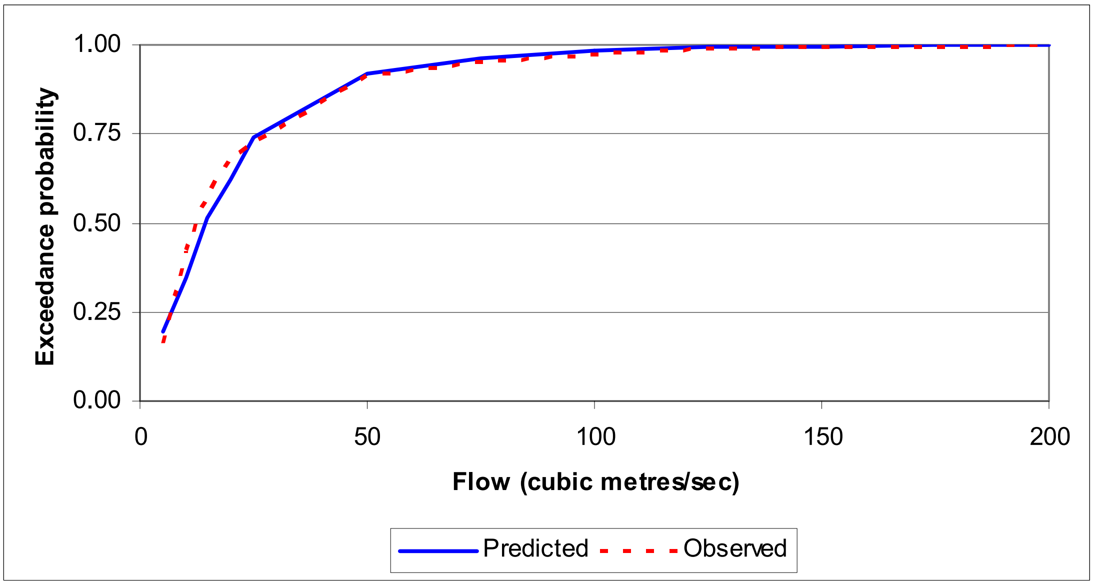

Fig 3.8 Flow exceedance curve for Thorverton, 1998-1999

Model calibration at Woodmill

Woodmill sub-catchment to the east of the Exe was the most difficult to calibrate, in large part because of a large groundwater contribution to flow in this area, combined with a moderate proportion of arable land for which uncertainty about crop types exists. Figs 3.9 and 3.10 show the time series and flow exceedance curve for this catchment for 1998-1999, whilst Fig 3.11 shows the IH turning points baseflow estimate and SWAT-2000 groundwater contribution to flow for the same period and Figs 3.12 and 3.13 show the evolution of soil moisture during 1998-99 for a wheat HRU and a pasture HRU, respectively.

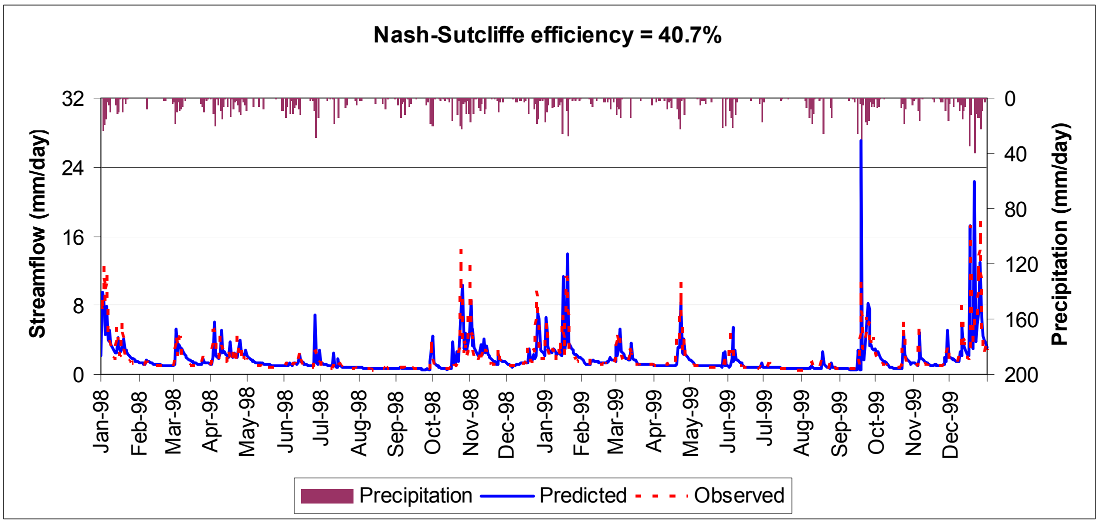

Fig 3.9 Observed and predicted river discharge for Woodmill, 1998-1999

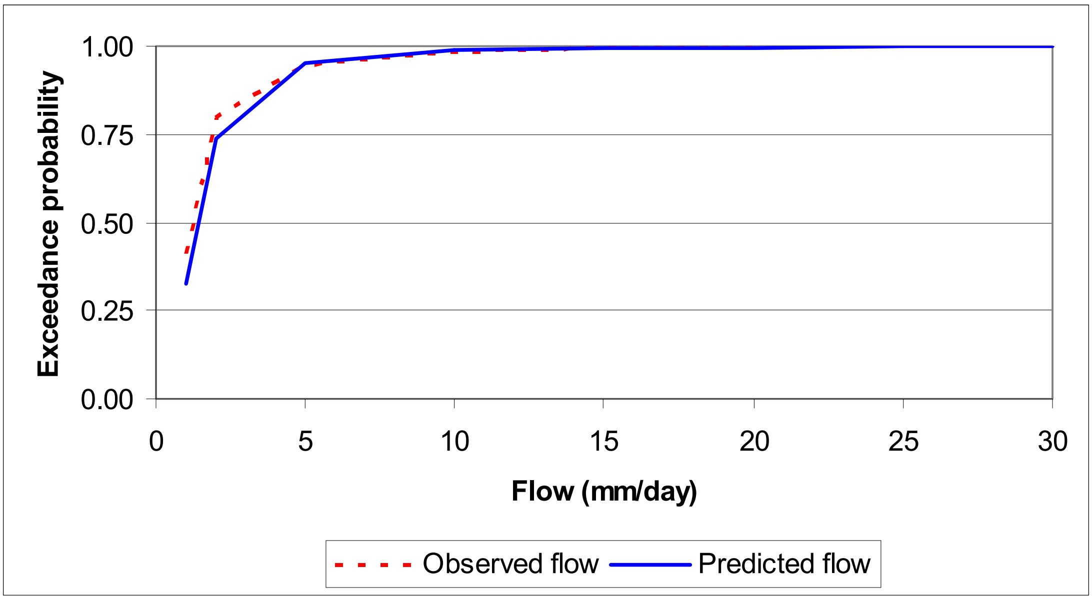

Fig 3.10 Flow exceedance curves for Woodmill, 1998-1999

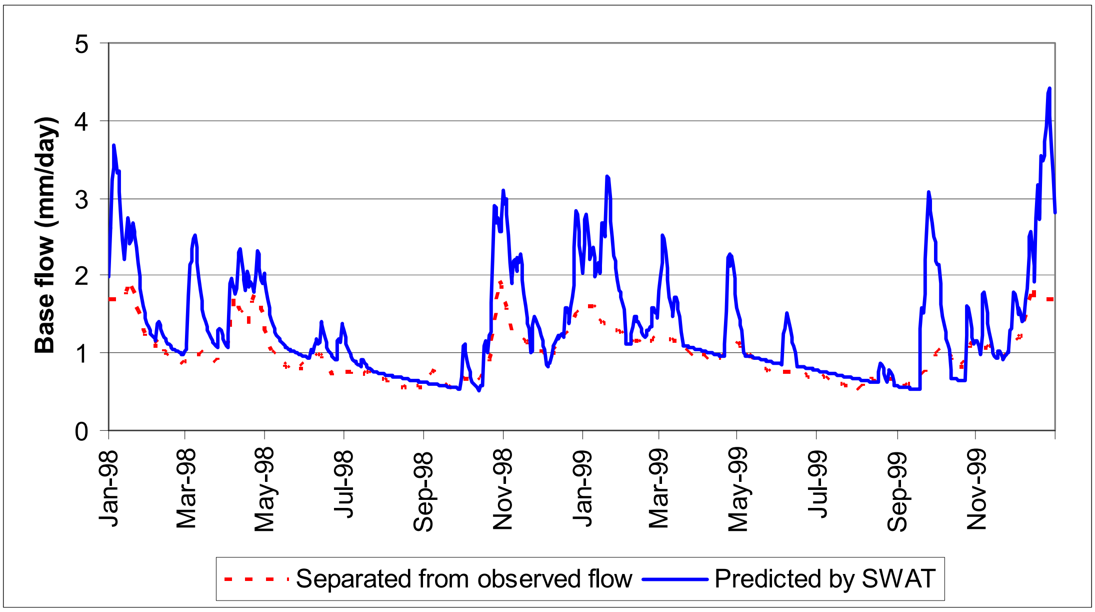

Fig 3.11 IH turning points baseflow estimate and predicted baseflow for Woodmill, 1998-1999

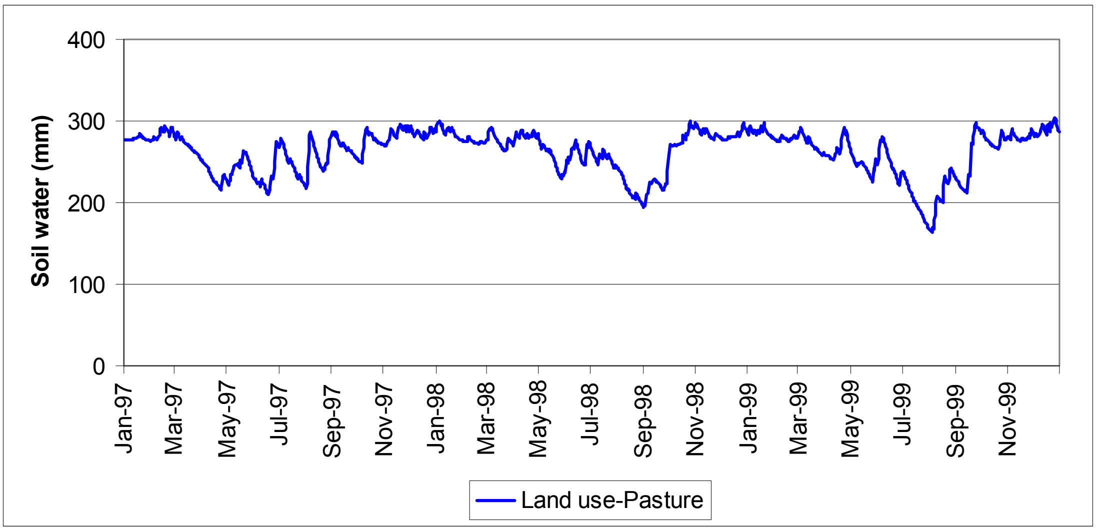

Fig 3.12 Soil moisture content for HRU40 (wheat), Woodmill sub-catchment

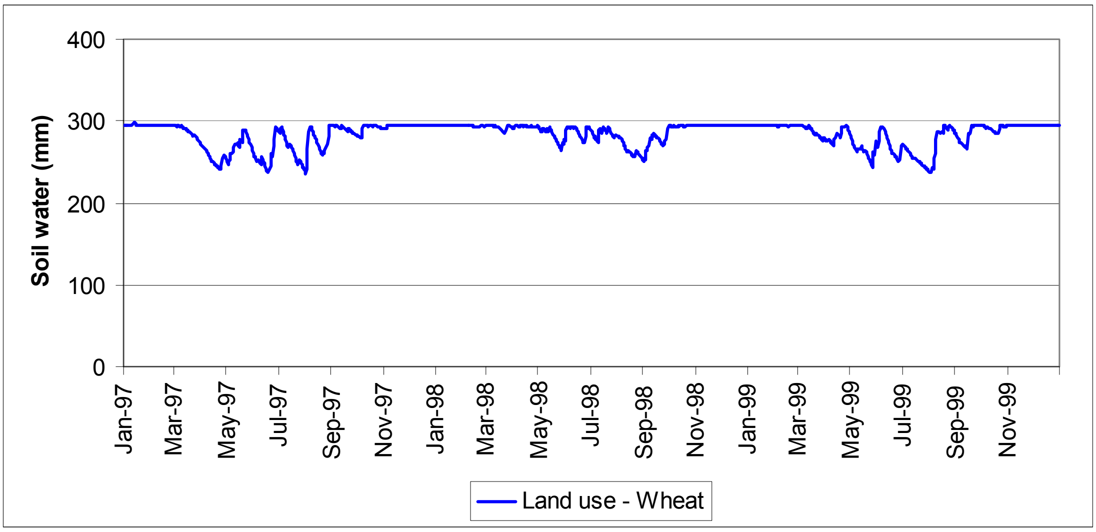

Fig 3.13 Soil moisture content for HRU43 (pasture), Woodmill sub-catchment

Table 3.7 shows the water balance components for 1998-1999 for Woodmill. For comparison with results for the same period at Cowley given in Table 3.1. Results are also given for the two HRU's illustrated above to show the different responses possible from different crop-soil combinations.

Table 3.7 Water balance components for Woodmill sub-catchment, 1998-99

	Rainfall (mm)	PET (mm)	AET (mm)	Surface flow (mm)	Lateral flow (mm)	Base-flow (mm)	Water Yield (mm)
Observed	1193.4	468.6					638.3
Sub-catchment			446.7	135.4	N/A	492.6	665.8
HRU40			460.7	170.7	25.4	456.1	648.9
HRU43			369.5	62.2	61.5	625.5	748.1

Modelling contaminant movement

Once the correct hydrological behaviour of the catchment had been confirmed, Mecoprop and Mecoprop-p were applied to appropriate crops in the catchment following the guidelines for application rate and the plant development stage, as outlined above . Inputs were checked against the temporal distribution detailed in Defra usage statistics. For arable crops pesticides were applied at a defined plant growth stage, the actual date of application was determined by climatic factors which allowed (or not) access to the land by farm machinery. The spatial distribution of pesticide application in a month was random within a particular crop type, however the total area of application as a percentage of total crop area, represented the percentage of annual application in a given month from the Defra statistics. For grassland pesticide is applied to randomly selected HRUs in each month in order to match the annual distribution to grassland shown in Defra statistics. Table 3.8 gives the application rates and HRU numbers for application to grassland in certain months for the 3-year model run, whilst Fig 3.14 shows the resultant monthly distribution compared with monthly Defra usage rates.

Table 3.8 Mecoprop and Mecoprop-p application schedule 3-year model run

	Mecoprop		Mecoprop-p	
Month	Application of pesticide to HRU nos:	Dosage (kgha^{-1} as)	Application of pesticide to HRU nos:	Dosage (kgha^{-1} as)
January	13	1.7	-	
February	-		-	
March	21	1.7	-	
April	2, 4, 11, 20, 29, 33, 36, 41, 52	1.7	28, 47	1.1
May	6, 35, 40, 42, 53	1.7	46	1.1
June	1, 5, 14, 27, 31, 34	1.7	-	
July	30	1.7	-	
August	-		-	
September	-		-	
October	-		15	1.8
November	-		32	1.8
December	-		-	

Recommended Mecoprop dosage for grassland 1.0-2.4 kgha^{-1} as; recommended Mecoprop-p dosage for grazing land 0.6-1.5 kgha^{-1} as, in autumn 1.8 kgha^{-1} as

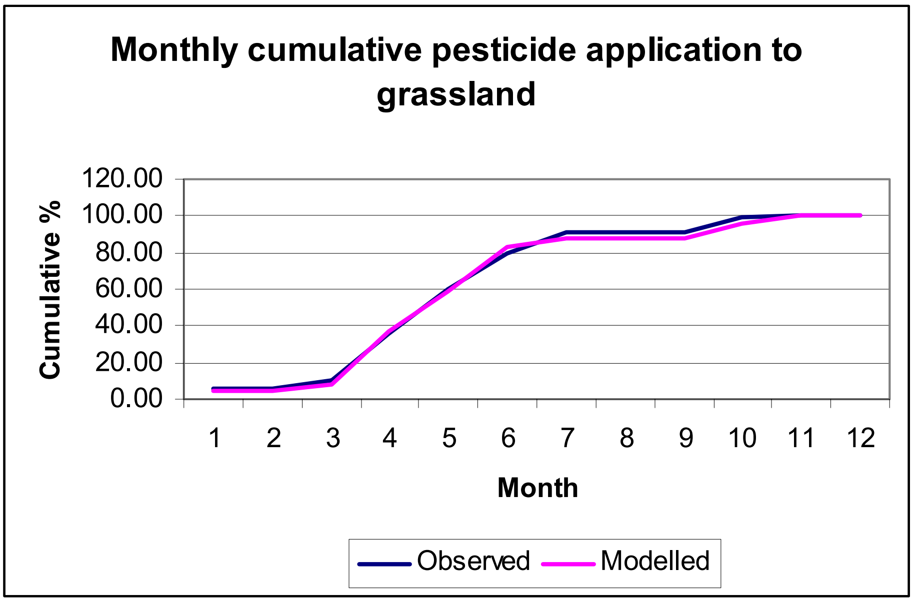

Fig 3.14 Monthly distribution of Mecoprop and Mecoprop-p application as compared with Defra statistics

Fig 3.15 shows the results obtained from applying Mecoprop and Mecoprop-p as defined above to all relevant HRUs, compared with measured data at Pynes water treatment works (between Trews Weir and Thorverton). It should be noted that this form of blanket application will be a worst case scenario. Defra usage statistics suggest that Mecoprop or Mecoprop-p is applied to between 5 and 9% of wheat fields, 12-20% of barley, 0.7-2% of permanent grass and 1.6-3.8% of new or temporary grass in the South Western region. The major losses will be from wheat rather than grassland as surface runoff is a primary transmission mode for Mecoprop. Therefore the comparison with Pynes data multiplied by 10 is reasonable.

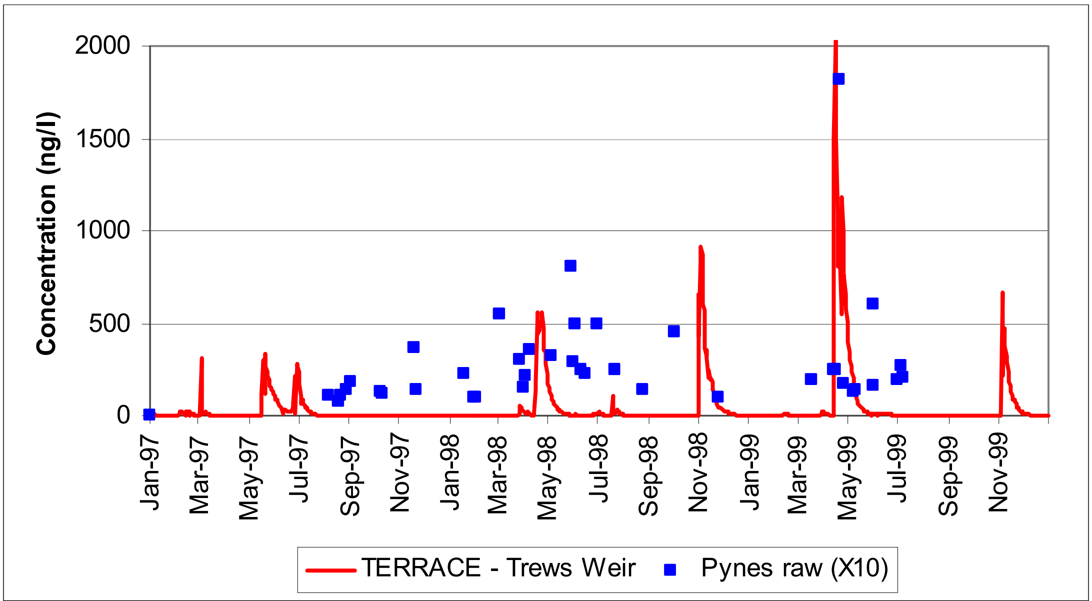

Fig 3.15 Predicted and observed Mecoprop concentrations, 1997-1999

3.4 Exe catchment modelling 1961-1990

After calibration of the model and testing for Mecoprop application, the model was set up to run for the 1961-1990 period for direct comparison with flow statistics from the LowFlows2000 package. In order to match flow duration curves for the two models the period of modelling must be concurrent.

3.4.1 Catchment discretisation

In this case the catchment was discretised by a sub-set of LowFlows2000 nodes, or river reaches, which are those that will be used within GREAT-ERII. The node list was provided by CEH Wallingford and used the following procedure:

- Identify all the consents held by South Water
- Identify all discharges (location, consented dry weather flow (DWF)) within the basin: only the discharges representing 95% of the total DWF were considered to build the reduced river network
- Identify the relevant sampling points: upstream and downstream of discharges, strategic locations to identify the boundary conditions

- Identify a suitable 1:50 000 river network: The location of the selected discharges defined the bulk of the river network. Only tributaries contributing to more than 10% of the main flow were modelled.
- Concerning the headwaters, at a confluence only the river stretch with the highest natural mean flow was selected.

This more detailed model set-up results in 63 sub-catchments and 306 HRUs (Fig 3.16). If all LowFlows2000 nodes were included the sub-catchment rises into the thousands and the model cannot properly represent sub-catchment areas due to a mis-match between topographic data scale and length of river reach.

At each GREAT-ERII node, equivalent to a SWAT sub-catchment outlet, a time series of flows and contaminant concentrations are produced. Flows can be converted easily into flow duration curves, whilst concentrations need to be multiplied by concurrent flow values to convert them to loads. A load duration curve can then be produced. This is the basic transfer required to GREAT-ERII. However, one further step is required as GREAT-ERII samples the in-river flow duration curve by percentile and it is necessary to know which percentile on the flow duration curve relates to a particular percentile on the load duration curve. Because of non-linearities in the flow-concentration relationship the percentiles will not be the same. The linkage between these two can be provide by plotting the load percentile against corresponding flow or flow percentile. Then either a function of this relationship can be defined or a Look-Up table can be produced linking certain flow percentiles to equivalent load percentiles.

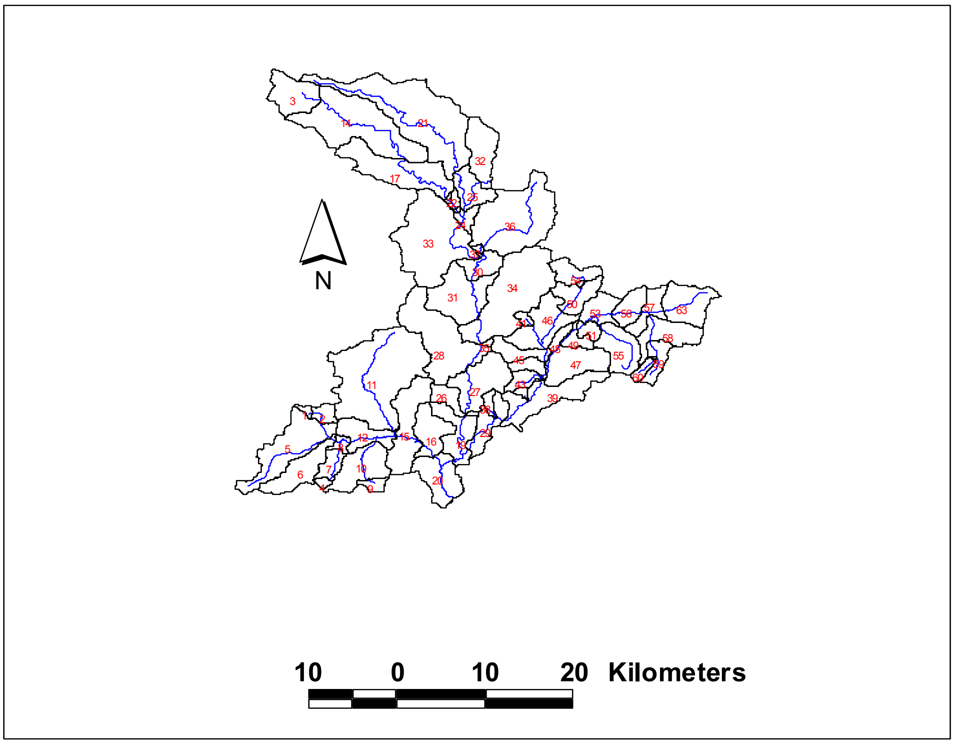

Fig 3.16 Complex Exe catchment model setup

3.4.2 Model inputs

Data inputs were as defined above. Model parameters and crop rotation patterns were kept the same as those for the 1997-1999 run. There will be some inaccuracy in this as land use, crops grown and rotation patterns, stocking density and so on will have changed during this period. However, the lack of reliable data sources means that any other pattern of land usage and crop type is likely to be just as inaccurate as that used. As ultimately the aim is to produce Predicted Environmental Concentrations for a range of climatic conditions for which data are available and a set of non-varying base conditions (soil, topography) the land use assumption is considered to be valid.

3.4.3 Wimbleball model

Wimbleball reservoir was impounded in 1982, therefore for the long model run it was necessary to simulate pre-reservoir outputs for the catchment. This was done by setting up a SWAT run for the Wimbleball catchment alone and calibrating against three small sub-basins upstream of the dam site (Bessom Bridge, Upton and Upton-tributary), for which historic flow data were available. The predictions of outflow from the Wimbleball catchment are then added to precede the time series of reservoir outflows available since 1982. These data then provide a boundary condition to the main catchment model. The Wimbleball model calibration followed the same strategy as described for the 1997-1999 run. Nash-Sutcliffe model efficiencies of 60%, 81% and 81% and corresponding R^2 values of 75%, 86% and 83% were achieved for the three gauging sites at Bessom Bridge, Upton and Upton-tributary, respectively.

3.4.4 Contaminant inputs

Table 3.9 shows the HRU and pesticide application pattern for the 1961-90 run. Note that only Mecoprop is used or this run as Mecoprop-p only came onto the market in the 1990's.

One successful run of the 1961-90 model has been made, however we have since improved the performance for the simpler 3-year set up considerably and will therefore present only methodological results here. A further 30-year run will be completed in the next two weeks so that flow and load duration curves with realistic data values can be presented for all nodes in the network.

Table 3.9 Mecoprop application schedule – 30-year model run

Month	Mecoprop	
	Application of pesticide to HRU nos:	Dosage ($kgha^{-1}$ as)
January	1, 2, 19, 40	1.7
February	-	
March	15	1.7
April	11, 24, 29, 30, 43, 46, 47, 48, 49, 54, 55, 60, 64	1.7
May	28, 36, 63	1.7
June	7, 13, 14, 22, 41	1.7
July	4, 6, 23, 27, 31, 42, 53, 62	1.7
August	-	
September	-	
October	18, 21, 32, 61	1.7
November	20, 25	1.7
December	-	

Recommended Mecoprop dosage for grassland 1.0-2.4 $kgha^{-1}$ as.

3.5 TERRACE to GREAT-ER linkage

In order to demonstrate the methodology results from the 3-year simple model set-up are given here for Woodmill. The first stage is to produce flow duration curves for a site for comparison with those from LowFlows2000 (Figs 3.17). Only annual data are presented here as with only two years of valid run the monthly level curves are not statistically valid.

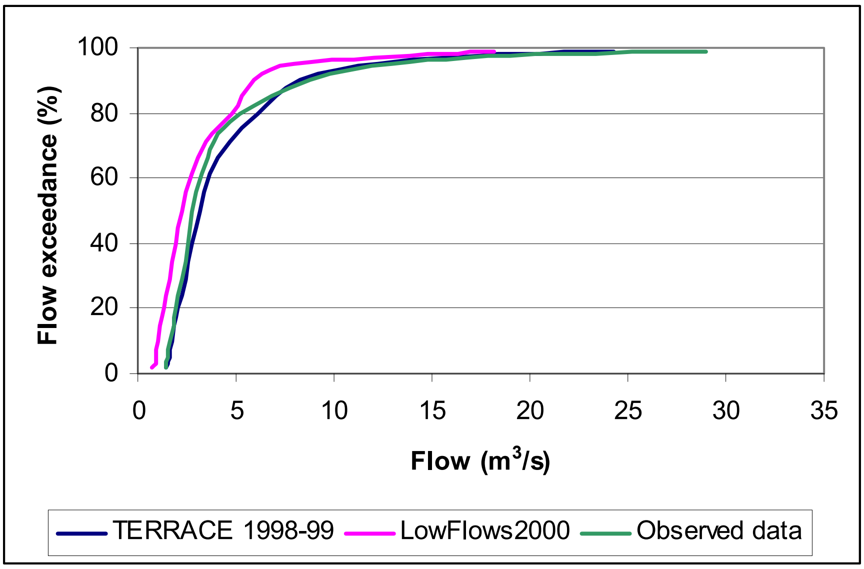

Fig 3.16 Flow exceedance curves for Woodmill

Mecoprop load duration curves are also prepared for the same sites (Fig 3.17). As may be expected there is little or no response at the low frequency end of the graph, indicating that Mecoprop is only moving in high flow events which will have a large surface flow component.

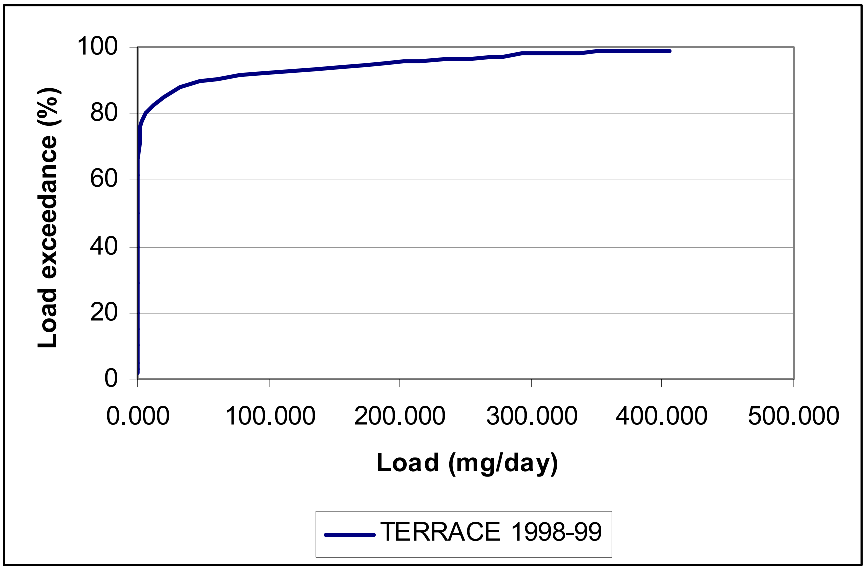

Fig 3.17 Load exceedance curves for Woodmill

The final step in the analysis procedure is to link the flow and load duration curves for each node. Again examples are given for Woodmill. Fig 3.18 shows the load exceedance-flow exceedance relationship for the site. This figure shows that it is only for flows between 5 and 10 m^3day^{-1}, corresponding to loads of less than $50mgday^{-1}$ when a linkage needs to be made. Fig 3.19 demonstrates the load versus flow relationship for all data and shows the strong influence of days with low or zero load data. This indicates that high water flows do not always relate to high Mecoprop loads. The additional control on the relationship is Mecoprop availability. Fig 3.20 presents the same data for loads of over 50mgday^{-1} by month of occurrence. This shows the improvement that will be obtained by looking at the data at a monthly level once the 30-year run is completed.

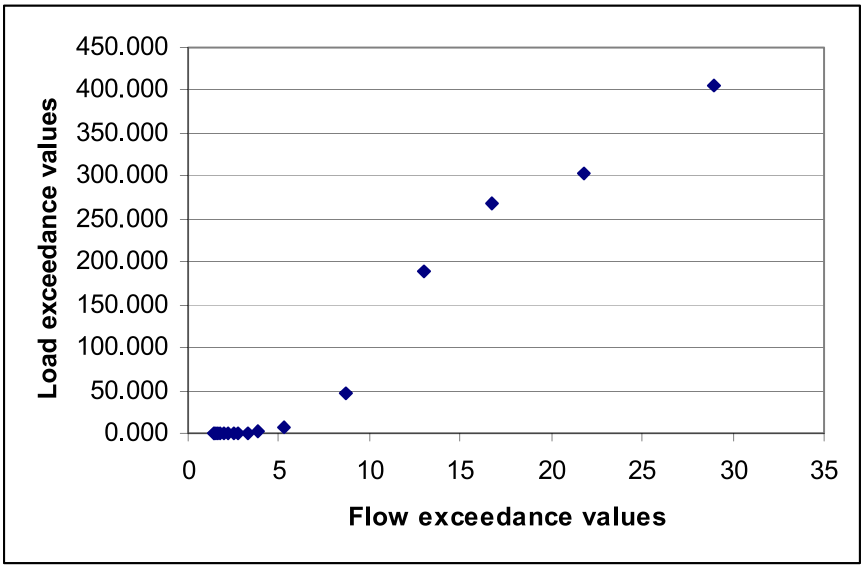

Fig 3.18 Linkage between flow and load exceedance for Woodmill, Cowley and Thorverton

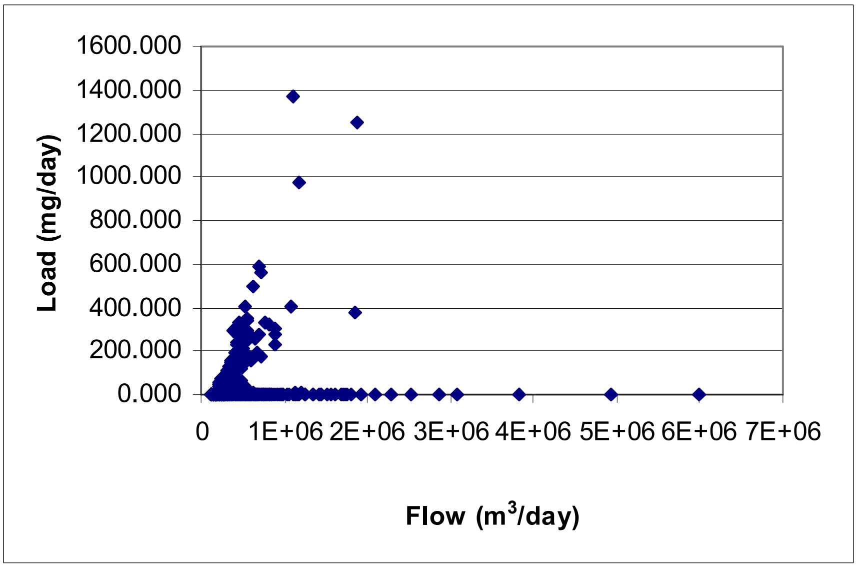

Fig 3.19 Flow versus load for Woodmill (all data)

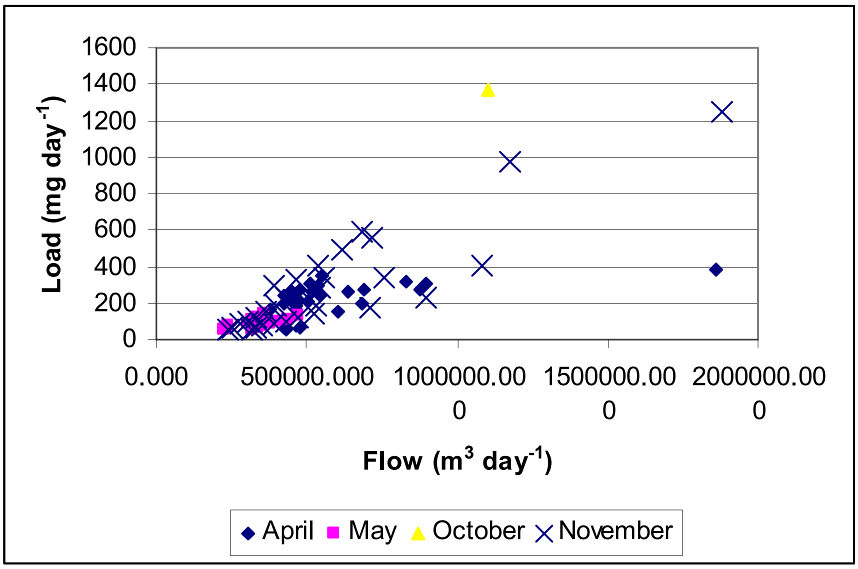

Fig 3.20 Flow versus load for Woodmill by month (only loads above 50mgday^{-1})

Thus one would start with a monthly flow duration curve being sampled in the GREAT-ER model. This would be linked to a particular flow rate. This flow rate would be applied to the flow versus load curve for a month to obtain a load figure. This would then be used with the load duration curve to link to a load exceedance. This load exceedance will relate to the flow exceedance sampled in GREAT-ER and is the level that should be sampled to give a load input for the reach in a particular month. A look-up table of flow exceedance versus load exceedance will be produced for each month once 30-year results are obtained.

4. TERRACE database

A database of information used for the TERRACE Exe application has been produced on CD. A separate user guide is provided with a copy of the CD.

It should be noted that many of the data sets are subject to licence agreements which restrict their use to this project or to research only. Details of IPR are given with the individual data sets.

5. TERRACE validation and implementation plan

5.1 Introduction

The impetus for the CEFIC-LRI programme has been the requirement by the EU for the chemicals industries to develop methodologies for demonstrating the likely impacts of chemicals in the environment via the estimation of Predicted Environmental Concentration (PEC). The EU has recently accepted in outline the approaches developed under LRI subject to “extensive validation”. This section outlines a recommended approach to such a validation exercise for TERRACE.

5.2 What is validation and what is it not?

The term "extensive validation" implies that the EU wish to see models tested and validated against monitored data for a range of environments and chemicals. In the case of a diffuse source pollution model, such an exercise should demonstrate several things:

- Ability of the model to reproduce the processes which are responsible for the supply and transport of pollutants;
- Responsiveness of the model to varying climate, land use, land management and chemical inputs;
- Robustness of the model for prediction of PECs

These things imply that validation should include an important component of quality assurance, including evaluation of results being carried out by teams independent from modellers, evaluation of data and parameter quality and consistency, evaluation of validation data and consistency of approach between model applications.

Although there is a place for widespread application of a model in order to "prove" its worth, this does not constitute validation. With a model as complex as SWAT-2000 inconsistencies in approach and data may well mask problems with the model or the particular application and will not result in credibility for the results. It is therefore recommended that a quality assured validation exercise be carried out as outlined in the following sections.

5.3 Validation of TERRACE within the context of the European Risk Assessment process

The first part of the exercise is to define the outputs which the model is expected to deliver and the accuracy that is required.

- Required end points
- What exposure estimates?
- For which compartments?
- To which level of accuracy?

It is then necessary to select a range of sites and environments for which the model should be tested. Such scenarios should include a full range of climates, chemicals, sources, land uses and land management and should incorporate sites where extreme responses would be expected.

Within the context of LRI, as opposed to TERRACE, the integration of models is also a matter which should be considered in terms of validation and error propagation. Any error in the atmospheric input to TERRACE may be magnified by TERRACE and so on through linkage to GREAT-ER and the estuary model, and may make results down the model chain meaningless. An evaluation of error propagation is therefore strongly recommended as part of the validation of the LRI environmental modelling programme. This would suggest that models should be applied to the same geographical areas.

5.4 Validation plan for TERRACE

A possible format for TERRACE validation is shown below (Fig. 5.1). A core group (tasks identified in the light blue boxes to the right) would first draw up a model application guide and validation protocol. This would define the data inputs to be used (and their quality requirements), the period to be modelled, the validation tests to be carried out and the acceptance level for model performance. This would be agreed by CEFIC before any further work was carried out.

This core group would also be responsible for selecting scenarios and catchments and for evaluating input and validation data. Once a set of sites have been identified and scenarios defined, one or more independent modelling groups would each be charged with application of TERRACE to one or more catchments. An individual application would follow a clearly defined methodology, with parameter estimation and adjustment for calibration being consistent between applications. Queries about model application would be fed back to the core group and application guidelines for all groups adjusted accordingly.

Results from model application and calibration exercises would then be fed back to the core group for independent validation, and results from all applications would be compared and evaluated. At this point all groups would meet to discuss outcomes from the validation exercise. If necessary a further iteration of the model application-validation exercise may occur at this point. The aim is to have not only a validated approach to estimation of diffuse source pollution for CEFIC, but also a series of validated sites around Europe for which new and existing chemicals can be tested. By rigorous validation of TERRACE for a range of environmental situations future application of the package becomes simpler and indeed possible for non-specialists.

Who will be involved?

We suggest:

- Core group
- User groups identified because of modelling capability and data availability (possibilities are):
- University of Giessen (Martin Bach) – SWAT user, detailed (daily level) pesticide data for 60km^2 catchment in northern Germany
- University of Uppsala (Nick Jarvis) – modellers with very detailed pesticide input/output data for a 9km^2 catchment, some (limited) possibility to move to larger scale modelling
- JRC (Giovanni Bidoglio, Roland Heiderer) – experience with SWAT for nutrient modelling, European catchment data sets
- University of Leuven – extensive experience with SWAT model
- ….others

The core group should:

a. Produce a TERRACE modelling package application guide
b. Define a validation procedure
c. Work as a user group for one catchment to ensure modelling protocols are implementable
d. Identify scenario gaps – i.e. those environments/contaminants not covered within this validation phase
e. Carry out validation for all modelling exercises

f. Identify modelling problems and missing process representation
g. Modify and improve the application guide
h. Supply a validated Tier II version of TERRACE and an online application guide for inclusion in the REACH system
i. Recommend how the modelling and validation procedures should progress into the future

User groups will:

a. Supply all data to be used for model running and validation to the core group before modelling starts (guarantees that data remain fixed throughout the process)
b. Run the TERRACE package following the steps laid down in the application guide for one catchment and an agreed set of contaminants
c. Provide feedback to the core on the application process and the guide
d. Provide all model output to the core group for validation
e. Attend workshops and meetings to assist in definition of project direction and final recommendations.

Resources and timescale:

1 x full-time research officer for 18 months in the core group
1 x full-time research officer for 12 months in each of the user groups

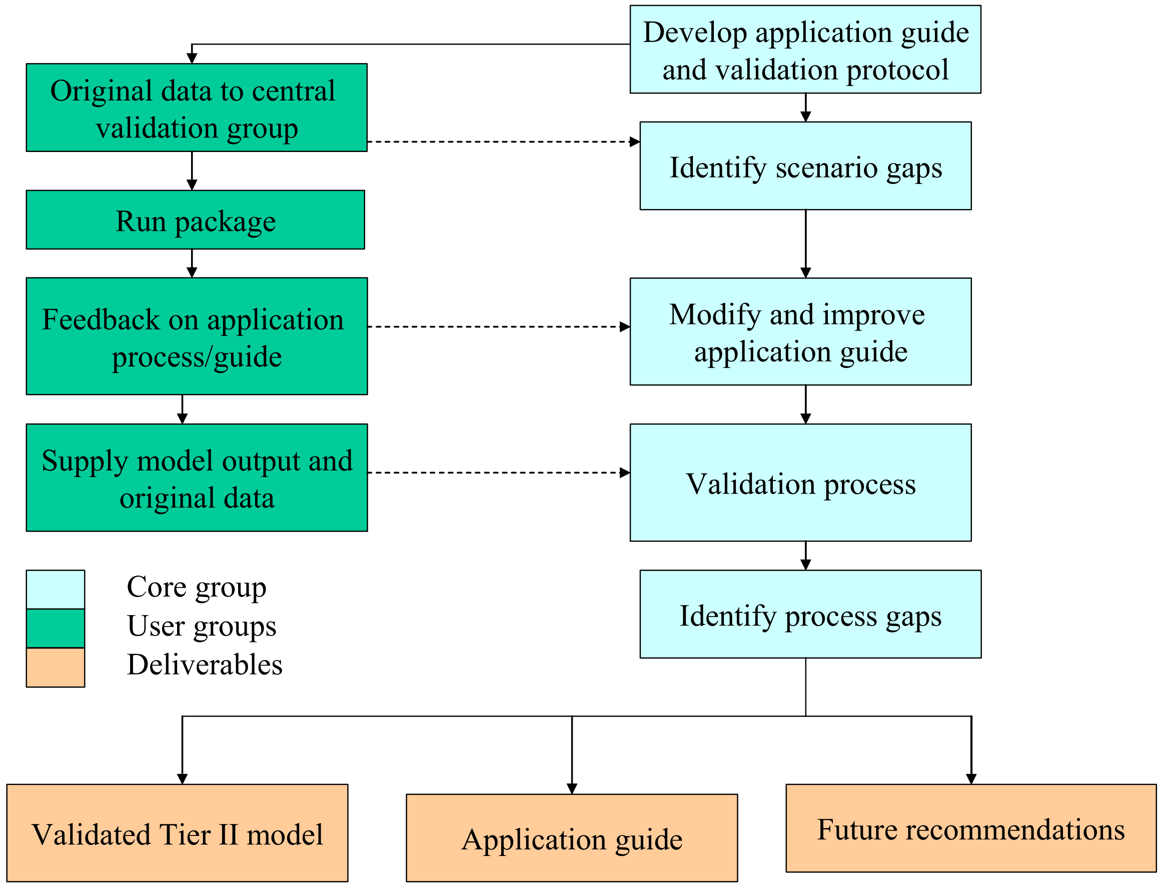

Fig. 5.1 Outline work plan for model validation

5.6 *Implementation*

Once the TERRACE approach is validated there is still the question about how it will be implemented and used within LRI and REACH-IT. SWAT-2000 is a complex model which requires a high level of hydrological expertise to set up, calibrate and validate for hydrological performance before any contaminant movement can be modelled. Our suggestion is that this is best achieved through a series of focus sites across Europe. These should be selected to represent key combinations of land use, climate, soil and land management. This approach is the same as that approved by the EU as part of their FOCUS initiative for both groundwater (vertical) and surface water (to edge-of-field) analysis of pesticide transfer. Details of the FOCUS scenario selection methodology are given in Appendix C. Such an approach fits well alongside the proposed validation scheme.

6. Discussion and conclusions

7. References

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Appendix A Defra usage statistics for Mecoprop and Mecoprop-p for the South Western Region 1994 and 1996

Appendix B EU Recommendations for Mecoprop and Mecoprop-p application

Appendix C Guidelines for FOCUS site selection

The objective of developing a set of scenarios suitable for calculating environmental exposure resulting from pesticide use as part of the Step 3 risk assessment process was to produce a limited number of "*realistic worst case*" surface water scenarios which were broadly representative of agriculture as practised in the major production areas of the EU. These scenarios should take into account all relevant entry routes to a surface water body (via spray drift, drainage and run-off), as well as considering all appropriate target crops, surface water situations, topography, climate, soil type and agricultural management practices. The lack of comprehensive databases that characterise most of these agro-environmental parameters at a European level meant that it was not possible to select representative worst-case scenarios in a rigorous, statistically-based manner. Instead, a pragmatic approach to selection was adopted, using very basic data sources together with expert judgement. In doing this it was recognised that the scenarios should reflect realistic combinations of run-off and drainage, recognising that these processes dominate in different parts of Europe. In addition, wherever possible, selected scenarios should be represented by specific field sites with monitoring data to allow subsequent validation of the scenario.

Data Sources.

Selection of representative realistic worst-case scenarios was based on a number of broad data sets that cover all areas of the European Community. The data sets are briefly described below, grouped according to the environmental characteristics they represent:

Climate

- *Average annual precipitation.*
  This data was calculated from data collated by the Climatic Research Unit (CRU) at the University of East Anglia, UK as part of the Climatic Impacts LINK Project funded by the UK Department of the Environment. The data are held at a resolution of 0.5º longitude by 0.5º latitude and include long-term monthly averages of precipitation, temperature, wind speed, sunshine hours, cloud cover, vapour pressure, relative humidity and frost days based mainly on the period from 1961 to 1990 (Hulme *et al.*, 1995). The database was derived from various sources and is based on daily data from between 957 and 3078 weather stations across Europe, depending on the specific variable.

- *Daily maximum spring rainfall.*
  Values were calculated by combining data for 'spring' precipitation derived from the GISCO databases with daily rainfall data for the years 1977-1991 for a set of European stations available from the National Climatic Data Centre at Ashville in the USA (Knoche *et al*, 1998).

- *Average spring (March, April, May) and autumn (Sept., Oct., Nov.) temperatures.*
  This data was calculated from the monthly temperature in the climatic dataset compiled by the Climatic Research Unit (CRU) at the University of East Anglia, in the UK as part of the Climatic Impacts LINK Project (see *average annual precipitation* section above).

- *Average annual recharge.*

Values for this parameter were calculated from a monthly soil-water-balance model using a uniform deep loamy soil as a standard. The data collated by CRU (see above) were used as sources for the model and the evapotranspiration input data was calculated according to the method of Thornthwaite (Thornthwaite, 1948; Thornthwaite & Mather, 1957)

Landscape characteristics

- *Slope*.
  Data for slope were calculated from elevation data obtained from the USGS. This dataset has a resolution of 120 pixels per degree and was used to create average slope within a 5km x 5km resolution grid. (Knoche *et al*, 1998).

- *Soil texture, drainage status and parent material*
  Information on general soil properties such as soil texture and parent material, together with those areas containing cropped soils with some type of field drainage system installed, were derived from the Soil Geographic Database for Europe (Le Bas *et al.,* 1998).

Land use and cropping

- *Land cover*
  Data relating to actual land use within Europe at a resolution of 1 km by 1 km was obtained from the United States Geological Service (USGS) EROS Data Centre as part of its Eurasia land cover characteristics database. It has been derived from the Normalised Difference Vegetation Index (NDVI) data from Advanced Very High Resolution Radiometer (AVHRR) satellite imagery spanning a twelve-month period from April 1992 through March 1993.

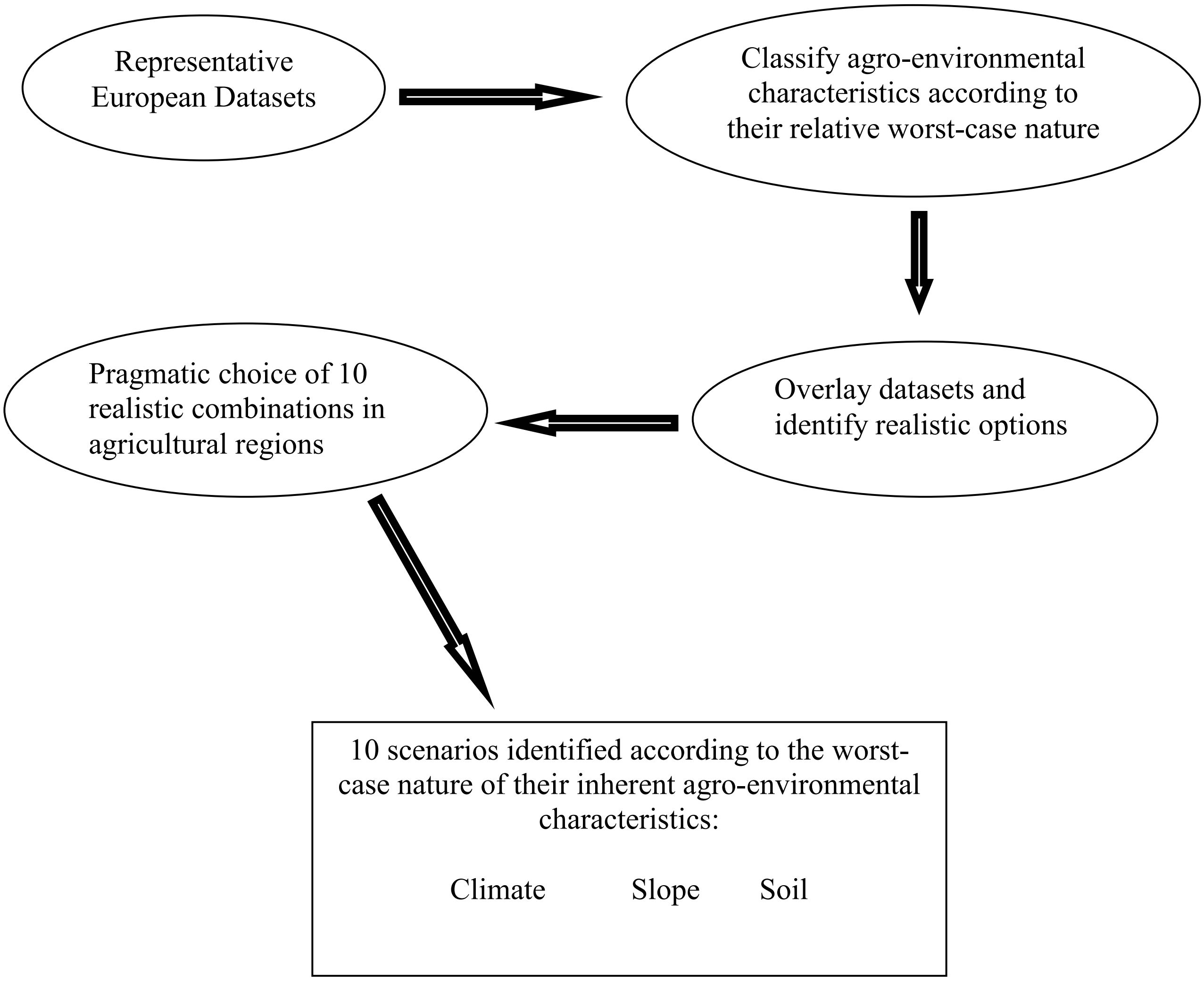
- *Cropping*
  Data on the main ranges of crops grown in different parts of the European union were derived from the REGIO databases collated and administered through the Statistical Office of the European Communities; EUROSTAT. Relevant data are held in two main data sets; *AGRI2LANDUSE* and *AGRI2CROPS*.

Methods

The pragmatic approach adopted to identify scenarios is illustrated in Figure 1. Initial scenario selection was based principally upon climate using temperature and recharge together with soil drainage status to identify broad drainage scenarios, and temperature and rainfall together with slope to identify broad run-off scenarios. The USGS land cover data was used to exclude non-cropped areas (pasture and forest) from consideration. Intersection of the data for land cover, slope, drainage status and climate showed that:

- Cropped land has a wide range of average autumn and spring temperature from less than 6.6^{o}C in the north to greater than 12.5^{o}C in the south.
- Cropped land occurs generally in areas with less than 1,000mm of average annual rainfall, but in marginal areas can have up to 1500mm.
- Cropped land with drainage occurs generally in areas with less than 250mm of average annual recharge, but in marginal areas can have up to 500mm.
- Cropped land does not occur in areas with average slopes greater than 15%.
- Cropped land with drainage occurs predominantly on areas with slopes of 4% or less.

Figure 1. *Pragmatic methodology for identifying realistic worst case surface water scenarios for Europe*



Based on this analysis, sets of climatic and slope ranges were defined to differentiate drainage and run-off scenarios as shown in Tables 1, 2 & 3.

Table 1 *Climatic temperature classes for differentiating agricultural scenarios*

AVERAGE AUTUMN & SPRING TEMPERATURE	
Range ^{o}C	**Assessment**
<6.6	Extreme worst-case
6.6 – 10	Worst case
10 – 12.5	Intermediate case
>12.5	Best case

Table 2 *Climatic classes for differentiating agricultural drainage and runoff scenarios*

AVERAGE ANNUAL RECHARGE (drainage)		AVERAGE ANNUAL RAINFALL (Run-off)	
Range mm	**Assessment**	**Range mm**	**Assessment**
>300	Extreme worst case	>1000	Extreme worst case
200 – 300	Worst case	800 – 1000	Worst case
100 – 200	Intermediate case	600 – 800	Intermediate case
<100	Best case	< 600	Best case

Table 3 *Slope classes for differentiating agricultural runoff scenarios*

SLOPE (RUN-OFF)	
Range %	**Assessment**
>10	Extreme worst case
4 – 10	Worst case
2 – 4	Intermediate case
<2	Best case

Appropriate soil types for either drainage or run-off scenarios were then identified using broad textural, structural and organic matter characteristics. Appropriate characteristics were considered to be those that represent a realistic worst-case for the identified input route, taking into account the models used to calculate inputs from that route. The soil characteristics used to classify relative worst cases for drainage and runoff are given in Tables 4 and 5.

Table 4 *Relative worst-case soil characteristics for Drainage*

Soil Characteristics	Assessment
Coarsely structured 'cracking clay' soils with extreme by-pass flow on impermeable substrates	Extreme worst case
Clays and heavy loams with by-pass flow over shallow groundwater	Worst case
Sands with small organic matter content over shallow groundwater	Worst case
Light loams with small organic matter content and some by-pass flow on slowly permeable substrates	Intermediate case

Table 5 *Relative worst-case soil characteristics for Runoff*

Soil Characteristics	Assessment
Soil hydrologic group D[3] (heavy clay soils)	Extreme worst case
Soil hydrologic group C [3] (silty or medium loamy soils with low organic matter content).	Worst case
Soil hydrologic group B [3] (light loamy soils with small clay and moderate organic matter content)	Intermediate case

By examining the combination of soil, climatic and slope characteristics across the European Union, 10 broad scenarios that integrate a realistic combination of inherent worst case characteristics for drainage and run-off were identified. Six of the scenarios characterise inputs from drainage and spray drift whilst four characterise inputs from runoff and spray drift. The selection process identified that scenarios combining extreme worst-case characteristics in every case do not occur in agricultural areas. This is because a combination of extreme environmental conditions means that most types of agriculture are not feasible. For example, a worst- or extreme worst-case soil for drainage scenarios precluded its combination with an extreme worst-case for recharge, because such extreme 'wet' climate and soil combinations restrict agriculture mainly to grassland.

Once the 10 broad scenarios had been selected, representative 'field sites' were identified for each one. In most cases these sites were chosen because extensive monitoring data was available to facilitate model parameterisation and possible future validation of PEC calculations.

At this stage, representative "edge of field" surface water bodies were identified for each of the selected 10 scenarios. In the absence of data bases mapping the characteristics of surface water bodies over the whole of Europe, expert judgement was used to identify three categories of "edge of field" surface water body that are common in Europe. The three categories are ponds (static or slow moving), ditches (relatively slow moving) and first order streams (fast moving). The presence or absence of these three categories of water body at each site was then assessed from

[3] Descriptions of soil hydrologic groups are according to the PRZM manual (Carsel *et al*, 1995)

local knowledge and validated by examining detailed field-scale maps of the relevant areas.

Finally, using local knowledge and the REGIO cropping databases, each of the 10 identified soil/climate scenarios were characterised in terms of the main range of crops they support.

Having identified a set of realistic worst-case scenarios, based on relevant agro-environmental characteristics, the distribution of each scenario within Europe was mapped using a GIS, to show their relevance to specific areas. The resulting maps indicate that in any of the areas highlighted, some part of the agricultural landscape corresponds to the soil, climate and at least one of the cropping characteristics of the specified scenario.

Finally, again using the pan-European databases described above, estimates were made of the percentage of total European agricultural land covered by each scenario, the percentage of European agricultural land with ‘worse’ or ‘better’ characteristics and the percentage of European agricultural land that would be ‘protected’ by each scenario.