THE DEVELOPMENT AND HARMONISATION OF RISK ASSESSMENT PROCEDURES TO EVALUATE THE ENVIRONMENTAL IMPACT OF TOXIC SUBSTANCES

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A thesis submitted to Brunel University for the degree of Engineering Doctorate

Research conducted within the Centre for Environmental Research, Brunel University and the National Centre for Ecotoxicology and Hazardous Substances, The Environment Agency.

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INTRODUCTION

The six-monthly reports are a record of progress toward the ongoing research objectives. These reports do not necessarily describe work at a conclusive stage, simply the progress made towards the deliverables. Project Gantt charts were reviewed updated on a six-monthly basis and included with each report. The six-monthly reports were submitted on the 1st of April and October each year.

At the end of the second year of registration, a dissertation, which subsumes the 24-month report, was completed and a copy of this dissertation is included. The progress towards achieving the aims and objectives of the EngD programme have also been reviewed in these reports.

6 Month Report

ENVIRONMENT
AGENCY

BRUNEL
UNIVERSITY

Engineering Doctorate in Environmental Technology

First 6 Monthly Report

1st April 1998

By
Nik Robinson

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Executive Summary

This report is the first six monthly report of my Engineering Doctorate. It contains an introduction and review of my work during this first six-monthly period. I have introduced the Environment Agency and briefly outlined its structure and where the National Centre for Ecotoxicology and Hazardous Substances fits within this structure. I have documented my time, which was initially with the Chemical Assessment Unit, and more recently with the Environmental Toxicology Unit. I have also summarised the modules that I have attended during this period. I have reviewed the aims and objectives that were set for this period and then laid down the new objectives for the next six-month period, as well as looking at more long-term aims. Finally a section containing some of the documentation that I have produced this period has been included, to indicate the type of work I am producing as part of my research and for modules, etc. There is also a glossary of terms included in this section to explain the many acronyms that are used in this field.

1 Introduction

This is the first six monthly report of my Engineering Doctorate program, which is intended to record a personal account of my progress, to-date as a Research Engineer sponsored by the EPSRC and the Environment Agency. The program followed to date has involved two distinct modes of study:

1. Introduction to research program
2. Attendance of four taught, week-long modules

Some discussion on each of these activities, not included in assignments already submitted to my portfolio, will be given. The overall aim in the first instance is to provide a comparative review of the activities of the Chemical Assessment Unit and the Environmental Toxicology Unit. The agreed objectives set for the first six months of the research program were:

- To familiarise myself with the structure and workings of the Environment Agency
- To develop an understanding of the current European Union notification system
  - To understand the methodology
  - To understand the models applied
- To accustom myself with the workings of the computer programme EUSES
- To select the necessary data from notification dossiers for use in comparative risk assessments
- To compare the results of manual and (EUSES) computer conducted risk assessments
- To complete a preliminary report on the activities of the Chemical Assessment Unit
- To familiarise myself with the operations and activities of the Environmental Toxicology Unit
- To ascertain the background to and method of producing Environmental Quality Standards
- To review reports on completed Environmental Quality Standards
- To attend the four skills based modules scheduled for this period, the Induction, Clean Technology, Project Management and Life Cycle Analysis Modules.

Box 1 - Objectives set for the first six months

All objectives have been met except for the completion of the preliminary report on the activities of the Chemical Assessment Unit. This report has been written and awaits review by my supervisors before submission to my portfolio. New objectives have been set for the next period.

This report has been constructed in two parts. The first part (Section 2), which follows this introduction, will begin by giving an outline of the Environment Agency's activities. Following this is a chronological review of work carried out within this first six-month period and my aims and objectives for the future, and in particular the next six months. I have also reviewed my work from the point-of-view of the course objectives and requirements, to indicate how I believe I am fulfilling these criteria. I have also included a review of the modules I have attended during this first six-month period to enable further comment and discussion and recording of work that was produced for the modules other than the assessment coursework. The second part (Section 3), comprises documents and other work I have produced. Although not all the work I have produced has been included in this section, a representative cross-section has been included in an attempt to convey the main emphasis of my work. In this section, a review of literature to date has been included, although this is by no means exhaustive and is growing daily. The table of literature references is more of an attempt to record papers I have read, referenced or intend to revisit, in order to more easily return to important and/or useful papers that I have come across during my work.

2 Review

2.1 The Environment Agency

The Environment Agency is a non-departmental public body established by the Environment Act 1995. The Agency became operational on the 1st April 1996 from which point it took over the functions of its predecessors – the National Rivers Authorities, Her Majesty's Inspectorate of Pollution, Waste Regulation Authorities and associated sections of the former Department of the Environment. The Environment Agency's work is divided into seven main functions, these being:

- Pollution Control
- Water Resources
- Flood Defence
- Fisheries
- Navigation
- Recreation
- Conservation

The Agency's overall aim of protecting and enhancing the whole environment contributes to the world-wide environmental goal of Sustainable Development, which has been defined as "Development that meets the needs of the present without compromising the ability of future generations to meet their own needs". The Agency has eight regional offices across England and Wales and head offices in London and Bristol; the regional offices are then sub-divided into areas. This structure resulted in expertise in the Agency being dispersed across a wide area and to counter this three national "Centres of Excellence" were set up, one of which being the Ecotoxicology and Hazardous Substances (EHS) National Centre, within which I am working. In Section 3.2 an organisational structure can be seen for the EHS, and where I fit within it. In line with the Agency's policy on printing and reports, all my assignment and reports are printed on paper produced from one hundred percent recycled and chlorine-free pulp.

2.2 Review of Work Carried Out to Date:

During the period from the 3rd November 1997 until 29th January 1998 I worked within the Chemical Assessment Unit (CAU), of the Environment Agency at Steel House, London. The CAU is part of the joint UK Competent Authority (CA) along with the Health and Safety Executive (HSE). Together these two organisations are responsible for the notification process in the UK, a process by which all companies marketing chemicals in the EU must indicate this intention and supply basic physical, chemical and toxicological data. All chemical substances fall under one of two categories:

New substances
Existing substances

Where a "new" substance is any chemical that was not marketed in the EC in the 10 years prior to 18th September 1981.

Due to this dividing date, all chemicals then come under one of two notification systems, these being:

NONS - Notification Of New Substances
ELINCS – European List of Notified Chemical Substances
ESRs - Notification of Existing Substances
EINECS – European Inventory of Existing Chemical Substances

My time at the CAU was spent mainly familiarising my self with the NONS system. ESRs are carried out on the basis of priority lists, from which Member States bid for chemicals to do notifications on. However, any company in the world wishing to market a chemical in the EU for the first time must notify the local country's CA of this intention and supply the required information, including physical and chemical data as well as human and ecological toxicity results. From these data a Risk Assessment (RA) is produced resulting in one of the four conclusions outlined below:

(i) *The substance is of no immediate concern for man or the environment.*

(ii) *The substance is of concern, further information required at next tonnage threshold.*

(iii) *The substance is of concern, further information required immediately.*

(iv) *The substance is of concern, risk reduction recommendations required.*

The approach used to perform these RAs is to calculate Predicted Environmental Concentrations (PECs) and Predicted No Effect Concentrations (PNECs) and then calculate the ratio of these two values (PEC/PNEC) which is termed as the Risk Characterisation Ratio (RCR) for each environmental compartment. If the RCR is greater than 1, further research or risk reduction may be required, as outlined in the conclusions above.

The methodologies involved in the calculation of these PEC and PNEC values are complex and for this reason considerable time was spent in gaining an understanding of them. Various areas of interest have arisen; there is extensive use of Quantitative Structural-Activity Relationships, (QSARs) where there is a lack of data or experimentally undetermined values. These QSARs based on chemical and physical knowledge, are well documented in the literature and many are available for difficult to measure values. They attempt to link families of like-structured chemicals to certain properties. For example below are three examples of QSARs for the prediction of the organic carbon-water partition coefficient (Koc) from the octanol-water partition coefficient (Kow):

Esters	$\log Koc = 0.49 \log Kow + 1.05$
Nitrobenzenes	$\log Koc = 0.77 \log Kow + 0.55$
Organic Acids	$\log Koc = 0.60 \log Kow + 0.32$

Test methods are also of interest, in their representation of actual environmental conditions and situations. Are the chosen species, tests and methods representative of the real environment? Are our environmental models (fate and behaviour etc.) indicative of the real environment? One of the ways in which the RA process takes account of these questions is through the application and use of Assessment Factors, (AFs). If results are only available for a few test species then AFs are applied to extrapolate these figures to the whole environment, to ensure protection of all species. Below examples are shown of AFs used in the calculation of various PNEC values.

Data Available	Assessment Factor
At least one short-term $L(E)C_{50}$ from each of three trophic levels of the base-set (fish, daphnia and algae)	1000
One long-term NOEC (either fish or daphnia)	100
Two long-term NOECs from species representing two trophic levels (fish and/or daphnia and/or algae)	50
Long-term NOECs from at least three species (normally fish, daphnia and algae)	10
Field data or model ecosystems	Reviewed on a case-by-case basis

Table 1 – Assessment factors for aquatic PNEC derivation

Data Available	Assessment Factor
$L(E)C_{50}$ short-term toxicity tests, (e.g. plants, earthworms, or micro-organisms)	1000
NOEC for one long-term toxicity test (e.g. plants)	100
NOECs for additional long-term toxicity tests of two trophic levels	50
NOECs for additional long-term toxicity tests for three species of three trophic levels	10
Field data or model ecosystems	Reviewed case-by-case

Table 2 - Assessment factors for soil PNEC derivation

The situation is even more complex for sediment PNEC and RCR calculation, with ecotoxicity data not always being available for sediment dwelling organisms, in which case the sediment PNEC is extrapolated from the aquatic PNEC value.

$$PNEC_{sed} = \frac{K_{sed-water}}{RHO_{sed}} \times PNEC_{aquatic} \times 1000$$

Equation 1

Where:

$PNEC_{sed}$	Predicted no effect concentration in sediment	$(mg.kg^{-1})$
$K_{sed-water}$	Sediment-water partitioning coefficient	$(m^3.m^{-3})$
RHO_{sed}	Bulk density of suspended matter	$(kg.m^{-3})$
$PNEC_{aquatic}$	Predicted no effect concentration in water	$(mg.l^{-1})$

The derivation of an RCR value then depends on what data were available for earlier calculations and appropriate ratios and AFs are then calculated.

Available measured data: PEC_{sed}	**Available measured data: $PNEC_{sed}$**	**Risk Characterisation**
$C_{pore\text{-}water}$	none	$\frac{C_{pore\text{-}water}}{PNEC_{water}}$
C_{bulk}	none	$\frac{C_{bulk} \times RHO_{sed}}{K_{sed\text{-}water} \times PNEC_{water} \times 1000}$
none	$PNEC_{sed}$	$\frac{K_{sed\text{-}water} \times PEC_{water} \times 1000}{PNEC_{sed} \times RHO_{sed}}$
$C_{pore\text{-}water}$	$PNEC_{sed}$	$\frac{K_{sed\text{-}water} \times C_{pore\text{-}water} \times 1000}{PNEC_{sed} \times RHO_{sed}}$
C_{bulk}	$PNEC_{sed}$	$\frac{C_{bulk}}{PNEC_{sed} \times RHO_{sed}}$

Where:

$C_{pore\text{-}water}$	Concentration in sediment pore water	$(mg.l^{-1})$
C_{bulk}	Concentration in whole sediment	$(mg.kg^{-1})$
$K_{sed\text{-}water}$	Sediment-water partition coefficient	$(m^3.m^{-3})$
RHO_{sed}	Density of moistened sediment	$(kg.m^{-3})$

Table 3 - Sediment risk characterisation, requirements and calculations

Difficulties are also encountered when dealing with substances with any of the following properties: low water solubility (e.g. <1 mg.l-1), toxicity at low concentrations, volatility, photolytic or hydrolytic instability, adsorption onto glass, coloured, not acutely toxic at limit of solubility, complex substances with known or unknown components, and highly lipophilic (log Kow >3) substances.

Substances that have any of these properties can prove very difficult to test in the laboratory, making risk assessment hard due to missing or poor quality data. QSARs (as well as OECD and EU test guidelines) are available for the prediction of these values.

I also spent a considerable amount of time reviewing the computer system called EUSES, (European Union System for the Evaluation of Substances). The 7th Amendment to the Dangerous Substances Directive (67/548/EEC) states the procedure and requirements of the notification process for both NONS and ESRs. The EUSES programme is intended to be an automation of the technical guidance documents that accompany this amendment. This computer system contains the necessary models needed to perform the risk assessment of chemicals, however as a result of poor documentation, generic modelling and a lack of transparency in its use, results obtained from the program rarely concur with those produced manually by risk assessors.

Towards the end of my time at the CAU I prepared a report on my work within the CAU and a full in-depth look at risk assessment as part of the EU notification system. Questions arising concerning risk assessment as part of the notification system and the strengths and weaknesses that were immediately apparent are discussed. Further discussion is intended in a later report in the light of information I gain while working within the Environmental Toxicology Unit.

After leaving the CAU at the end of January I moved to the Environmental Toxicology Unit on 16th February 1998. This unit is sited at, Wallingford, in the EA's Ecotoxicology and Hazardous Substances National Centre, which has proved very advantageous, due to the wealth of scientific knowledge which is concentrated in the centre, the Direct Toxicity Assessment, Pesticides and Nutrients groups. The Environmental Toxicology Unit (ETU), is responsible for dealing with regional enquiries on chemical standards and data held by the Agency, and the production of Environmental Quality Standards (EQS) for chemical substances. On arrival at the ETU I aimed to start reviewing the structure and methodology of the EQS system, and to analyse and understand the significance of ecotoxicology endpoints, including their meaning, statistical validity and confidence limits. In the longer term I aim to have identified strengths and weaknesses in the EQS system as well as comparing this approach to that of the CAU's notification system.

I have since had a meeting with the manager of the ETU (Dr. Geoff Brighty) and my academic supervisor (Dr. Sue Grimes) and have agreed a set of objectives for at least the next three months, which can be seen later.

Overlapping with my time within these two units of the EA's Ecotoxicology and Hazardous Substances National Centre, I have attended three weeks of modules. These modules were as follows:

Induction Module 15th to 19th September 1997
Clean Technology Module 20th to 24th October 1997
Project Management/Life Cycle Analysis Modules 8th to 12th December 1997

The Induction module, included attendance of the 1997 Engineering Doctorate Conference, where the first year Research Engineers (REs) make a fifteen minute presentation on their work to date, while second and third year REs make poster-board presentations. Attending the conference dispelled any doubts I may have had about the course. I felt that the REs made professional and inspiring presentations and were able to competently defend their work to a mixed audience of their peers including academic and industrial sponsors, other REs and members of the Management Committee. Also as part of the induction module we were taught presentation skills, Belbin team roles, and how to form and work within a team. The presentation skills that were outlined have been of great use and I have implemented them at subsequent modules and for my academic department. I have produced a fifteen-minute presentation for the other researchers in the group and a poster-board presentation for the new Chancellor's visit, both on my work at the CAU (see Sections 3.13 and 3.14).

The Clean Technology was a very interesting module, in which my beliefs in technology, progress and the environment were all questioned. I enjoyed the opportunity to have knowledgeable debate with my peers on subjects such as pigs being used for transplants and the protection of one species to the detriment of another. I came away from the module confused but with a burning need to find answers to questions that had been raised.

The Project Management module covered many practices that had been previously covered to greater depth in my undergraduate management courses, however some of the exercises were interesting and good application of the required skills. The Life Cycle Analysis module that ran for the second half of the week, was interesting, however there were both problems with the Surrey University computer network and the PEMS software that made the module unduly arduous. I found the outline to the methodology interesting but would have enjoyed the chance to discuss the relative merits of the method to greater depth. Particularly in the light of my research project and where risk assessment and LCA stood in relation to one another, aquatic toxicity levels being hinted at in some parts of LCA methods.

2.3 Proposed Work for Next Period:

Now that I am within the ETU I shall continue with my work in this group for at least the next three months, at which point a review meeting is to be held with my industrial supervisor (Dr. Jim Wharfe) and my academic supervisor. My objectives while in the group and for the next three months are as outlined below. However, I anticipate spending possibly one if not two months of my time on the Kennet and Avon incident which came up suddenly and has thrown up a lot of questions about the methods used in these types of incidents. Not least is the fact that the National Centre was not informed of the events until two days after the initial incident..

- To review structured methodology of the EQS system
  - How chemicals are chosen for assessment
  - Data collation
  - Data interpretation
  - What happens after the assessment has been carried out
- To analyse and understand the significance of ecotoxicology endpoints
  - EC_{50}/LC_{50}
  - NOEC/LOEC
  - Their meaning, statistical validity and confidence limits
- To write a report on the National Centre's response and handling of the Kennet and Avon incident
  - Involvement in pollution incident
  - Chemical information, used/needed
  - Point at which National Centre should be informed
  - Thought processes
    - what was needed
    - what was used
    - what else would have been useful
- To identify the learning points from the incident and to develop and propose a management system for coping with incidents

Box 2 - Objectives for next three months in the ETU

Minutes of my meeting on the 30th January 1997 with my industrial supervisor, can be found in the third section of this report and outlines the manner in which Dr. Jim Wharfe intends me to review the approaches to risk assessment within the Agency. Some longer-term aims that were indicated are as follows:

- To understand toxic modes of action
  For aquatic life there are only between 8 and 12, toxic modes of action, and therefore if chemicals mode of action can be assessed, cumulative effects may be able to be considered.

To become accustomed to the methods of direct toxicity assessment

This would mean that the toxicity of whole effluent samples would be considered. It would probably take longer and involve more work, but would be more protective of the environment.

To conduct sensitivity analysis using case studies

Sensitivity analysis needs to be carried out on all risk assessment processes to see which steps prove to be the sensitive ones and where assessment factors have the greatest effect on the final assessment figures.

To compare manual vs. EUSES risk assessment calculations

As was previously mentioned, EUSES has its problems for risk assessment compared with manual assessments, or does this indicate that manual assessments are too site specific.

To consider site specific vs. generic risk assessment

Which method of risk assessment leads to greater protection of the environment? Is there a place for both in risk assessment practices?

To compare risk assessments conducted in the CAU vs. ETU

Draft assessment documents are available for nonylphenol, acrylomide, tri-/per- chloroethylene and acetonitrile, which have been conducted under each system. What does a comparison of the results suggest? Is either method more protective than the other, and are the results of one as applicable to the customers of the other results?

Box 3 - Longer-term aims for work within the EHS

2.4 Glossary

Many terms, references and acronyms have come to light during the work I have carried out to date. Where possible I have defined these the first time I have used them in this report, however a full glossary is included (Section 3.16) for ease of reference.

2.5 Aims and Objectives of the Engineering Doctorate Program:

The Engineering Doctorate (EngD) in Environmental Technology, Course Handbook, outlines aims and objectives of the course in both Section 3 under Objectives and Appendix 1, The Joint Regulations, under Section 2.1. Below I have listed these aims and objectives in a table and have summarised how I feel my research work will demonstrate and meet, if not exceed these attributes.

Aims and Objectives of EngD Program	**How Attributes Will Be Demonstrated**
REs should: (i) be equipped as engineering research-designers to plan and lead flexible and innovative R&D programmes that respond to customers' needs.	I aim to firstly outline the strengths and weaknesses of the existing Risk Assessment systems and methodologies and then research, propose and implement, integrated sustainable practices for the risk assessment of hazardous substances, mindful of the effects these systems have on chemical industries.
(ii) be able to work effectively, and to form, work within and where necessary lead teams with a multi-disciplinary background to tight time schedules.	I shall be addressing this aim in two ways. The forming of and working with of multi-disciplinary teams will be necessary in both the organisation of the 1998 Engineering Doctorate Conference, and in my work on the Risk Assessment systems, where biologists, ecotoxicologists and business managers among others will all have inputs and constraints on my work.
(iii) possess comprehensive expert knowledge of the field of Environmental Technology, of the techniques needed to balance social and economic benefit against resource utilisation and environmental impact, and of the processes of technology transfer needed to ensure the application of research into practice	Expert knowledge of environmental technology and in particular risk assessment, ecotoxicty and environmental legislation will be of great importance throughout my research. I will also need to balance not only social and economic but also environmental benefit, in all developments my research produces. And finally the methods of technology transfer, particularly in the development of transparent risk assessment methodologies will also be of great importance, to ensure the proper use of risk assessment systems in industry.

Table 4 - Aims and objectives of the Engineering Doctorate

Aims and Objectives of EngD Program	How Attributes Will Be Demonstrated
(iv) have demonstrated ability for originality and for. innovation	In any methodologies and systems I design or development, I will show my flair for originality and innovation, creating systems which are tailored towards the needs of both the Environment Agency and industry (the customer).
(v) possess a working knowledge of project management and business methods and their implications for research and development	The project management module served as an introduction to project management practices and their power in the planning, implementing and tracking of not just projects but all work. These new skills I have learnt I shall practice and improve through their use in the running of my research and more immediately the organisation of the 1998 Engineering Doctorate Conference.
(vi) possess and have demonstrated a high level of communication and presentation skills	These skills that I find to be continually developing the more work I produce shall be demonstrated not only at the annual conference, but also in all the reports I produce as well as papers and poster presentations I intend to get involved in during my research project.

Table 4 - Aims and objectives of the Engineering Doctorate (continued)

The University of Surrey and Brunel University Joint Regulations (Appendix 1, Section 4.4.1, Assessment and Progression Criteria), also outline criteria that are necessary for eligibility to graduate as a Doctor of Engineering. Many of these are assessed as part of the taught modules, however two criterion of particular note are to be tested in the final *viva voce*, but I feel should be considered here and throughout the degree program are to:

- Demonstrate evidence of innovation and a contribution to knowledge via research into either:
  - (i) novel understanding of the environmental consequences of systems for providing or using goods or services, or;
  - (ii) novel methods of improving the environmental performance of systems for providing or using goods or services thereby contributing to more sustainable development.

- Demonstrate an understanding of the context of the research: this must include the scientific context and, where appropriate should include the commercial and social context.

Further to these is the consideration that the work should meet the criterion of environmental technology, which is unique to the Brunel/Surrey Engineering Doctorate program. I feel I will meet these criteria in the following ways:

My innovation and contribution to knowledge shall primarily be in the area of risk assessment. Through the initial study of the existing systems, strengths, weaknesses, and possible synergies will be outlined. Novel methodologies will then be researched, devised and documented. The contribution to knowledge clearly being in the generation of newly improved, risk assessment practices, systems and methodologies. These will be transparent to both implementers and users, protective of the target environmental compartments and the environment as a whole. However, they will also endeavour not to over regulate or be over protective, which can result in the hindrance of industry and loss of faith in risk assessment practices. An understanding of the environmental consequences of the systems and methodologies will be necessary and should result in an improvement in environmental performance and a move towards more sustainable development.

An understanding of the context of the research will be necessary and demonstrated in the transparent nature of the developed systems, due to their use by industry and scientists at different levels. An understanding of the scientific context will be demonstrated in the application of the novel systems to ensure the protection of the environment, with good use of data and knowledgeable interpretation of results. As mentioned earlier, the commercial and social context will also have to be considered, being careful not to over regulate, or over protect, as well as constructing transparent methodologies and systems to ensure easy application and use.

Finally, my research is at the core of the Environment Agency's Ecotoxicology and Hazardous Substances National Centre's activities. As such I believe I shall demonstrate environmental technology in the construction of novel risk assessment practices that, while still ensuring protection of the environment, don't over regulate, to ensure the practices are workable in industry, making them more able to apply sustainable practices.

3 Documentation

3.1 Introduction

On the following pages are documents that I have produced during the course of my research and work to date, included is some of the work that I carried out for the modules both in preparation and while at the modules. The actual assignments have not been included here but are available for viewing as part of my portfolio, and a short comment on each module was included in Section 2 earlier. A cover sheet has been included with each document in way of a brief introduction to the context in which the work was carried out, when, why and who the customers or audience of the work was intended to be. A list of the included documents follows:

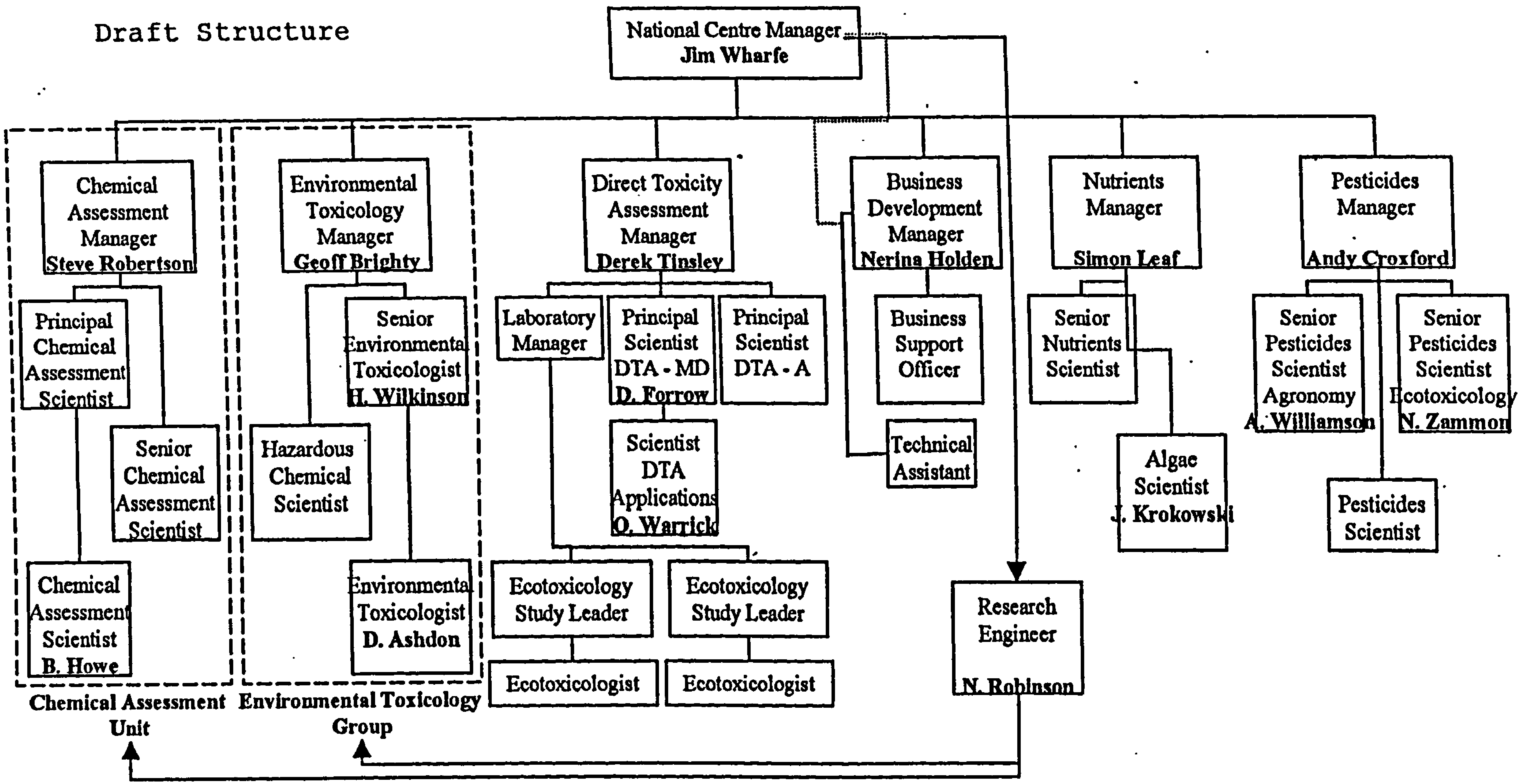
Section	Document
3.2	Organisation Chart of the National Centre for Ecotoxicology and Hazardous Substances
3.3	Notes on EUSES
3.4	Clean Technology Module – Pigs for Transplants Discussion
3.5	LCA Module – Exercises
3.6	LCA Module – Presentation
3.7	Project Management – Presentation
3.8	Minutes of Meetings with Jim Wharfe and Geoff Brighty
3.9	1998 Conference – Agenda for Meeting
3.10	1998 Conference – Budget
3.11	1998 Conference – Minutes of Meeting
3.12	1998 Conference – Notes on 1997 Report
3.13	Notification Process – Presentation
3.14	Notification Process – Poster-board
3.15	Literature Review – To Date
3.16	Glossary

3.2 Organisation Chart of the National Centre for Ecotoxicology and Hazardous Substances

This is a draft structure that I have drawn up from similar internal draft structures. Where positions remain blank this because they have not been appointed at this date. The reason for this lack of clarity is due to the infancy of the Ecotoxicology and Hazardous Substances National Centre, the final structure should be clarified later this year.

Ecotoxicology And Hazardous Substances National Centre

Draft Structure



3.3 Notes on EUSES

When I started my work on EUSES, many questions came to light. I took these questions to the Building Research Establishment (BRE), who under contract to the Environment Agency, carry much of the ESR work out. Members of BRE are also on the EUSES working group and so were able to give me knowledgeable accounts on the programme's working and implementation. A short report of some of the points that came to light follows.

EUSES
European Union System for the Evaluation of Substances

EUSES was made to automate parts of the Technical Guidance Document (TGD).

However EUSES doesn't deal with all chemicals and care must be taken in its use.

Changes to the EUSES program are decided at technical meetings, those that effect the written TGDs must go before a committee. The three types of changes are as follows:

Bug Fixes - Problems in the programming that are high priority changes to ensure a working program.

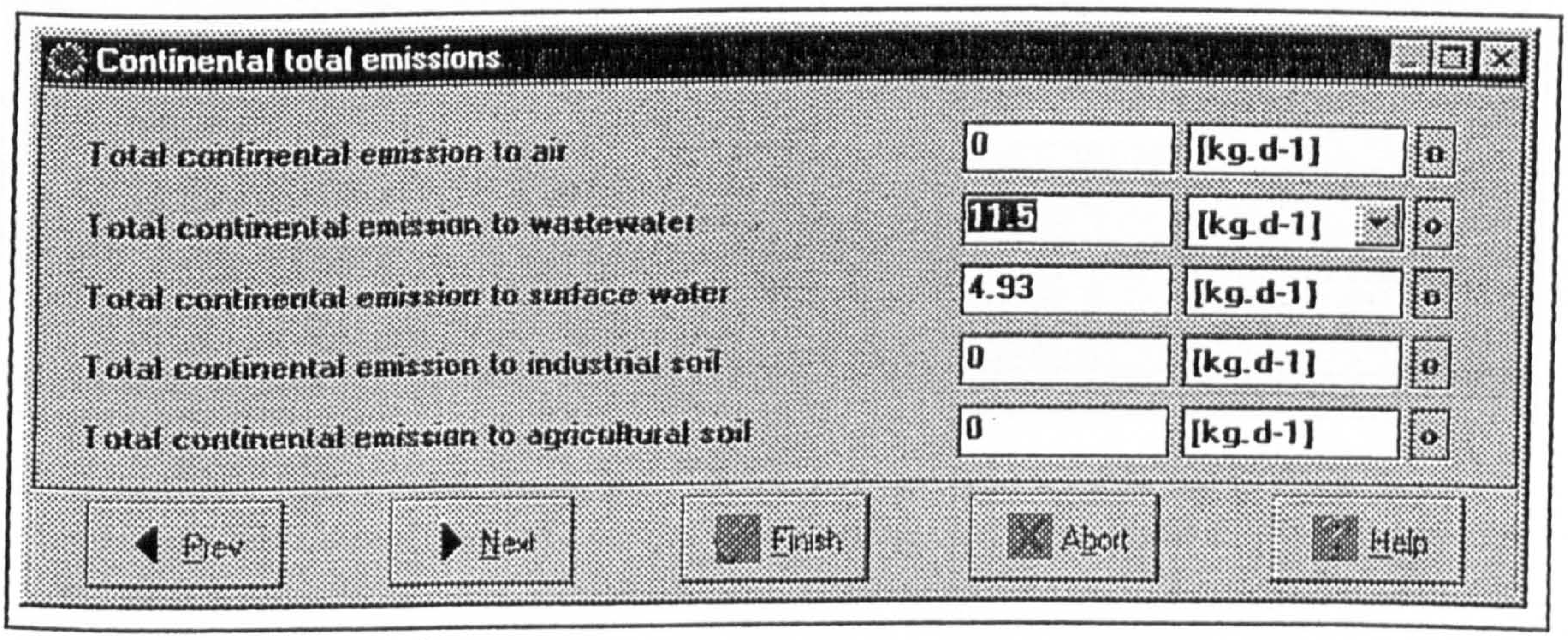
Problems - These are usually numerical inaccuracies or formula mistakes that produce erroneous results.

Wish List - Changes that would like to be made if budget, and time allows, mainly aesthetic and user friendliness changes. These obviously have the lowest priority.

TGDs are re-released approximately at 5 year intervals, the EUSES program will be updated at a more regular interval.

Problems and Tips that have come to light:

Continental figures,

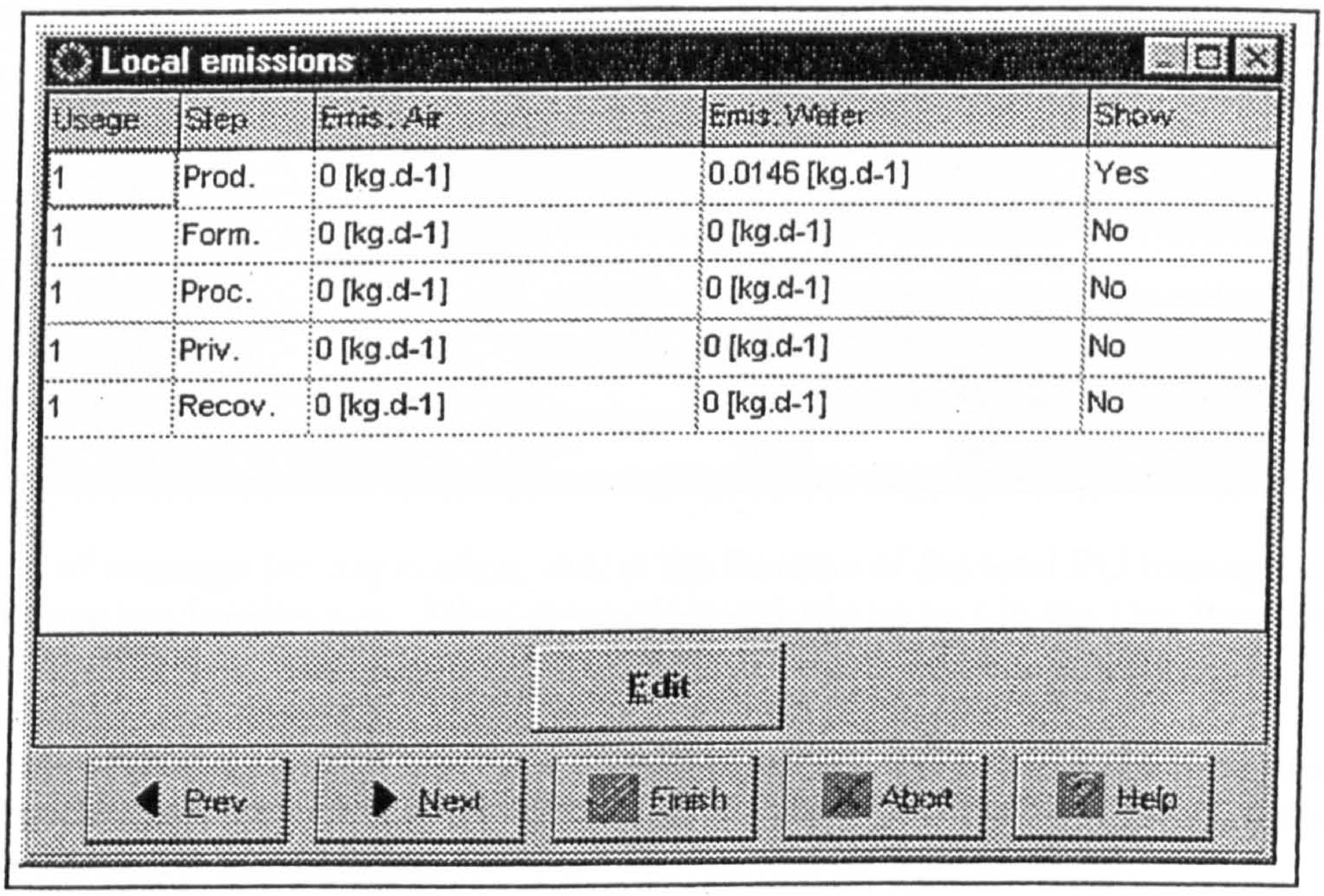


Continental total emissions

Total continental emission to air	0	[kg.d-1]
Total continental emission to wastewater	11.5	[kg.d-1]
Total continental emission to suface water	4.93	[kg.d-1]
Total continental emission to industrial soil	0	[kg.d-1]
Total continental emission to agricultural soil	0	[kg.d-1]

If values are known for continental emissions, or if they can be calculated it is best to enter them here at this point than use the calculated ones.

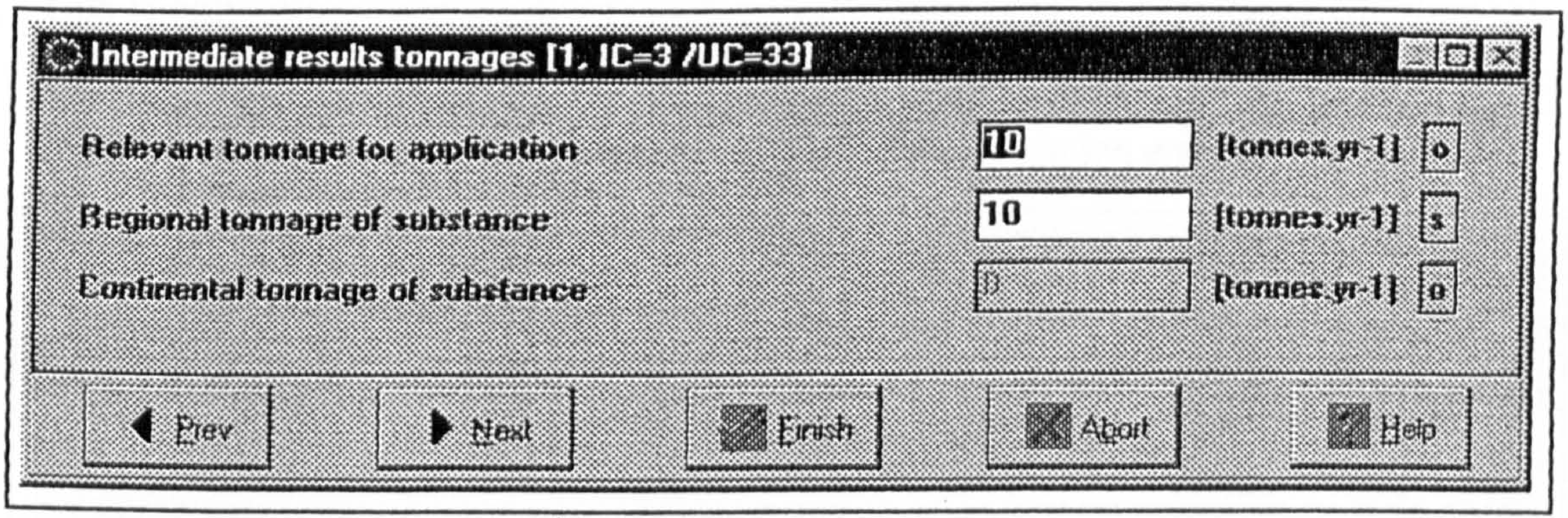
Local emission figures,



Usage	Step	Emis. Air	Emis. Water	Show
1	Prod.	0 [kg.d-1]	0.0146 [kg.d-1]	Yes
1	Form.	0 [kg.d-1]	0 [kg.d-1]	No
1	Proc.	0 [kg.d-1]	0 [kg.d-1]	No
1	Priv.	0 [kg.d-1]	0 [kg.d-1]	No
1	Recov.	0 [kg.d-1]	0 [kg.d-1]	No

This again should be edited in at this point as weight per day data is more likely to be available than percentage use and emission days per year figures.

If use is at a single site then the full tonnage can be entered under the regional value.



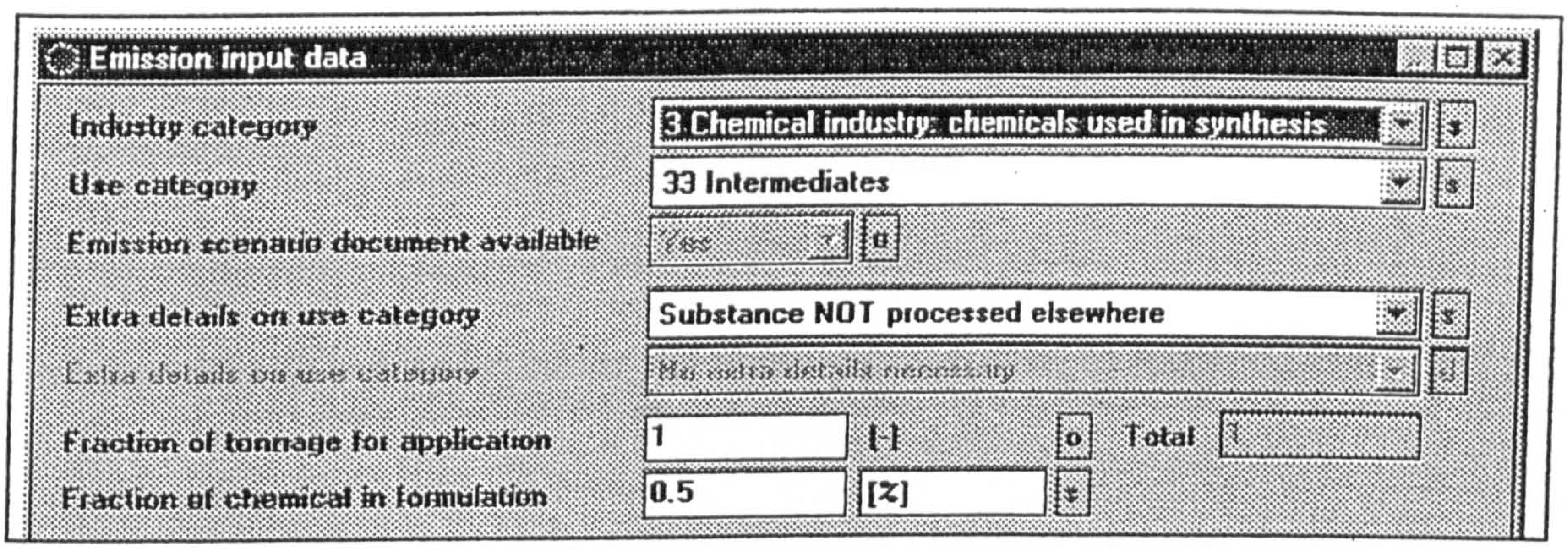
Relevant tonnage for application 10 [tonnes.yr-1] o

Regional tonnage of substance 10 [tonnes.yr-1] s

Continental tonnage of substance 0 [tonnes.yr-1] o

If there are < 10 sites in EU for a use, use largest site for regional value.

Fraction for application and formulation.



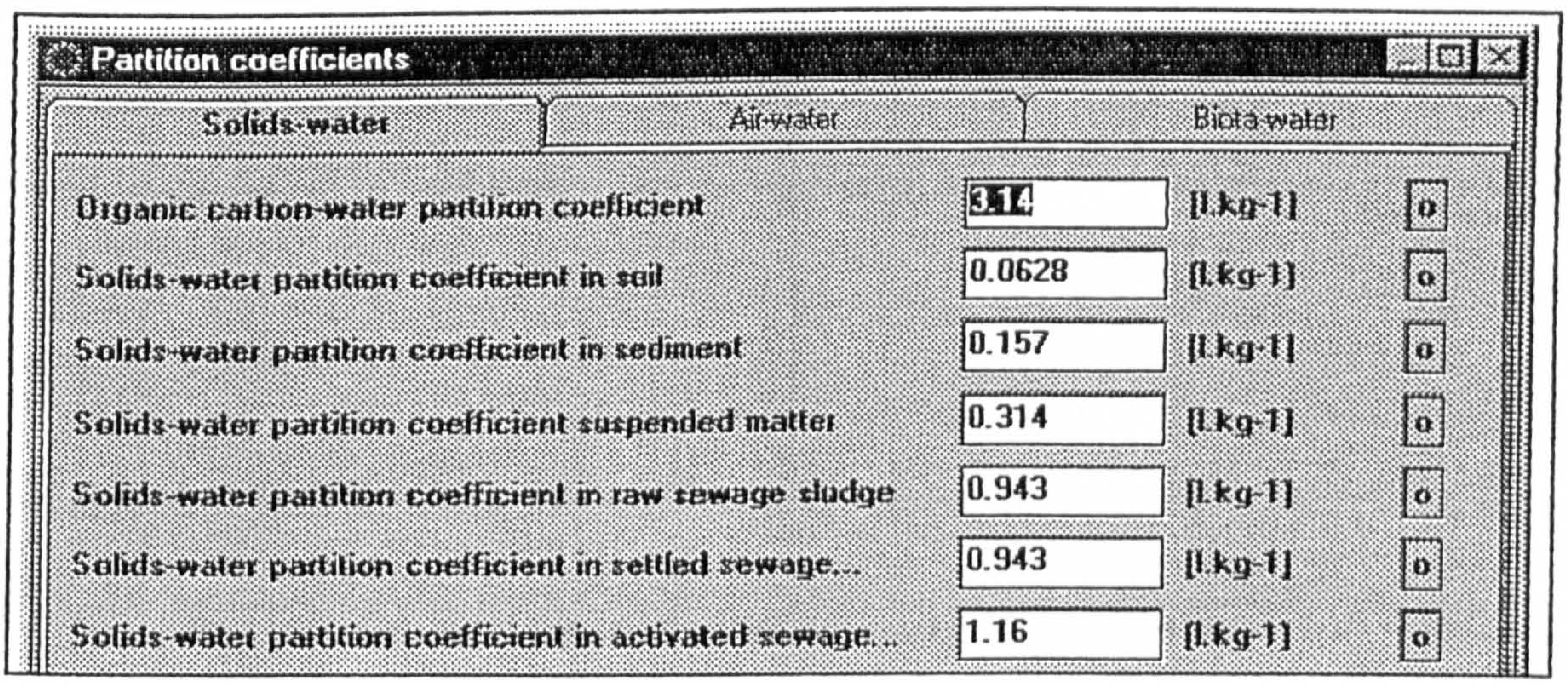
Industry category: 3 Chemical industry: chemicals used in synthesis
Use category: 33 Intermediates
Emission scenario document available: Yes
Extra details on use category: Substance NOT processed elsewhere
Extra details on use category: No extra details necessary
Fraction of tonnage for application: 1 [-] Total 1
Fraction of chemical in formulation: 0.5 [%]

Fraction of tonnage for application, this is the fraction of the total EU tonnage used in this application for this use. These figures should add up to 1 in the Use Pattern screen, but it is sometimes easier to have all production fractions adding up to 1 and all processing and other uses adding up to 1 therefore a total of 2.
The fraction of chemical in formulation, is the fraction compared to the total weight of the batch material, this figure is then used in the A and B tables of the Simpletreat model (Version 3 in EUSES).

The value for the Koc is calculated from the Kow value using the equation below,

$$\log Koc = 0.81 \log Kow + 0.10$$

This is only one of many suggested QSARs from the TGD. If a different equation is believed to be a better approximation or an actual figure is recorded for the Koc then this should be entered straight into the Partition Coefficients screen. An item on the Wish List for EUSES is the possibility to chose which sorption equation is used.



Organic carbon-water partition coefficient: 3.14 [l.kg-1]
Solids-water partition coefficient in soil: 0.0628 [l.kg-1]
Solids-water partition coefficient in sediment: 0.157 [l.kg-1]
Solids-water partition coefficient suspended matter: 0.314 [l.kg-1]
Solids-water partition coefficient in raw sewage sludge: 0.943 [l.kg-1]
Solids-water partition coefficient in settled sewage...: 0.943 [l.kg-1]
Solids-water partition coefficient in activated sewage...: 1.16 [l.kg-1]

Any value when changed can be replaced with the following,

D	Replaces cell with default value
O	Replaces cell with calculated value
?	Replaces cell with default value

STP discharge rate, a calculated value should be entered here.

Emission days from A and B tables, when entered do not back calculate!
Release fractions from A and B tables, when entered do not back calculate!

Internet address,
`http://www.ei.jrc.it/ecb/facilities/euses/index.html`

3.4 Clean Technology Module – Pigs for Transplants Discussion

As part of this course, we discussed various topics in groups, including the one that my group presented for which the notes overleaf were produced. I found these discussions very interesting, the pigs for transplants discussion brought up many arguments, including that of vegetarianism, farming and its sustainability, and animal rights and welfare. Another debate, on how to resolve a situation where two protected species were on an island (goats and a spices of plant), also brought up interesting argument about the value and/or comparative value of different species. Along with this, ideas such as species diversity, trophic levels and food-webs were discussed.

Pigs For Transplants And Meat

There is current controversy over the creation of genetically engineered pigs.

The current donor card system does not meet organ demand. The government found no ethical objection to the use of pigs for organs, but did find the same use of primates objectionable.

Animal rights activists are against breeding pigs for organs, saying it's wrong to create animals for human ends. They also say that there is no relevant difference between using pigs or severely mentally handicapped humans for organs. And that more human organs could and should be found.

Supporters of pig transplants argue that there will never be enough organs and that the interests of humans should take priority over pigs. After all transplants are a better breeding reason than bacon is.

Solutions:

Irreversible Donor Registration

Reversed Donor System

Mechanical / Genetic Alternatives

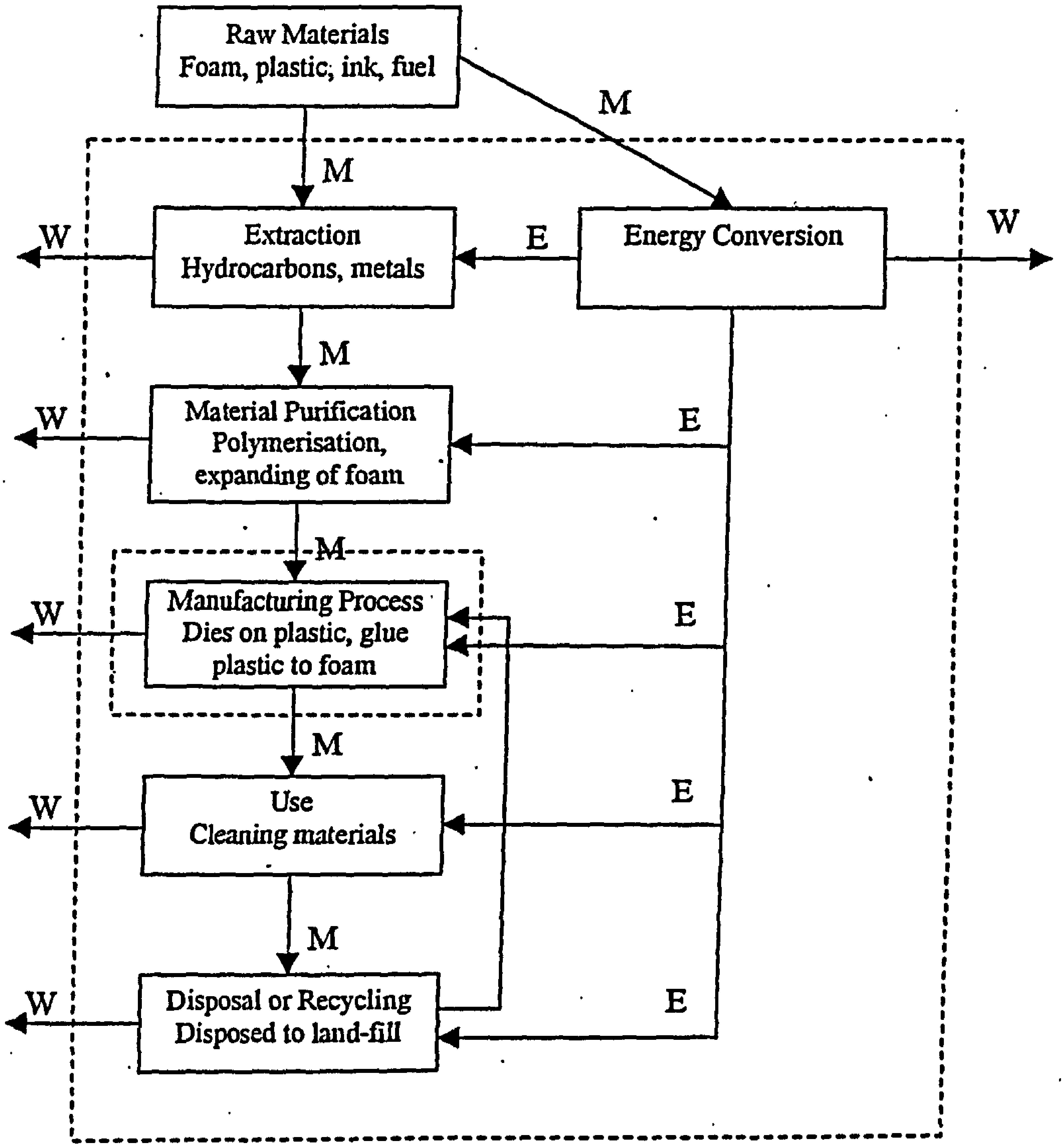
3.5 LCA Module – Exercises

Before attending the LCA module we were sent a short document to prepare us for the module. I found this very useful and worked through some of the exercises that were given. I felt it unfortunate that these exercises were not discussed or re-visited during the process of the module. I have included my notes on these exercises on the following pages. The exercises were:

1. Outline a life cycle of a product indicating the environment boundary, and any waste, material or energy transfers.
2. Suggest some base units for the comparison of similar products or services through life cycle analysis, and explain what is meant by spatial scale.
3. Suggest point of comparison for two similar products or services.
4. Discuss the use of political and scientific standards for the protection of the environment.

Exercise 1:

Mouse Mat

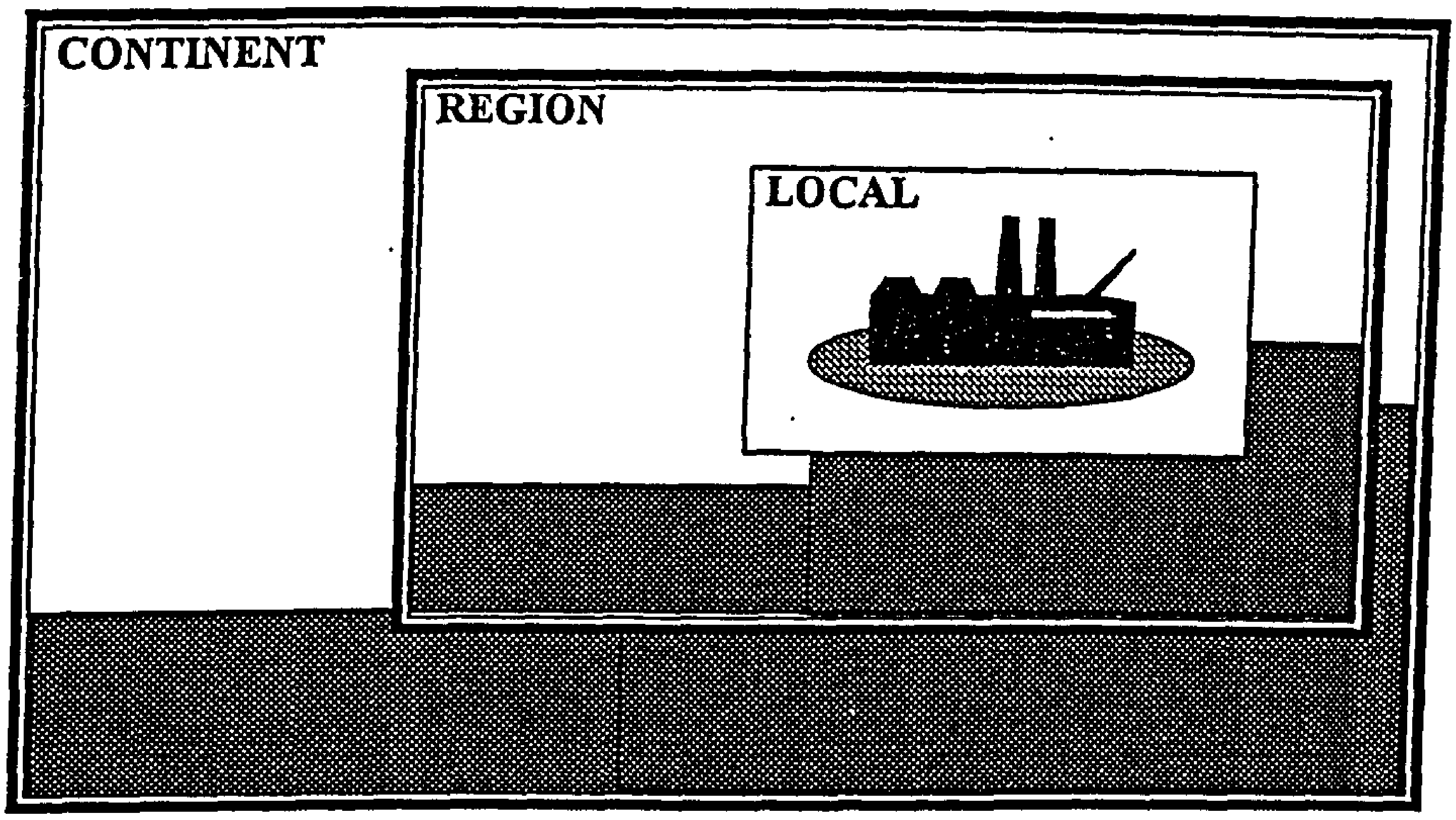


Exercise 2:

1. Floor covering, per m^2 or per m^2 per year (takes account of durability)
2. Paper/ plastic carrier bags, per kg, per ave. weekly shop, or monthly shop (taking account of re-use)
3. Work travel, by car, bike or bus, distance per pound per minute per environmental detriment unit (to take account of pollution of car and bus)

To the left is a diagram explaining the relationship between the different spatial environments which are considered in the risk assessment of chemicals.

It can be seen that the continental, regional and local calculations must be done in order, the local scale receiving it's background from the regional and the regional it's background concentration from the continental value.



Exercise 3:

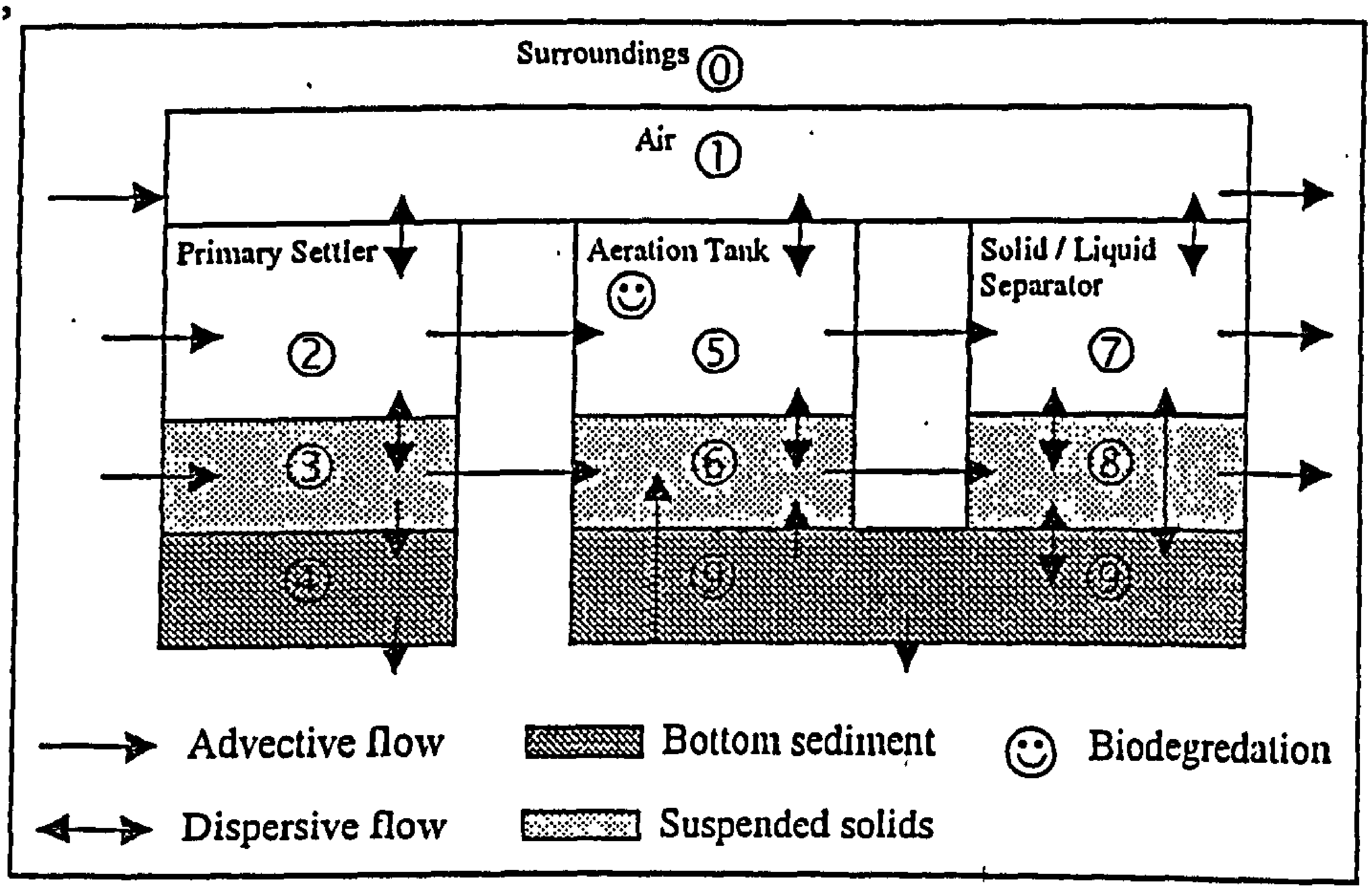
Two types of washing machine
Categories - Material usage, power consumption, recycle re-use ability

Exercise 4:

NOECs are far more scientific, being directly measurable, whereas political standards can be vote and party donation dependant. Also a political standard would be harder to implement internationally, whereas PECs, NOECs, PNECs and RCRs are already internationally accepted within the EU.

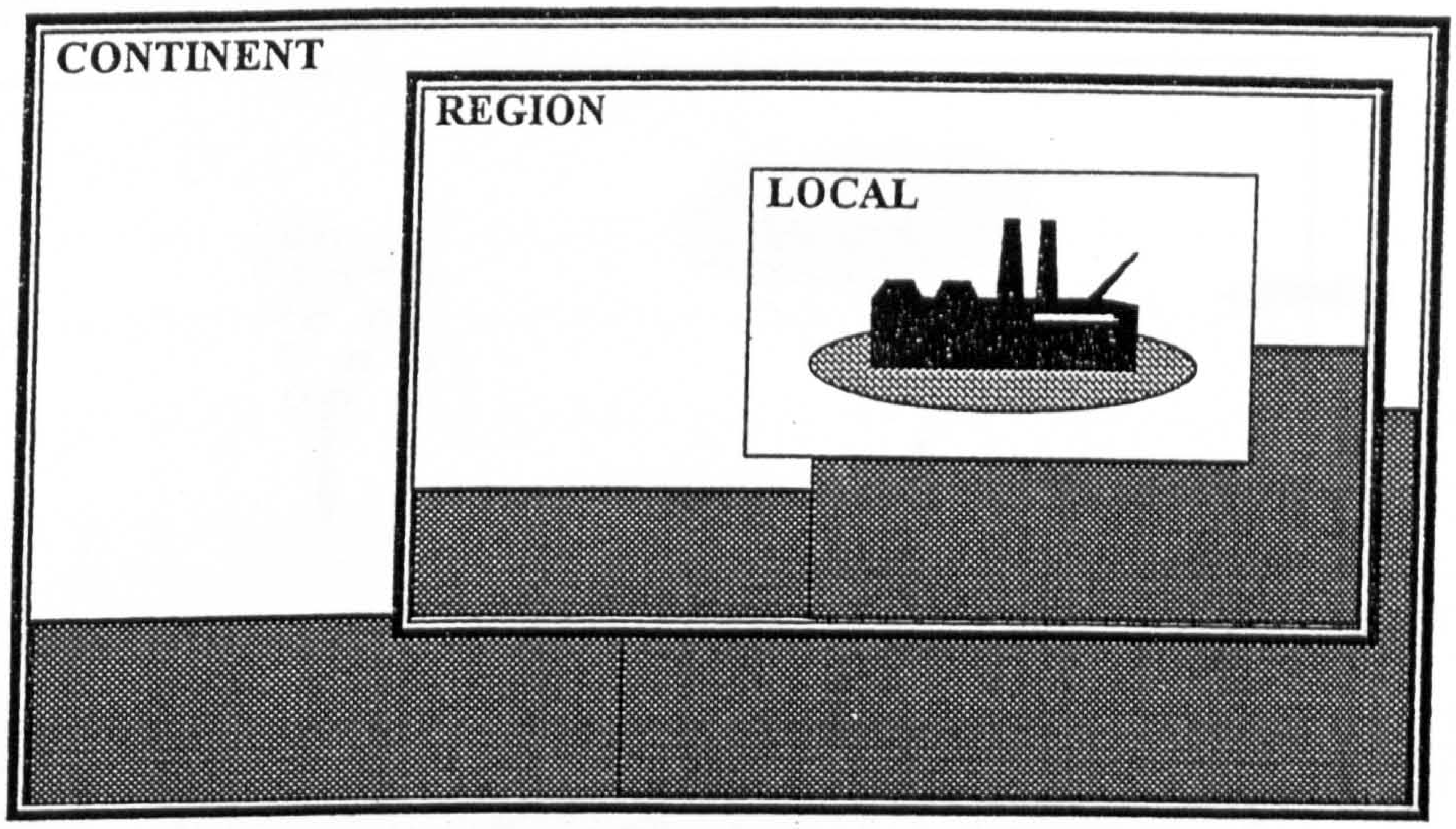
OECD and the US also use an HC_x model as well.

Compartment models, Simpletreat model for compartments linked to the sewage treatment plant.



Spatial scale of a system:

To the left is a diagram explaining the relationship between the different spatial environments which are considered in the risk assessment of chemicals.



It can be seen that the continental, regional and local calculations must be done in order, the local scale receiving it's background from the regional and the regional it's background concentration from the continental value.

Exercise 3:

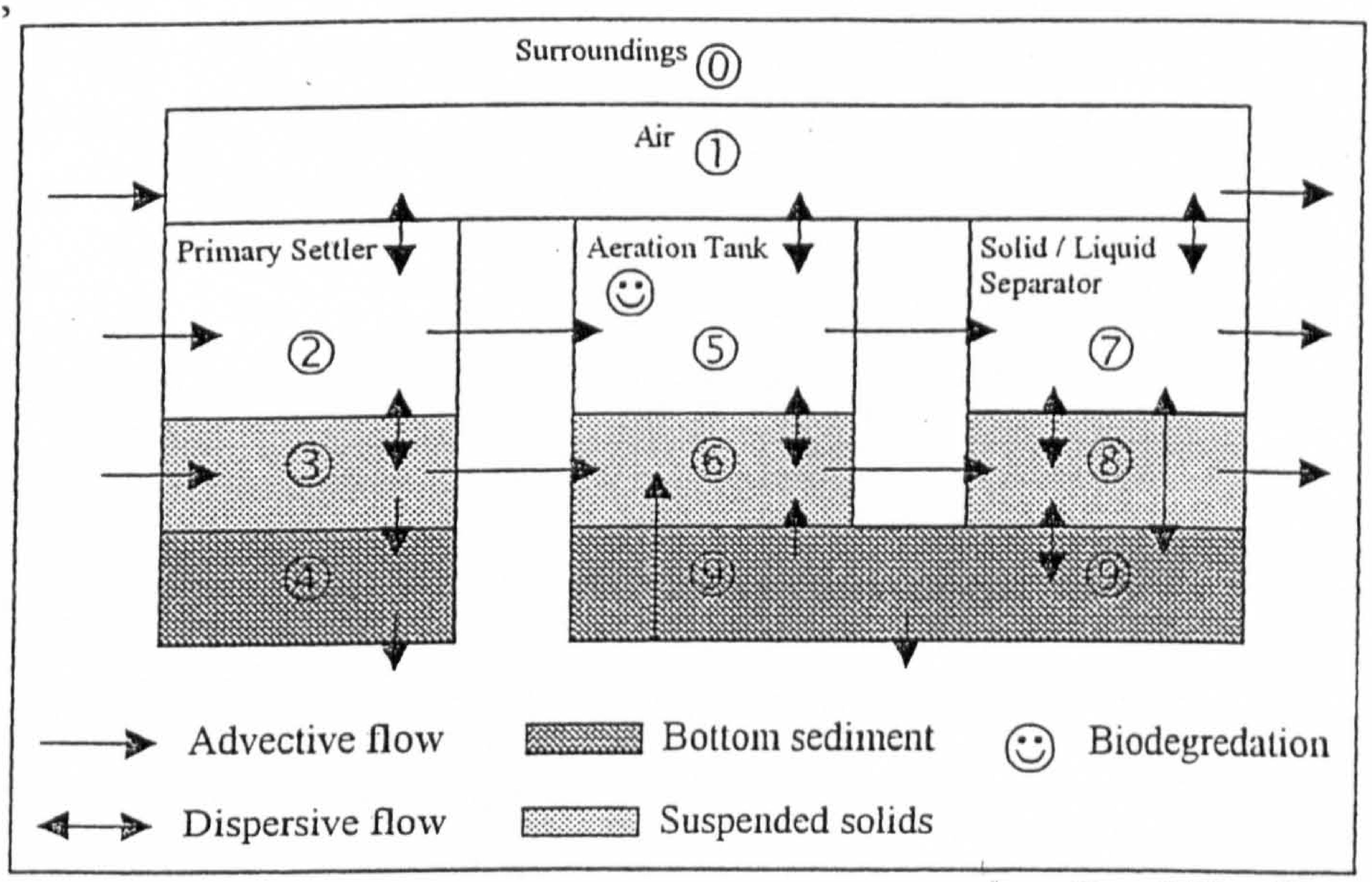
Two types of washing machine
Categories - Material usage, power consumption, recycle re-use ability

Exercise 4:

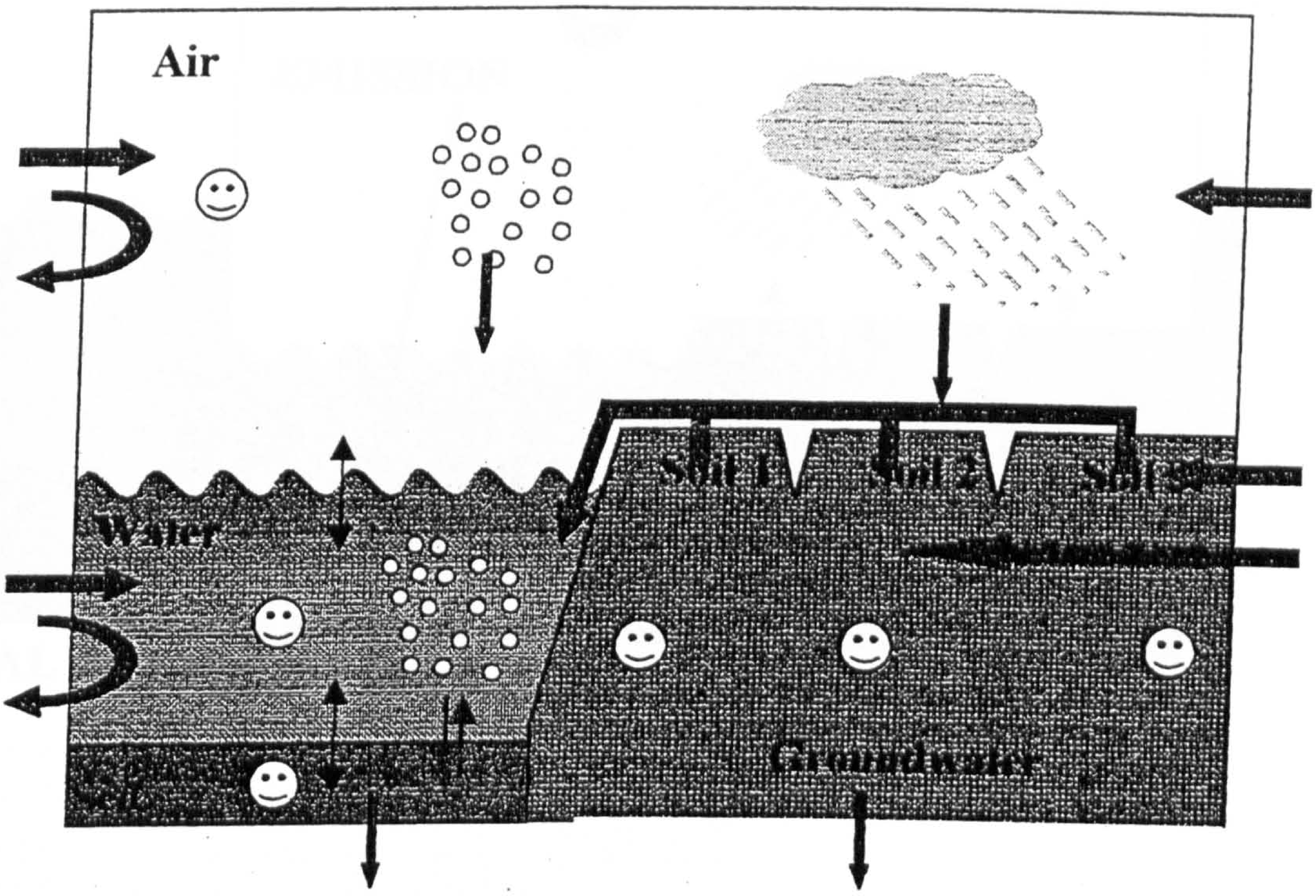
NOECs are far more scientific, being directly measurable, whereas political standards can be vote and party donation dependant. Also a political standard would be harder to implement internationally, whereas PECs, NOECs, PNECs and RCRs are already internationally accepted within the EU.

OECD and the US also use an HC_x model as well.

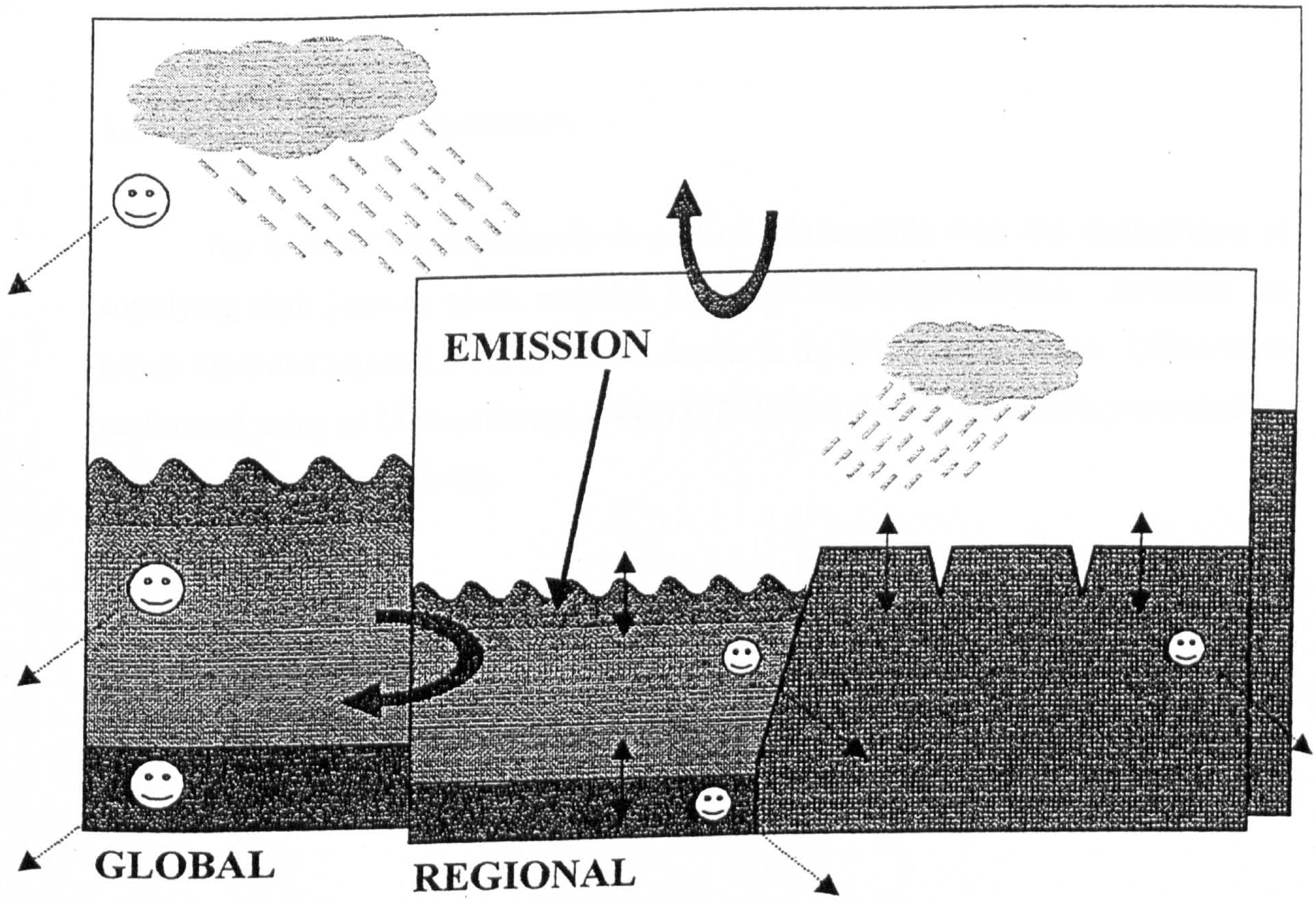
Compartment models, Simpletreat model for compartments linked to the sewage treatment plant.



Most "multimedia" models consider six compartments, these being air, water, suspended solids, sediment, soil and aquatic biota. Early models were suggested by Mackay. The three soil compartments are agricultural, industrial and grassland.

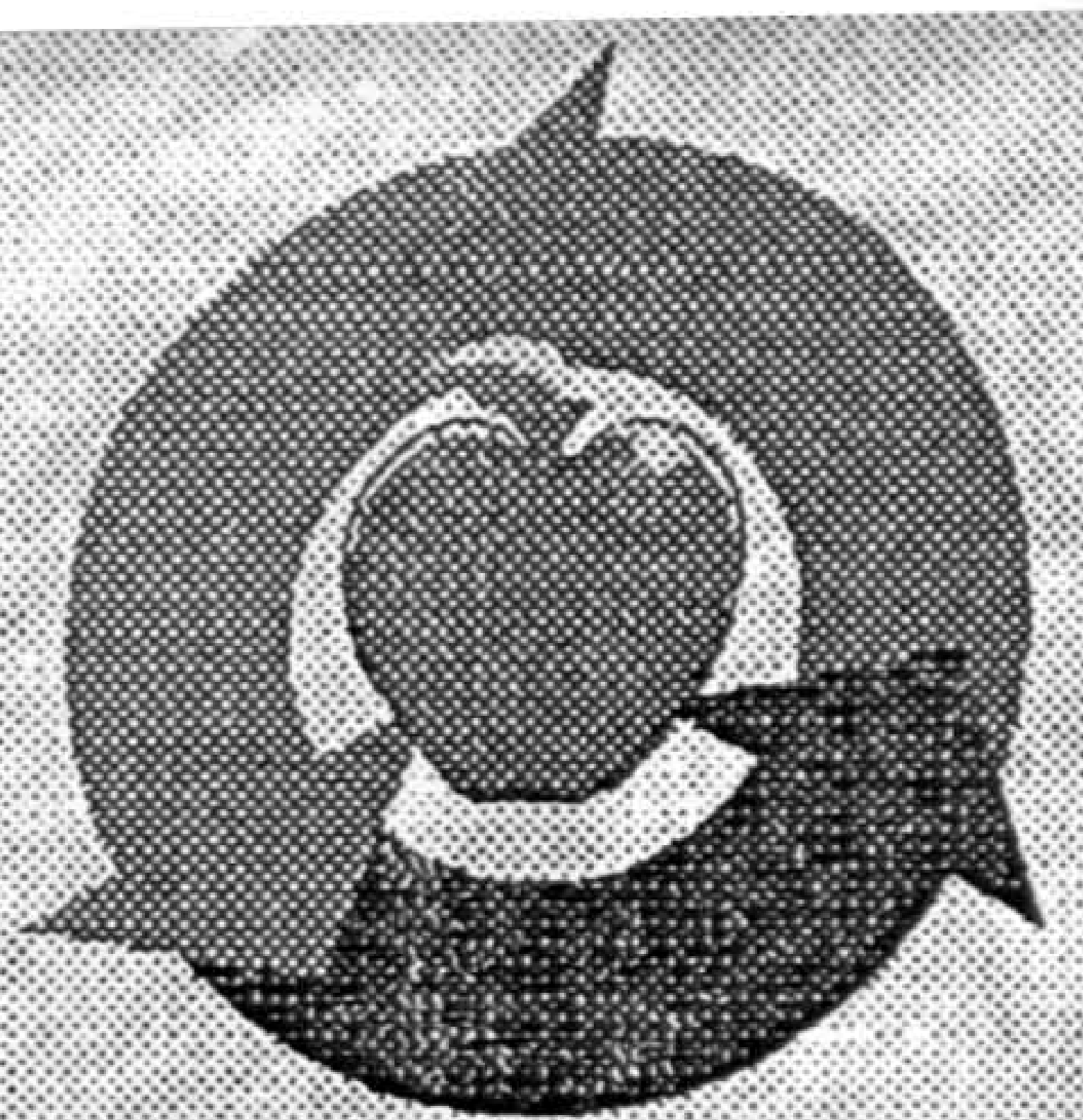


On the next page is a nested multimedia model


EMISSION
GLOBAL
REGIONAL

3.6 LCA Module – Presentation

An exercise we performed, as part of this module was the comparison of supplying fruit juice in glass, recycled glass and tetra-pack cartons. Between the group local and regional models were looked at in the UK and in France. LCAs were performed using an LCA software system (PEMS4) and then the results presented by each group the next morning.



LCA of UK Rural Juice Supply

AFeatures

Fruit-Juice-Is-Us

T 'n' T and Mick and Nick Supplies

Oh, and Athier

Features
Manufacture

Supply
Specs

Price List
Recycle

UK Rural Scenario

- Glass Bottles
  - Virgin
  - 40% Recycled
- Tetra-Pak
- Process Sites
  - Manufacture at Albert Square Wks. London E3
  - Filling plant in Glasgow, Scotland
  - Retail / consumption at Fruit-Juice-Is-Us, Blythe Bridge

Features

Manufacture

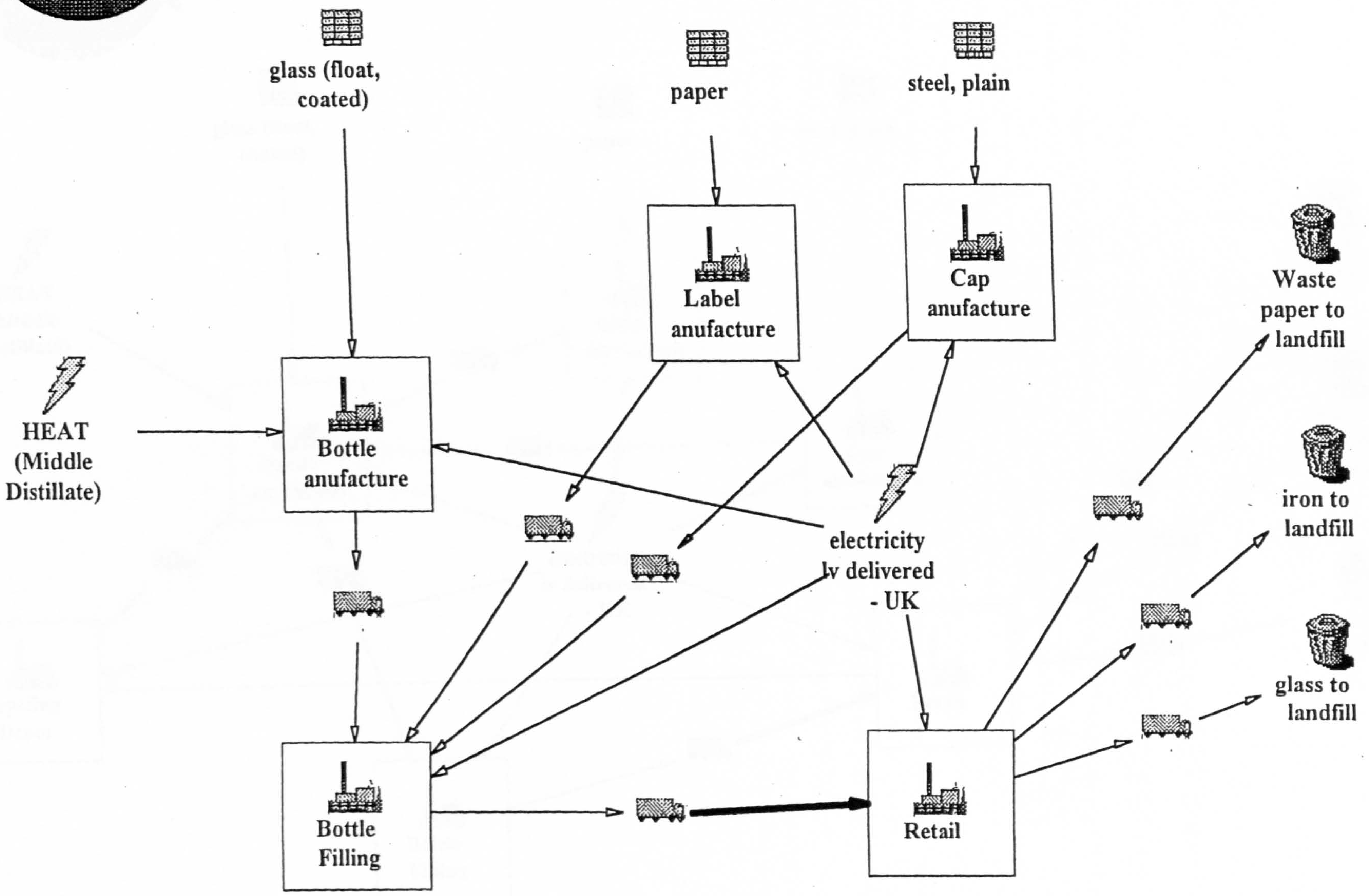
Supply

Specs

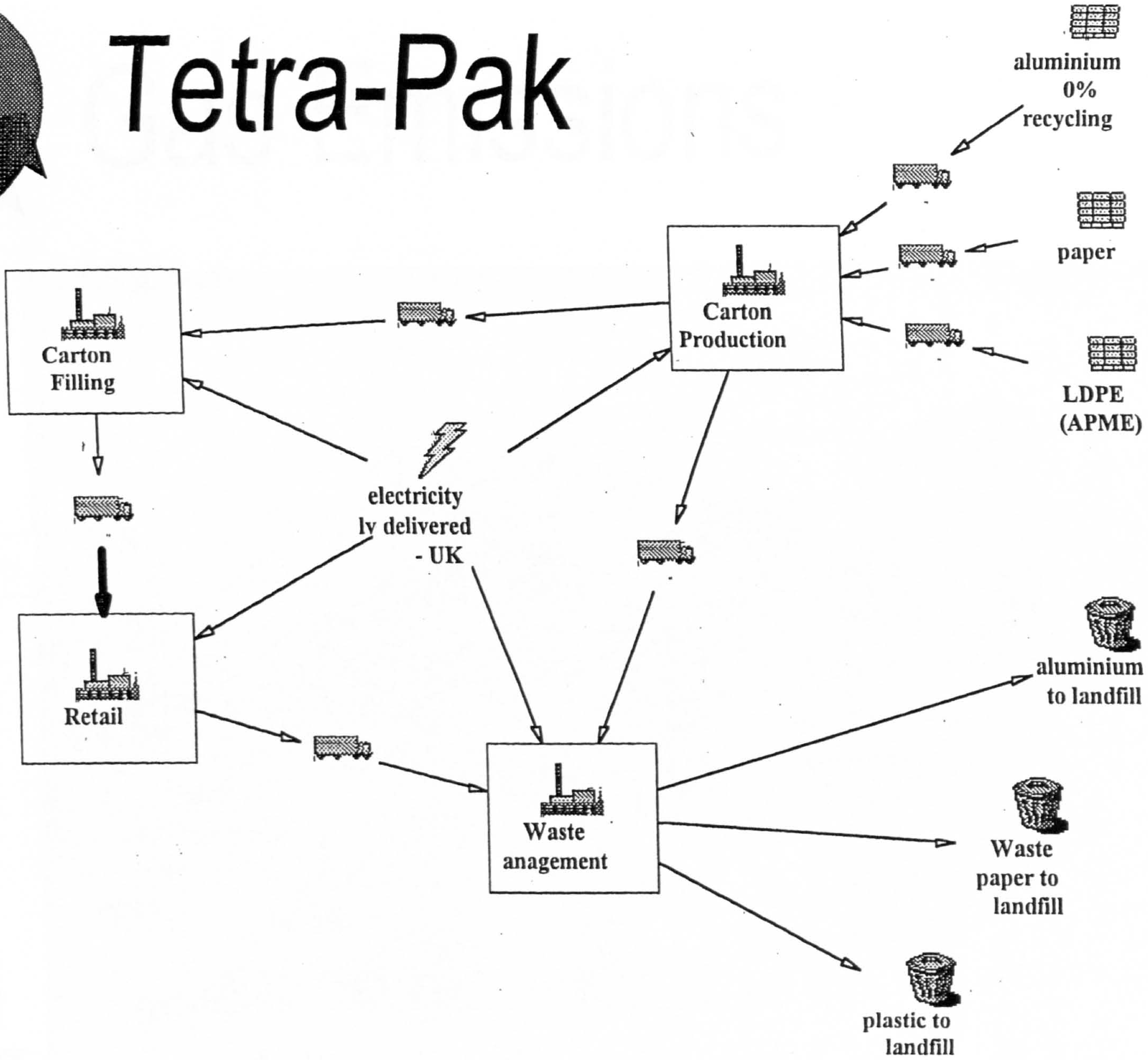
Price List

Recycle

Glass, 100% Virgin



Tetra-Pak



aluminium
0%
recycling

paper

LDPE
(APME)

Carton
Production

Carton
Filling

electricity
lv delivered
- UK

Retail

Waste
anagement

aluminium
to landfill

Waste
paper to
landfill

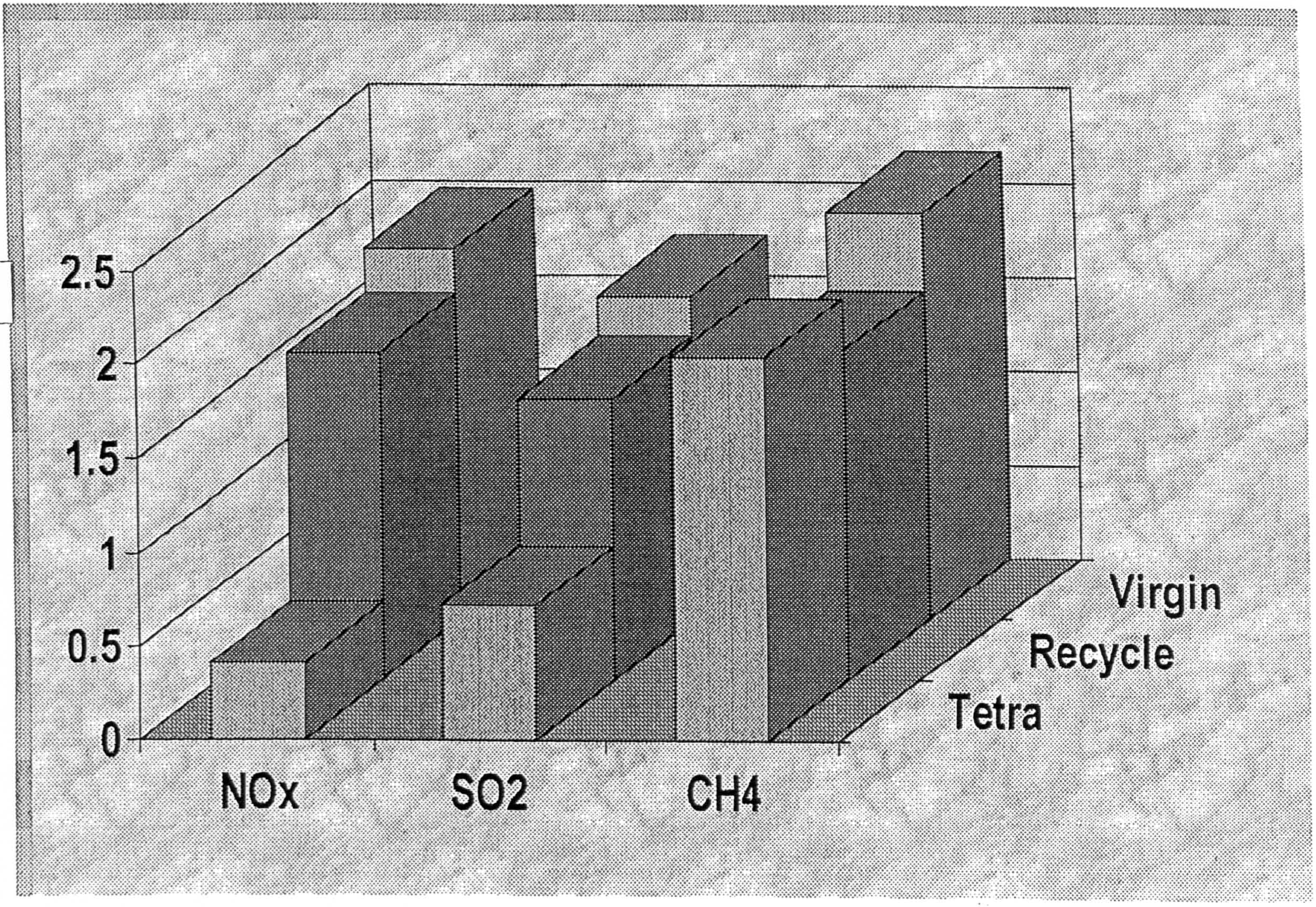
plastic to
landfill

Gas Emissions

Features Manufacture

Supply Specs

Price List Recycle



Extracted Energy

Features

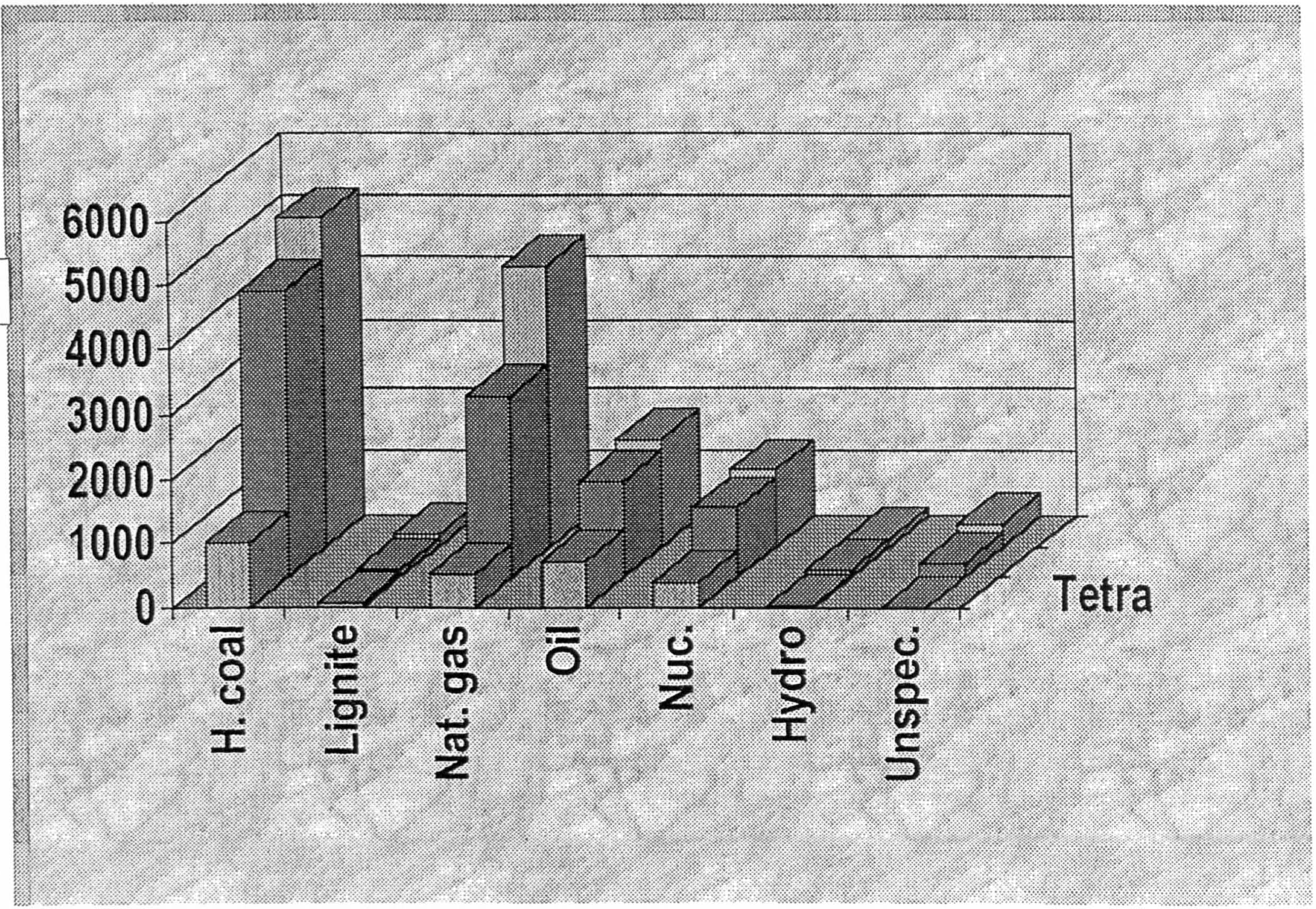
Manufacture

Supply

Specs

Price List

Recycle



LCA of UK Rural Juice Supply

Features
Manufacture

Supply
Specs

Price List
Recycle

Any Questions?

3.7 Project Management – Presentation

As part of this module we were set the task of proposing an integrated transport policy in groups. Our proposal was to include a Gantt chart indicating the time-scales for our proposed project. The following presentation was how my group presented its proposal to the class the following day.

Tender for

UK's Integrated Transport Policy

By

Nik Robinson, Faith Oliver, Tanguy Lenoir, Michael Bennett and Athier Alani

Outline Of The Problem

ROAD	LAND	SEA	RIVER	AIR
Car	Walking	Boat	Canal boat	Helicopter
Cycle	Climbing	Ship	Barge	Plane
Tram	Train	Submarines	Gondola	Airship
Lorry	Tube	Hovercraft	Boat	Air Balloon
Motorbike	Monorail			
Bus				
Van				

Problems

- Pollution
- Lifestyle
- Stress
- Safety
- Cost (Perceived Cost)
- Time (Waste)

Structure of Tender

- **How to Approach Each Topic**
  - Working Groups
  - Visits to functioning Integrated Transport Systems
  - Training within the DETR
  - Interdepartmental Studies in the Government
  - Establish National Plan by process of review
  - SEA & LCA Use

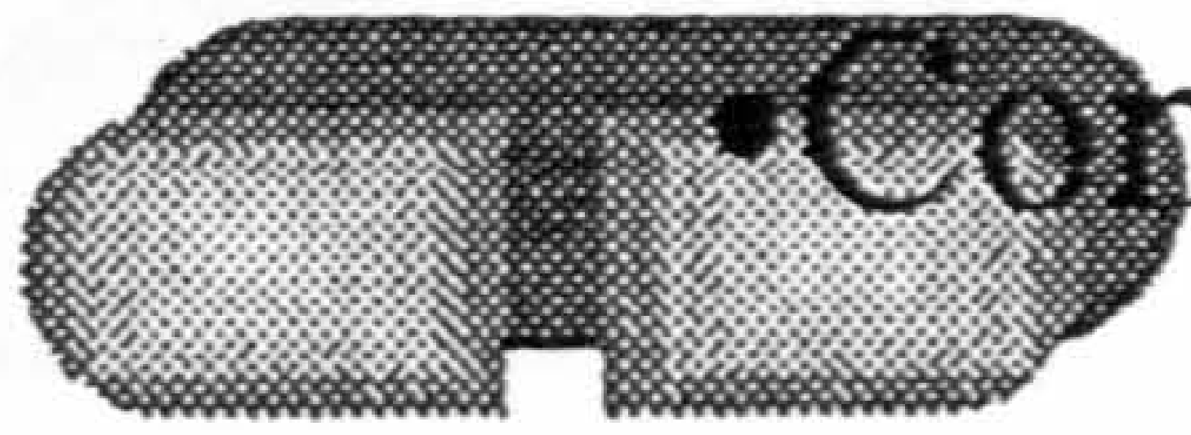
- **Benefits**
  - Health
  - Reduce Environmental Effects
  - Change Attitudes to Transportation

Canals

- Already in existence
- Underused
- Feasibility study
- Improvements to infrastructure

Reducing Of Cars

- Why reduce cars.
  - Environmental Improvement.
  - Safety
  - Congestion
  - Time Wasting.
- Proposed Solutions.
  - Convenient business facilities
  - Bus lanes



  - Company buses

Trains

- Use for long distance.
- Business facilities.
- Re nationalise (gradual).
- Investment in improving trains.

Trams And Buses

- Short and medium length journeys
- Buses
    - company financed buses
    - separate buses from main traffic flow
    - improve reliability
    - provide storage facilities
- Trams
    - dedicated tram and light rail lines
        - no emissions at point of use

Hire Vehicles

Cycles
Cars
Lorries

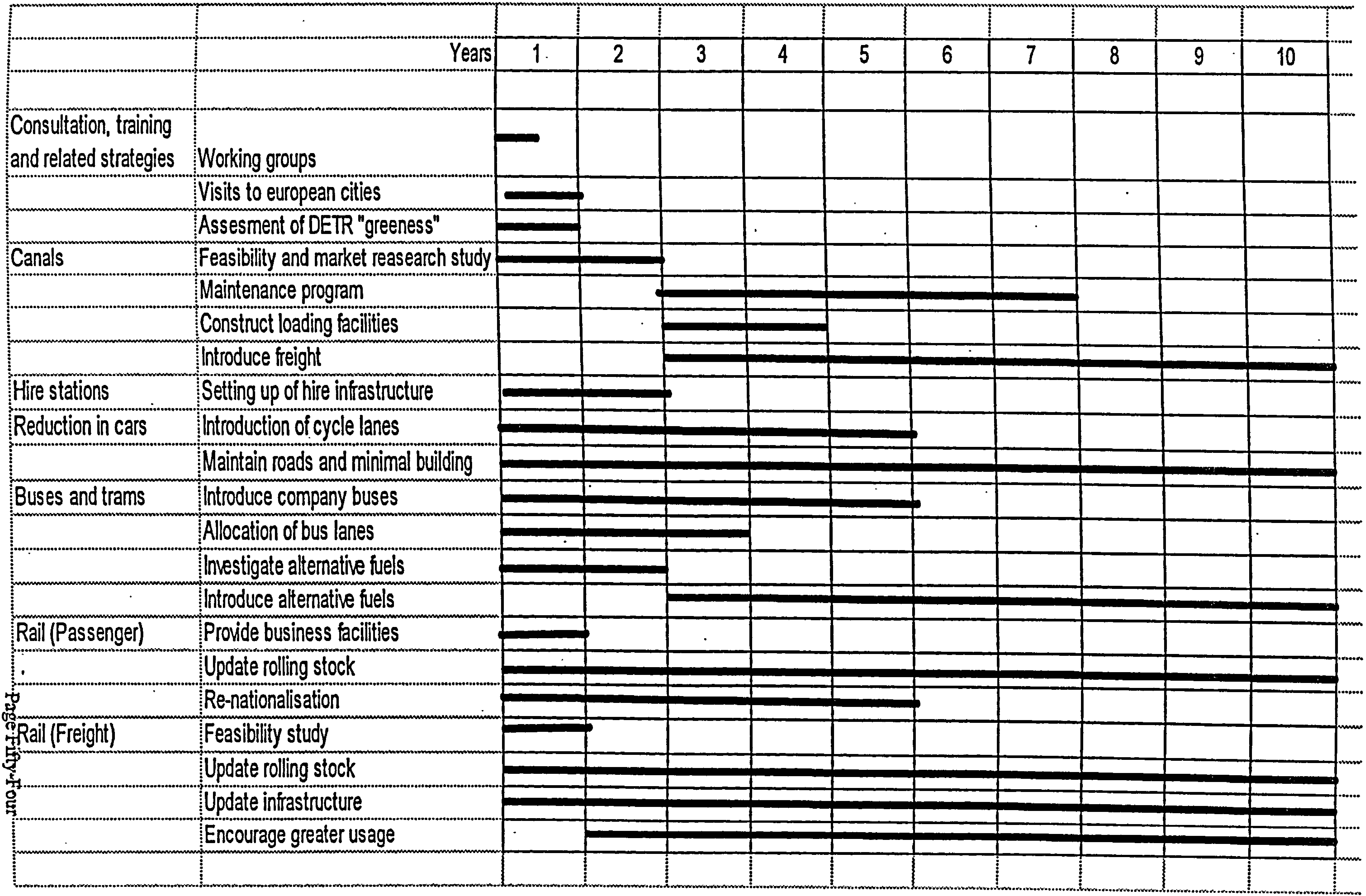
}

- Charge by time
- National hire network
- Scaled charges

Related Strategies

- **Planning System**
- Smart Card System

Gantt Chart


Years
1
2
3
4
5
6
7
8
9
10
Consultation, training and related strategies
Working groups
Visits to european cities
Assesment of DETR "greeness"
Canals
Feasibility and market reasearch study
Maintenance program
Construct loading facilities
Introduce freight
Hire stations
Setting up of hire infrastructure
Reduction in cars
Introduction of cycle lanes
Maintain roads and minimal building
Buses and trams
Introduce company buses
Allocation of bus lanes
Investigate alternative fuels
Introduce alternative fuels
Rail (Passenger)
Provide business facilities
Update rolling stock
Re-nationalisation
Rail (Freight)
Feasibility study
Update rolling stock
Update infrastructure
Encourage greater usage

Summary

- Focus on public transport, not roads
- Improving the existing infrastructure
- Moving freight off the roads
- Consideration of urban planning

3.8 Minutes of Meetings with Jim Wharfe and Geoff Brighty

This is the first set of minutes I took after meeting with my Industrial supervisor and the manager of the new group I was going to be joining. I have since gained much experience and picked up many ideas and good practices for the producing of minutes. This can be clearly seen when this document is compared to the later Conference documents that I have included in subsequent sections. The content of these minutes also indicates the longer-term aims that Jim Wharfe intends me to pursue.

MINUTES OF MEETING

DATE OF MEETING:
30/01/98

TAKEN BY:
Nik Robinson

PRESENT:
Dr. J. Wharfe, also had meeting with Dr. G. Brighty

Meeting With Jim Wharfe:

There are two different measurements for environmental standards, the EQS (Environmental Quality Standard) and the PEC/PNEC or RCR (Predicted environmental concentration/Predicted no effect concentration ratio, also called a risk characterisation ratio).

Management of the environment - What success measures are there (Goals)?

Water framework directive – environmental benefit.
Substance specific controls
    Substance doesn't enter environment as such.
    What are the effects of combinations and reactions?
    Are PNEC values cumulative?
Consented inputs (EQS or Levels)

Need an evaluation of approaches,

Substance Specific Controls vs. Whole sample / Direct Toxicity Assessment

SSC:

EQS vs Notification system (CAU)

The overlaps and interests between the groups.

Approach		Method		Result
CAU	→	Target	→	Regulations
EQS	→	Application	→	Pollution control

SWOT of CAU approach and EQS approach.

- Have completed time at CAU, need to finish writing report on practices of the group and knowledge gained. [1]
- After three months with the ETU (Environmental Toxicology Unit) need to write similar report.
- Third report should be written comparing the two units and coming to conclusions on the two approaches their strengths and weaknesses and where any synergies may lie between the two groups.

1 - Independent assessment of CAU

Strengths and weaknesses of PEC values	-	Synergy etc.
	-	Lack of info
	-	Fate/behaviour
	-	Sensitivity analysis
Strengths and weaknesses of PNEC values	-	Lab. Tox. assessment
	-	Species selection
	-	Lab. Method
	-	Quality of method
	-	NOEC vs. LOEC
	-	End points
	-	Sub lethal responses

Also consider
- Toxic modes of action, only 8-12
- Whole toxicity treatment (DTA)
- Case studies of sensitivity analysis
  - Manual vs. EUSES calculation
  - Site specific vs. generic assessment
  - CAU vs. ETU (draft docs. available for nonylphenol, acrylomide, tri-/per- chloroethylene and acetonitrile)

Geoff Brighty, Introduction To The ETU:

This group is the regional contact for chemical data.

As part of the national centre they have wider source of information as well as a technical service contract with WRc (Water Resource Centre) who do further EQS work.

Group deals with chemical specific enquiries.

- Technical service - What improvements could be made?
- New customers - Primarily aquatic compartment (moving towards terrestrial comp.)
  (new services) - Other compartments

Computer databases in use :-

SIS - Substance Information System
EASIS -

Possible assessments of systems.

Geoff Brighty:
BSc. – Marine biology
PhD – Fish reproduction
Worked for - Fisheries (NRA)
- R&D on endocrine disrupters
- Manager of ETU

Helen Wilkinson (Env. Toxicologist):
BSc. – Biology
MSc. – Ecotoxicology
Worked for - Thames region (NRA)
- ETU

3.9 1998 Conference – Agenda for Meeting

As an elective module Andrew Horsley and myself have opted for the Project Management – Conference Organisation module. For this module we must organise the 1998 Engineering Doctorate Conference. I have included this agenda to show how my project management skills are being implemented since attending the Project Management module.

ENGINEERING DOCTORATE PROGRAME

ENVIRONMENT
AGENCY

BRUNEL
UNIVERSITY

FACSIMILE TRANSMITTAL SHEET

TO: Alex Roberts

FROM: Nik Robinson

COPIES Darron Dixon-Hardy, Carole Carr, Caryl Brown.

DATE: 01/04/98

FAX NUMBER:

TOTAL NO. OF PAGES INCLUDING COVER: 1

PHONE NUMBER:

SENDER'S TELEPHONE NUMBER: 01491 828542

RE: Agenda for meeting on 6/3/98

SENDER'S FAX NUMBER: 01491 828427

Dear Alex,

Andrew and I propose the following agenda for our meeting on Friday:

				Duration
1.	Review of Gantt chart	(i)	Dates/deadlines	20 min
		(ii)	Durations	
		(iii)	Events	
2.	Costings	(i)	Howell Theatre	20 min
		(ii)	Accommodation	
		(iii)	Catering	
		(iv)	Printing	
		(v)	Other budget/finance matters	
3.	Letter to REs	(i)	Content	5 min
		(ii)	Dates (also above 1)	
		(iii)	Who to go out from	
4.	Other matters arising			15 min

See you at the meeting, 10:30, Friday 6th March, 32AB22, Surrey University.

Yours sincerely,

Nikki Robinson

1 ANCHOR COTTAGES,
HIGH STREET COWLEY

3.10 1998 Conference – Budget

This is the budget proposal that was put to the Conference Committee outlining, and were appropriate justifying expenditures for the 1998 Engineering Doctorate Conference.

Monday, 16 March 1998

Last year's conference budget (Conference 1997) is outlined below,

No.	Item	Supplier	Quantity	Cost	Total
1	Printing of proceedings	Basingstoke Press	300	£9.05	£2715
2	Other Printing	AVS	2000	£0.05	£100
3	RE Accommodation	Conference Office	80	£23.95	£1916
4	Delegate Package (RE)	Conference Office	120	£10.95	£1314
5	Delegate Package (Other)	Conference Office	120	£12.95	£1554
6	Additional Room Hire	Conference Office	6	£50.00	£300
7	Camcorder & Microphone	AVS	1	£98.00	£98
8	Name Badges	Central Stores	200	£0.13	£26
9	Document Wallets	Central Stores	200	£1.12	£224
10	Poster boards	Conference Office	45	£6.00	£270
11	White boards	Dome Ltd.	56	£2.31	£130
12	Postage	Central Stores	300	£0.20	£60
	TOTAL				**£8707**

Table 1 - 1997 Conference Budget

On line 2 the other printing costs are assumed to include mail shots to REs and Delegates.

The RE accommodation (3) for 80 delegates seems to include the new intake or Yr. 0 REs, the cost of which, in our budget has been ignored, this coming from a different budget from the conference one.

The Delegate Package (4 and 5) is an inclusive cost for conference rooms, lunch. Lines 3-6 together cover the whole facilities booking as far as food, rooms and accommodation are concerned. The original rates were quoted as below,

B&B for 214	@ £23.95	=	£5125.30
Day rate for 360	@ £10.95	=	£3942.00
Extra Conference Rooms 2 for 4 days	@ £50.00	=	£ 400.00
			£9467.30

This eventually ended up at the following rates,

B&B for 80 (16 Yr. 0 REs for 5 days)	@ £23.95	=	£1916.00
Day rate for 120 (Students)	@ £10.95	=	£1314.00
Day rate for 120 (Non-Students)	@ £12.95	=	£1554.00
Extra Conference Rooms 2 for 3 days	@ £50.00	=	£ 300.00
			£5084.00

This lower figure, results from savings such as that of £100 pounds from extra room hire for only 3 days not 4. Also a reduction in the B&B numbers, although with 50 REs for 2 nights this figure would be believed to be £2395.00 not £1916, but this is not clearly explained in the conference report.

The white boards were used to mount poster presentations prior to mounting on poster boards, the cost of the white board coming out of the conference budget.

The 1998 conference budget follows and notes on the figures can be found under this table.

No.	Item	Supplier	Quantity	Cost	Total
1	Printing of proceedings	Brunel	300	-	£3406
2	Other Printing	-	300	£ 0.04	£ 12
3	RE Accommodation	Conference Office	82	£ 21.28	£1745
4	Conference Rooms (H001)	Conference Office	2	£437.50	£ 875
5	Conference Rooms (H004)	Conference Office	2	£ 90.00	£ 180
6	Conference Rooms (H005)	Conference Office	2	£ 60.00	£ 120
7	Catering	Conference Office	-	-	£1610
8	Camcorder & Microphone	Conference Office	2	-	£ 100
9	Name Badges	-	200	-	£ 26
10	Document Wallets	-	200	-	£ 224
11	Poster boards	-	45	£ 6.00	£ 270
12	White boards	-	56	£ 2.30	£ 129
13	Postage	-	300	£ 0.22	£ 66
	TOTAL				£8763

Table 2 - 1998 Conference Budget (Draft)

1 – The printing quote has only been received by Brunel as yet and is approximately £700 more expensive than last year. Further quotes are being expected and £3000 has been set as a maximum cost for the printing.

2 – Other printing has been assumed to be the mail shots to REs and Delegates, however, in the first mail to REs the use of E-mail has been encouraged to reduce this cost and this is expected to be the absolute maximum other printing cost.

3 – The RE accommodation, for 41 REs for 2 days at £21.28 B&B represents the lowest the university could offer us having already lowered the cost from £28.94 (approximately 25% reduction). The 41 REs does not include the 16 new intake (Yr. 0) REs, whose accommodation is being arranged separately.

4 – This room is the main lecture theatre, and has been hired to us at a 50% discounted rate.

5 – This is one of the two seminar rooms which will be used for poster boards and food.

6 – This is the other of the two seminar rooms which will be used for poster boards.

4-6 – There is an option to have alternative rooms in the main lecture centre rather than the Howell centre at zero cost, a total saving of £1745 compared to the Howell centre.

7 – The catering costs break down as follows:

Early morning coffees for 50 @ £0.95 both days	=	£ 95	
Mid morning coffees for 100 @ £0.95 both days	=	£ 190	
Lunch FB1 buffet for 100 @ £5.30 both days	=	£1060	
Lunch drinks for 50* @ £0.75 both days	=	£ 75	*(charged as required)
Afternoon coffees for 100 @ £0.95 both days	=	£ 190	
TOTAL	=	£1610	

VAT is not required to be added as all moneys are going through an internal account.

8 – Audio-visual equipment has not been quoted for as yet but an initial estimate in relation to last year's cost has been included.
9 – Name badges of various types all represent a standard cost of £26 for 200.
10 – Document wallets are being looked into although their worth versus cost is being considered, estimated cost from last year has been included.
11 – Poster boards will be sourced from the Runnymede campus of Brunel and are not expected to cost, although last years cost has been budgeted.
12 – White boards will be needed and are yet to be sourced, but an estimate using last years cost has been budgeted for.
13 – Postage has been budgeted for the mail shots going second class, however the sending of proceedings to delegates (suggested last year) has not been budgeted for, this is believed to entail excessive and unnecessary cost. As with the printing for mail shots, the use of E-mail will reduce the postage cost, meaning the cost budgeted for will be the maximum cost envisaged.

New this year is the concept of sponsorship, particularly for the printing of the proceedings, if this were successful this would result in a significant reduction in the expenditure for the conference. Below the budget figures are revisited, with reductions and sponsorship considered.

		Costs			
No.	**Item**	**Budget**	**1**	**2**	**3**
1	Printing of proceedings	£3000	£3000	£ 0	£ 0
2	Other Printing	£ 12	£ 6	£ 6	£ 6
3	RE Accommodation	£1745	£1745	£1745	£1745
4	Conference Rooms (H001)	£ 875	£ 875	£ 875	£ 0
5	Conference Rooms (H004)	£ 180	£ 180	£ 180	£ 0
6	Conference Rooms (H005)	£ 120	£ 120	£ 120	£ 0
7	Catering	£1610	£1610	£1610	£1610
8	Camcorder & Microphone	£ 100	£ 0	£ 0	£ 0
9	Name Badges	£ 26	£ 26	£ 26	£ 26
10	Document Wallets	£ 224	£ 0	£ 0	£ 0
11	Poster boards	£ 270	£ 0	£ 0	£ 0
12	White boards	£ 129	£ 129	£ 129	£ 129
13	Postage	£ 66	£ 33	£ 33	£ 33
	TOTALS	**£8357**	**£7724**	**£4724**	**£3549**

Table 3 - 1998 Conference Budget Plans

The first column of costs "budget" are as in the draft budget but reducing the printing cost to the stipulated maximum cost of £3000. The "1" costs consider savings on printing and postage through use of E-mail (50% reduction), the ability to get the audio-visual equipment and poster boards free of charge and that the Conference wallets will be free or not used. This represents an overall saving of just of £600. If sponsorship is gained for the printing of the proceedings (2), up to £3000 could be saved bringing the conference cost down to under £5000. And finally use of Theatre D and the lecture centre instead of the Howell centre, or sponsorship to cover the cost of the Howell centre results in a further saving of £1175 lowering the total cost of the conference to just over £3500.

3.11 1998 Conference – Minutes of Meeting

These minutes again prepared for the 1998 Engineering Doctorate Conference, show how through clear minutes and recording of actions, we are keeping the project up-to-date, and on-course.

MINUTES

Meeting of Tuesday 3rd February

Present: AR, AH, NLR, CA, MN

After the meeting was opened AR requested an agenda, the following were outlined,

1) Finance
2) Project Plan
3) Timescale
    (i) Proceedings
    (ii) Papers
    (iii) Printing
4) Media Equipment

CA and MN handed over report for last year's conference, pointing out points of interest in questionnaire results and discussion in section 5.

1) The budget is to be £8000 and a draft budget is to be submitted at next meeting.

Act.1.1 NLR, AH

2) Project Plan,
Work to an end date. Source and use some form of project management software.
Papers have no float, this will ensure deadlines are kept more rigidly.
Consult printers early, consider, kind and colour of cover, number required (REs + Man. Comm. + Supervisors)

Act.1.2 NLR, AH

3) Timescale:

-	Titiles and subject area	9/5/98
-	Abstract and Biography	6/6/98
-	Final Paper	15/8/98

Subject areas needed to help grouping of papers.
Thanks and praise for chairs, need info for introductions 9/6/98
Possibly a Eng.D. graduate as a chair, R.Peters, D.Francis.

Type of binding for proceedings is called "perfect binding"
Last year 300 for £2714
Enquire into spine printing, ISBN number.

Act.1.3 NLR, AH

4) Media Equipment
26+ boards for poster presentations
≈ 3 rooms for displaying poster boards.
Booking of Howell centre mentioned, AR questioned audibility at back.
Numbers approximately 120 each day inc. REs.

Yr.1 will need LCD projector, 2nd and 3rd will need standard OHP facilities.
Map and info. board including siting of individual poster boards.
Poster board presentation adverts, no point having them in the last session, think about organisation and timing of presentations. Grouping, will need titles.

Arrange for assessment of poster boards. 2/3 for each presentation/poster-board.

Audio-visual equipment,
    Video camera, and operators
    Microphone
    Speakers for microphone
Remind REs to bring video tapes.
Specify presentation package, use of mouse, remote, etc.

Need people to met and greet at door, a master of services.

Evening celebration, only if money permitting!

For next meeting:

1) Gantt chart
Act.1.2 NLR, AH

2) Letters to REs with deadlines
Act.1.4 AH

3) Layout of Howell centre
Act.1.5 NLR

4) Costings/budget
Act.1.1 NLR, AH

Next meeting Friday 6th March at Surrey.

3.12 1998 Conference – Notes on 1997 Report

These are notes that were drawn up from the report of the previous year's conference. The report brought up many good points for improvement and lessons learnt, so hopefully they will not be repeated.

NOTES FROM 1997 CONFERENCE REPORT

Meeting on Wednesday, 01 April 1998

Purpose of event:

- REs to gain experience in the writing and presenting of papers
- Supervisors, management committee and other interested parties able to see RE's progress

Innovations:

- Papers format sent out to REs – more uniform look to proceedings
- Keyword index – for easier referencing of papers
- Coloured cover printing on proceeding
- Registration pack in "smart blue wallet"
- A delegate list was included in registration pack
- Feedback questionnaires were produced and analysed
- Conference spit into four parts or topic groups
- Plants hired as decoration for lecture theatre
- Conference Dinner on first night for REs and Management Committee
- Helpers from same Eng.D. year were designated tasks
- Hand-over meeting organised with next conference organiser

Questionnaires:

23 out of the 80 that were distributed to delegates (not REs) were returned.

Q1. How did you hear about the conference?

Mainly colleagues and direct mail, no response from posters or advert in Surrey Matters.

Q2. Assessment of conference's content.

Content and format overall were thought to be good/v.good.
Comments inc.: References or map for poster boards
Less fine print on poster boards
Better balance of viewing time needed
Question times, were best part of conference

Q3. How important were the proceedings?

Almost every body thought they were very important

Q4. Assessment of the conference's administration and organisation.

All aspects were deemed to be good → v.good although there was thought to be room for improvement in the liaison with delegates pre-conference.
Comments inc.: Proceedings could go out 1-2 week in advance (postage?)

Page references for ease of finding papers, particularly linking them to aural presentations
Proceedings on the world-wide-web!?
Formal conference welcome

Q5. Standard of conference facilities.

Theatres and catering were deemed to be good.
Comments inc.: Improvement to sound quality needed
The blocking off of some seats could help to concentrate the audience

Q6. Accommodation.

The majority of delegates did not require accommodation.

Q7. Would you consider paying a small fee to attend the conference?

50% said yes with the average figure quoted being £28.
Academics deemed the attendance of the conference part of their job ∴ felt they should not have to pay.
Some industrialist felt that the sponsoring companies already contributed enough.
Charge would also add complexity to organisation of the conference.
Possibility of a contribution to the cost of lunch (≈£2).

Q8. Aims and objectives of attending the conference.

Assess RE
Personal Knowledge
Support RE / Eng.D. program
Understand issues/work/thoughts
Introduction to the Engineering Doctorate program
Information on environmental thinking and industry
To network

50% of delegates were positive about the fulfilment of their objectives.

Recommendations:

- Split work from an early stage, and plan holidays so as to avoid overlap
- Invite delegates earlier (July 14^{th}-18^{th} 1997) than last year, NB late responses
- More time needed for compiling/printing etc. of proceedings
- Mail-shots can be and are time consuming (up to 4 hours)
- Main publicity was by mail and word-of-mouth. Word-of-mouth should be encouraged with "this conference is open to all who are interested in environmental technology" and/or "bring-a-friend" statements
- There was no responses from the poster adverts or the advert in "Surrey Matters"
- Internet/E-mail advertising should be considered
- A list of delegates to attend needs to be created at an early stage – conference delegates mail list

- Poster boards – many REs turned up late (9pm) to put up poster boards – enforce deadline e.g. by 6pm
- Helpers, preferably from the same year as organisers due to rapport
- Poster boards grouped by topic – map needed for easier locating of poster boards
- Sound quality needs improving, improper use of microphone
- Subject grouping was good, post boards questions were also good
- Time needed for viewing poster boards
- Poster board adverts?
- Proceedings, 100% completion, strict deadlines,
  no leeway,
  rumours of tight deadlines
- Foreword in proceedings
- ISBN number
- Submission to British Library
- Order of papers to reflect order of talks
- Page numbering was found to be confusing but very hard to resolve, numbering at printers?
- An abstracts brochure could be produced for posting to delegates and interested parties
- Conference report to be written and submitted ready for hand-over meeting with next year's conference organisers.
- Exact reason for conference, its aims and objectives need to be clarified, there is a potential for the conference to become more than just a dry run at paper presentations.
- Greater profile for conference, greater profile for Eng.D. program and its students
- Is a more professional conference worth the extra cost?

3.13 Notification Process – Presentation

This presentation was one that I prepared for the other researchers in my department at Brunel, the Centre for Environmental Research. It was to be a fifteen-minute presentation on the notification process, and my work at the CAU. I am to give the presentation on the 27th April.

BRUNEL
UNIVERSITY

ENVIRONMENT
AGENCY

The Notification Process

Nikki Robinson

Year 1 Engineering Doctorate Program
at Brunel & Surrey Universities

Sponsored by: EPSRC
Environment Agency

Topic Structure

- Dangerous Substances
- Competent Authority
- Existing Substances
- New Substances
    - Level Of Notification
    - Base Set Information
    - Technical Guidance Document
    - Ecotoxicology
    - (Q)SARs
    - PECs & PNECs
- EUSES
- Risk Assessment
- Difficult Substances

Dangerous Substances

- 7th Amendment Directive
  - Dangerous Substances Directive 67/548/EEC
- Europe Single Market
- CA, Competent Authorities
- NONS, Notification Of New Substances
- ESRs, Existing Substances Regulations

The UK CA

- HSE, Health and Safety Executive

- CAU, Chemical Assessment Unit
  - EA, Environment Agency

  formerly
  - DoE, Department of the Environment

NONS & ESRs

- NONS - Notification of new substances

  ELINCS,

  European List of Notified Chemical Substances

- ESRs - Notification of existing substances

  EINECS,

  European Inventory of Existing Chemical Substances

Where a "new" substance is any chemical which was not marketed in the EC 10 years prior to 18th September 1981.

NONS

A company or importer putting a new substance on the EC market must,

- Notify the CA of their intention to market a new substance

- Provide the CA with required information on the substance

The NONS Dossier

- Data
  - Physical & Chemical
  - Human Toxicology
  - Environmental Toxicology

GLP, Good Laboratory Practice

Level Of Notification

Level 2	>1000 t/a or >5000 t acc.	Base Set, plus additional toxicity, inc. birds, and long term soil and water data, and further degradation tests.
Level 1 (upper)	>100 t/a or >500 t acc.	Base Set, plus chronic, long term and bio toxicity data and sorption characteristics.
Level 1 (lower)	>10 t/a or >50 t acc.	Base Set, plus some relevant data from Level 1 (upper) tests.
VII A	>1 t/a or >5 t acc.	Base Set data
VII B	>100 kg/a or >500 kg acc.	Reduced Base Set, phys-chem data, biodegradation and acute toxicity.
VII C	>10 kg/a or >50 kg acc.	Reduced Base Set, chemical identity, indication of use and acute toxicity.

Base Set Information

0 Manufacturer and notifier identity and location of production site
1 Identity of the substance
2 Information on the substance
3 Physio-chemical properties
4 Toxicological studies
5 Ecotoxicological studies
6 Possibility of rendering substance harmless
7 Risk Assessment
9.1 Declaration of unfavourable effects on man and environment
9.2.1 Proposed classification and labelling
9.2.3 Proposed safety data sheet

TGD,
Technical Guidance Document

Part 1 - General Introduction
- Risk Assessment for Human Health

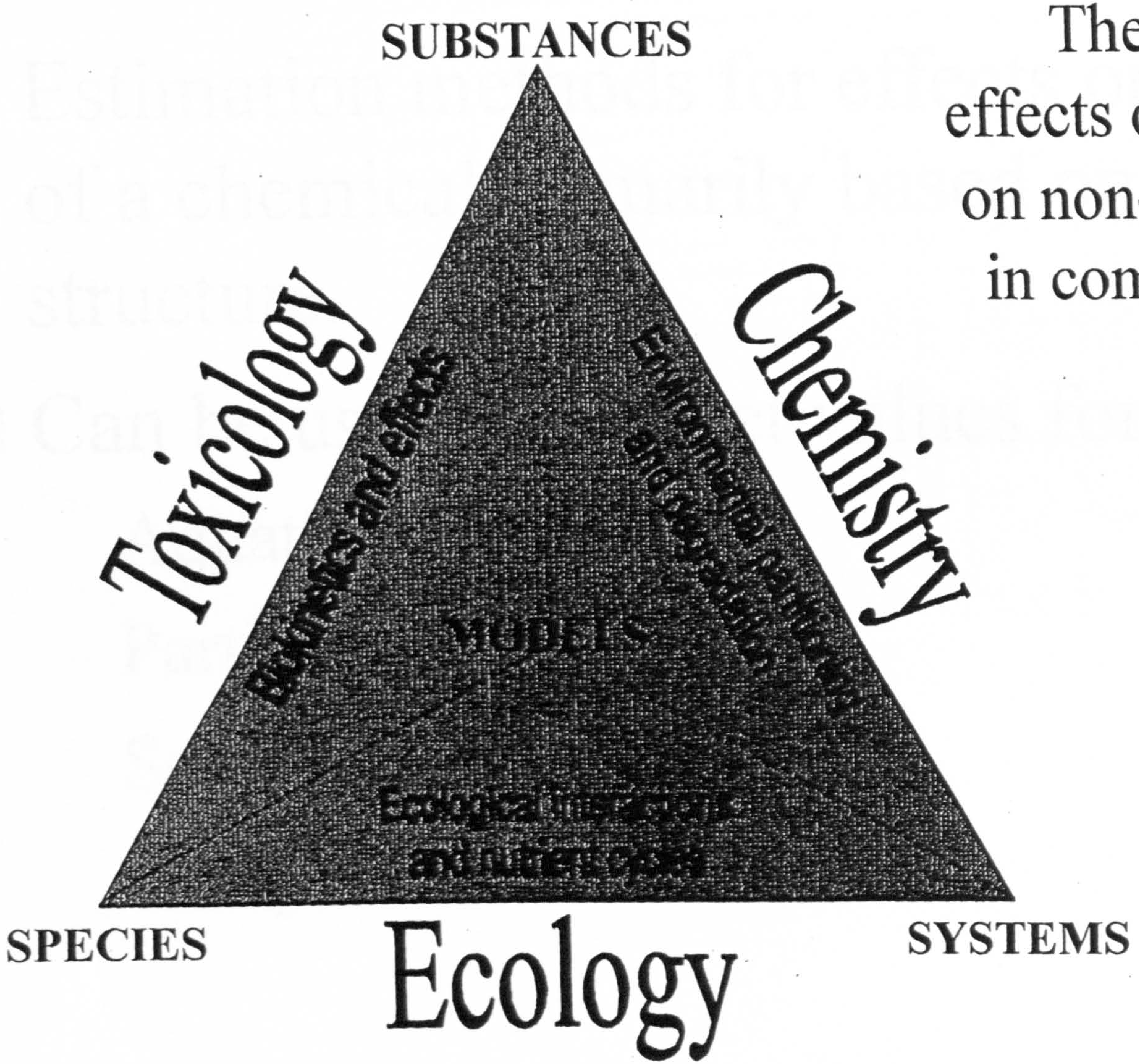
Part 2 - Environmental Risk Assessment

Part 3 - Use of (Q)SARs, (Quantitative) Structure Activity Relationships
- Use Categories
- Risk Assessment Report Format

Part 4 - Emissions Scenario Documents

Ecotoxicology

The study of toxic
effects of SUBSTANCES,
on non-human SPECIES,
in complex SYSTEMS.



(Q)SARs

- Estimation methods for effects or properties of a chemical primarily based on it’s structure.
- Can be used to predict values for:
  - Aquatic effects
  - Partition coefficients
  - Soil and sediment sorption
  - Henry’s Law constant, etc.

(Q)SARs For Sorption

Chemical Class	Equation
Predominantly hydrophobics	$\log \mathrm{Koc} = 0.81 \log \mathrm{Kow} + 0.10$
Non-hydrophobics	$\log \mathrm{Koc} = 0.52 \log \mathrm{Kow} + 1.02$
Alcohols	$\log \mathrm{Koc} = 0.39 \log \mathrm{Kow} + 0.50$
Amides	$\log \mathrm{Koc} = 0.33 \log \mathrm{Kow} + 1.25$
Anilines	$\log \mathrm{Koc} = 0.62 \log \mathrm{Kow} + 0.85$
Esters	$\log \mathrm{Koc} = 0.49 \log \mathrm{Kow} + 1.05$
Nitrobenzenes	$\log \mathrm{Koc} = 0.77 \log \mathrm{Kow} + 0.55$
Organic acids	$\log \mathrm{Koc} = 0.60 \log \mathrm{Kow} + 0.32$

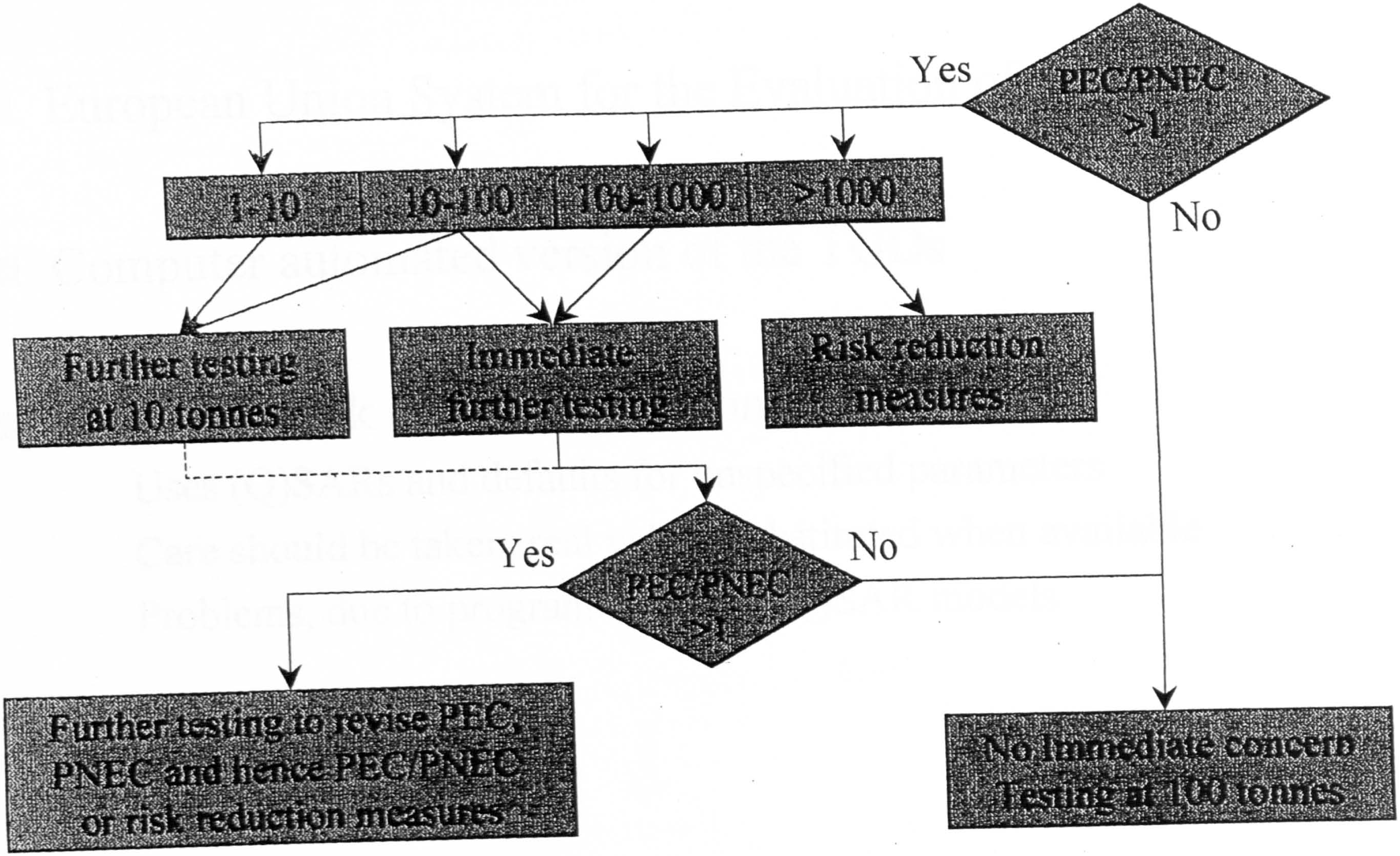
PECs & PNECs

- PEC - Predicted Environmental Concentration
- PNEC - Predicted No Effect Concentration

- $\frac{PEC}{PNEC}$ or RCR

  - Risk quotient used to express the risk posed by a chemical, if > 1 further testing may be necessary.

PEC/PNEC Ratios


PEC/PNEC >1

Yes

No

1-10

10-100

100-1000

>1000

Further testing at 10 tonnes

Immediate further testing

Risk reduction measures

PEC/PNEC >1

Yes

No

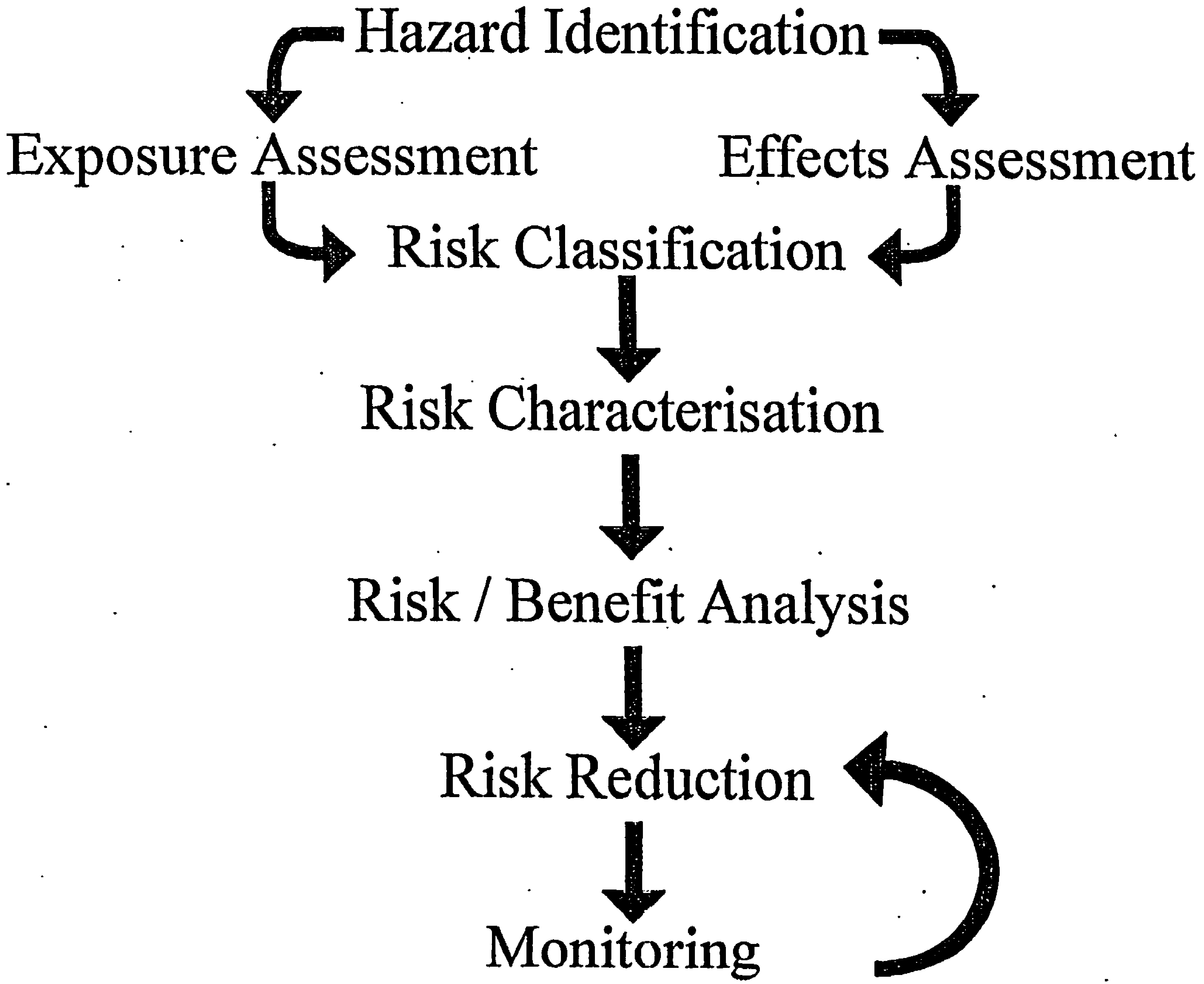
Further testing to revise PEC, PNEC and hence PEC/PNEC or risk reduction measures

No Immediate concern Testing at 100 tonnes

EUSES

- European Union System for the Evaluation of Substances
- Computer automated version of the TGDs
- Calculates risk classification from entered data
  - Uses (Q)SARs and defaults for unspecified parameters
  - Care should be taken, real values substituted when available
  - Problems, due to programming and (Q)SAR models

Risk Assessment



Hazard Identification

Exposure Assessment

Effects Assessment

Risk Classification

Risk Characterisation

Risk / Benefit Analysis

Risk Reduction

Monitoring

Difficult Substances

- Many substances are termed “difficult” due to inherent problems with testing them

- Poor water solubility
- Photolytically unstable
- Hydrolytically unstable
- Complex mixtures
- High volatility
- Ionisable
- Coloured

Ionising Substances

For some organic acids and bases,

- water solubility
- bio-availability
- measured toxicity

can all be influenced by relatively small changes in pH, due to its affect on the balance of dissociated and un-dissociated forms.

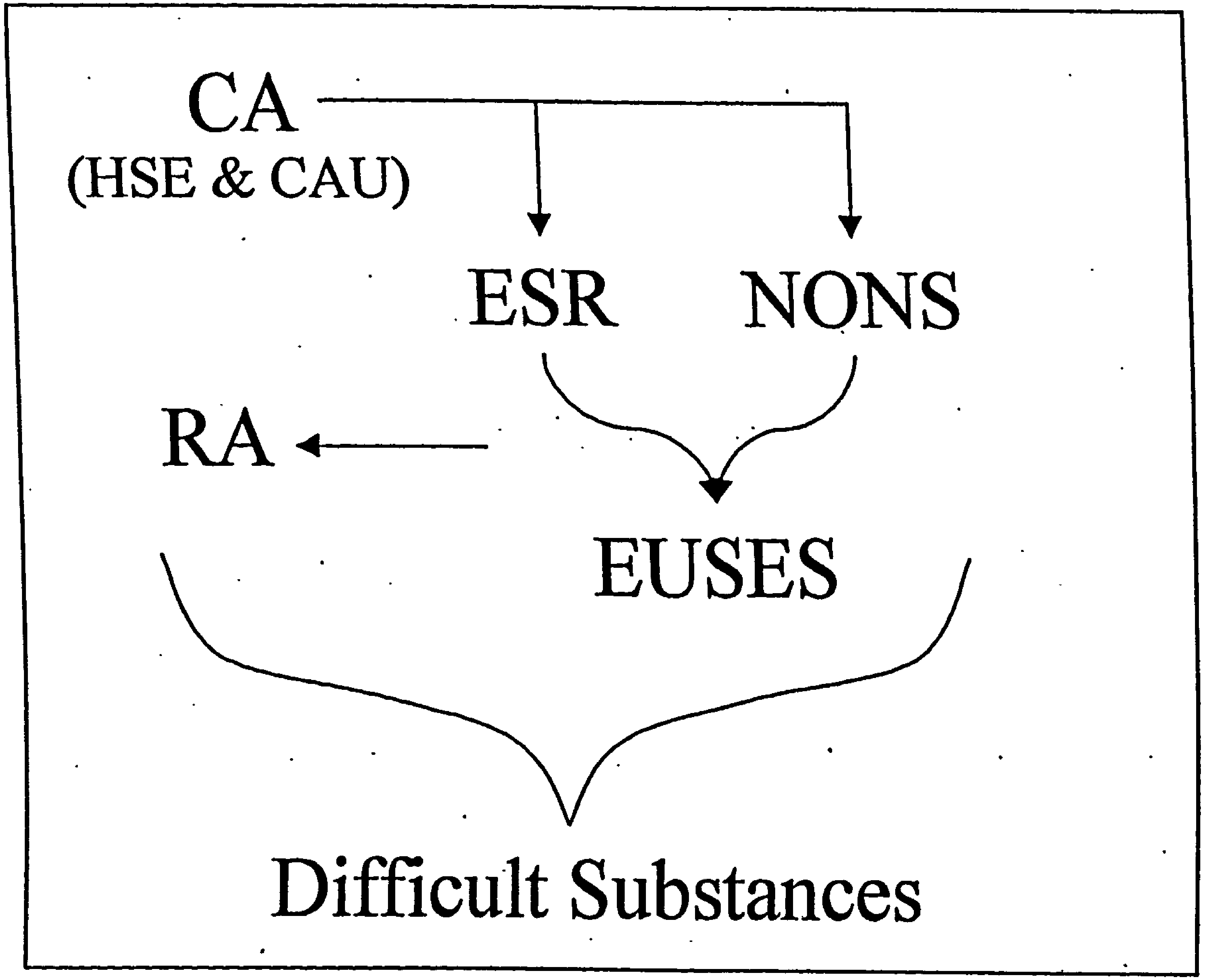
Definitive tests will be at a pH where toxicity is greatest

Areas of Possible Research

- Irreversible binding of anilines to soil, causing bio-accumulation
- QSARs
  - Henry's Law Constant
  - Ecotoxicity
  - Mixtures
  - Aerobic Biodegradation

Summary

Notifications



CA
(HSE & CAU)

ESR

NONS

RA

EUSES

Difficult Substances

Any Questions?

3.14 Notification – Poster-Board

This poster-board was prepared for the new Chancellor's visit to the university, and will be displayed on 31st March. Again like the oral presentation it was outlining the notification process and my work within the CAU.

The Notification Process

By Nikki Robinson
Year 1 EngD in Environmental Technology
at Brunel &Surrey Universities
Sponsored by: EPSRC
Environment Agency

There are two types of notification as outlined in the 7th Amendment to the Dangerous Substances Directive (67/548/EEC) which states the procedure and requirements of the notification process for both NONS and ESRs.

NONS - Notification Of New Substances,
Contained on, *ELINCS,*
European List of Notified Chemical Substances

ESRs - Existing Substances Regulations,
Contained on, *EINECS,*
European Inventory of Existing Chemical Substances

Where a "new" substance is any chemical which was not marketed in the EC in the 10 years prior to 18th September 1981

The CAU has carried out approximately 1100 NONs notifications to date with maybe 170 being performed a year at present.

Of approximately 103,000 substances on EINECS, Competent Authorities (CAs) in EU Member States are currently assessing 110 of them under ESR. The CAU having a commitment to 20 of these chemicals:

- 8 on the first priority list
- 5 on the second priority list
- 7 on the third priority list

A fourth priority list is being drawn up.

A company intending to market a new substance must notify the CA and provide a technical dossier containing the following details:

- Data on its chemical identity
- Estimate of quantity being placed on EC market
- Details of the substance's functions and uses
- Physiochemical, tox- and ecotox-icological data
- Precautionary, disposal and emergency measures
- Classification & labelling, and a safety data sheet

The notifier may either submit their own Risk Assessment (RA) or the CA will prepare one from the data supplied in the notification

Hazard Identification

Exposure Assessment   Effects Assessment

Risk Classification

↓

Risk Characterisation

↓

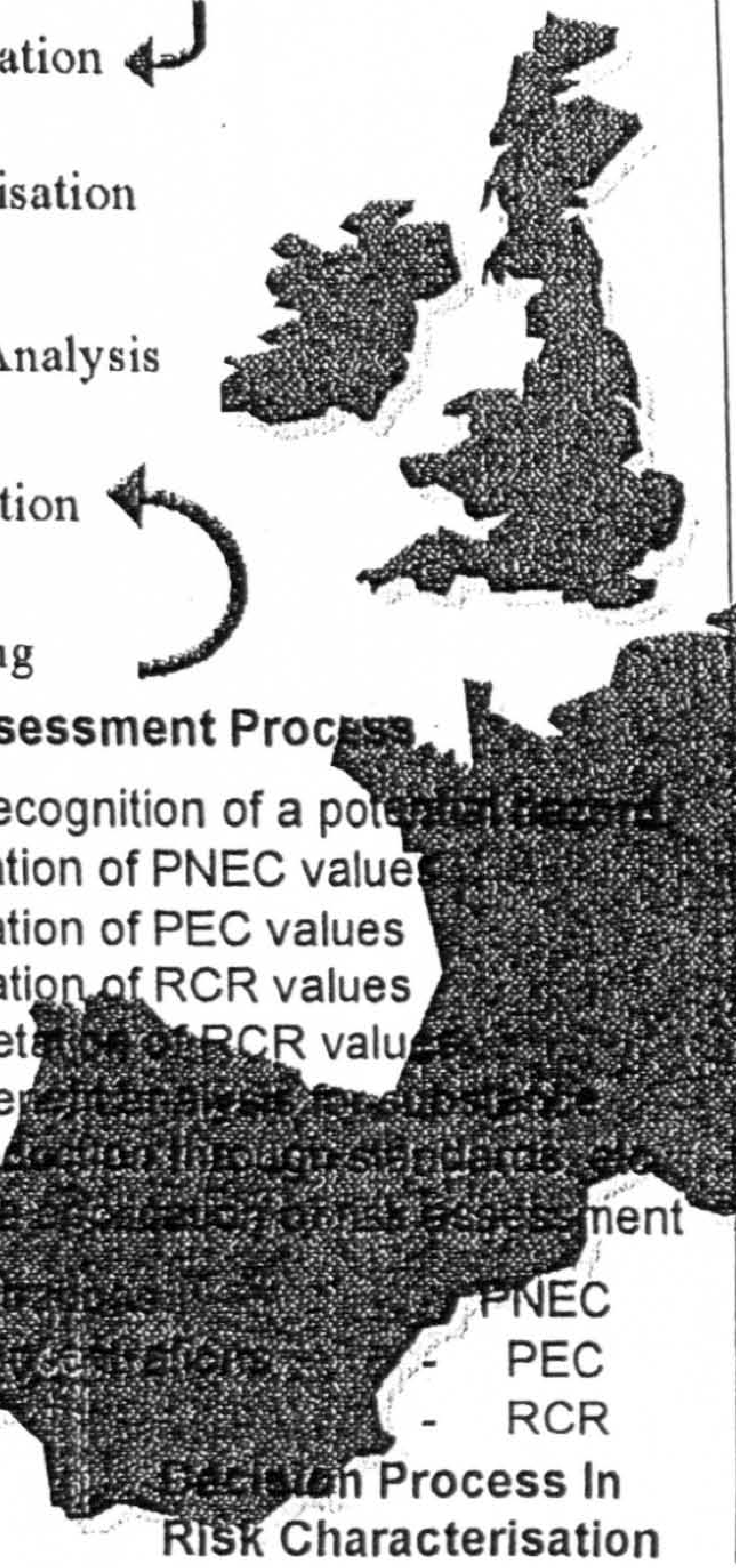
Risk / Benefit Analysis

↓

Risk Reduction

↓

Monitoring

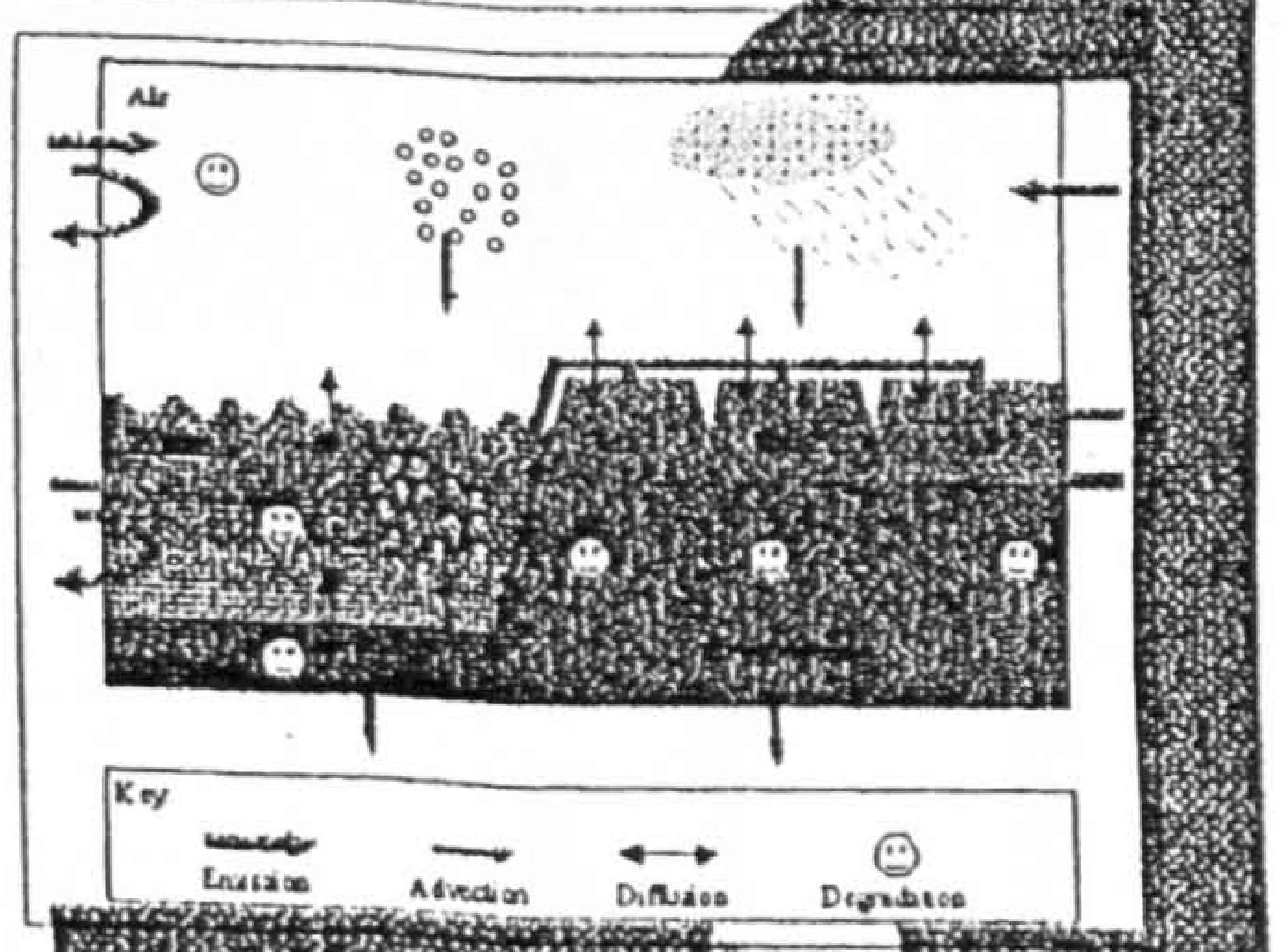


Stages To The Risk Assessment Process

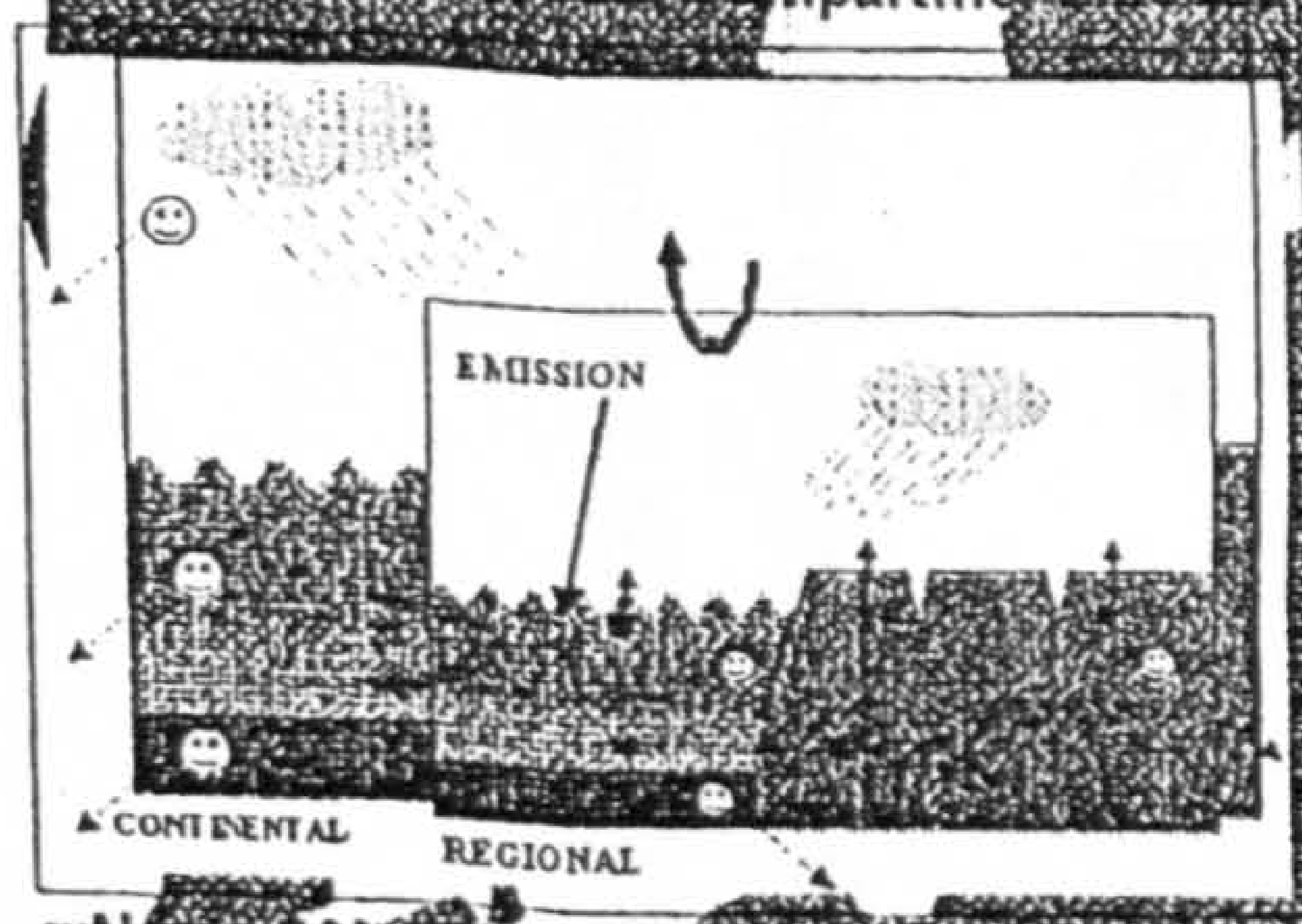
Hazard Identification	- Initial recognition of a potential hazard
Effects Assessment	- Generation of PNEC values
Exposure Assessment	- Generation of PEC values
Risk Classification	- Calculation of RCR values
Risk Characterisation	- Interpretation of RCR values
Risk Benefit Analysis	- Cost/benefit analysis [illegible]
Risk Reduction	- Risk reduction through standards, etc
Monitoring	- Iterative [illegible] assessment

Predicted No Effect Concentration	-	PNEC
Predicted Environmental Concentrations	-	PEC
Risk Characterisation Ratio	-	RCR

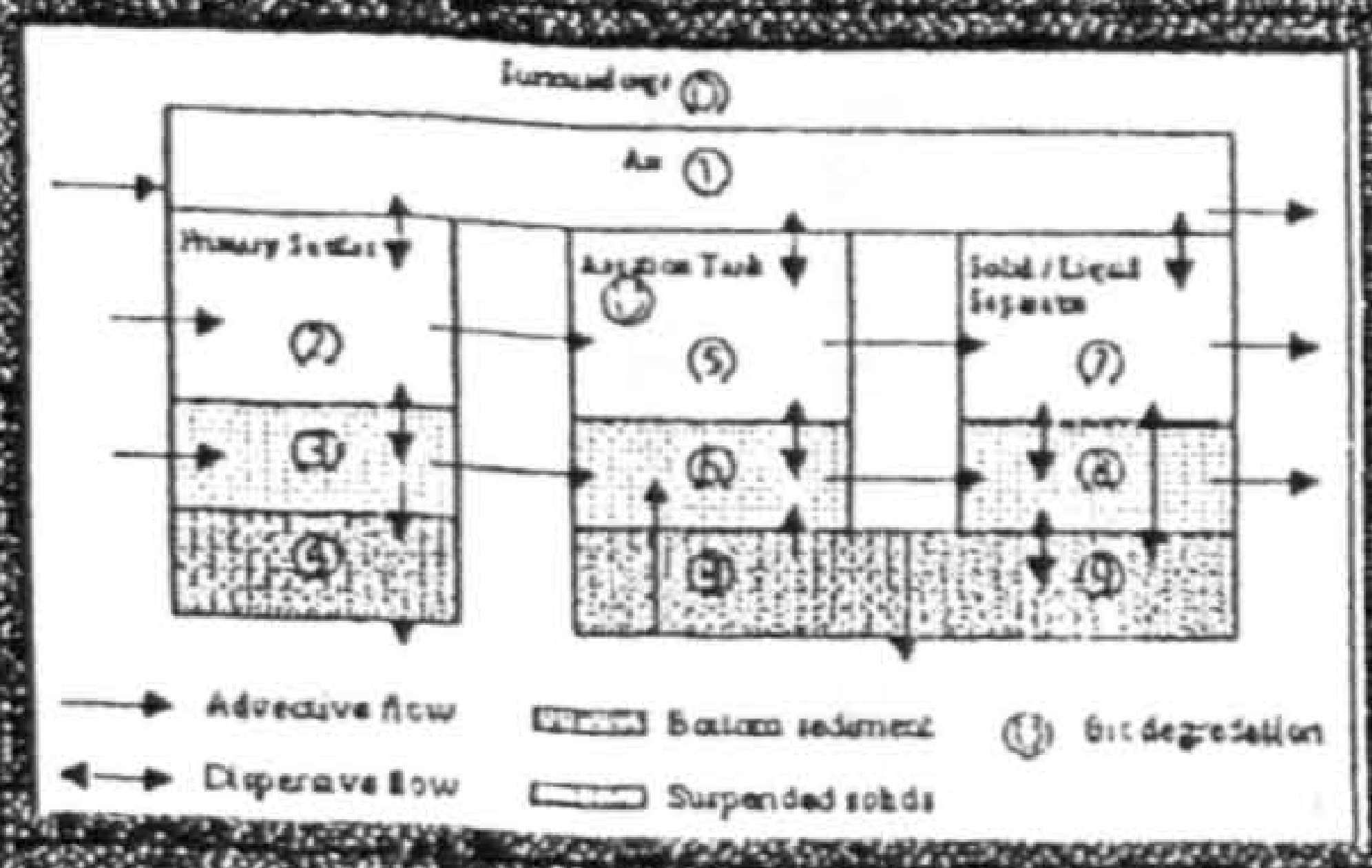
Compartment Models Used in Risk Assessment



Multimedia Compartment Model



Nested Multimedia Compartment Model



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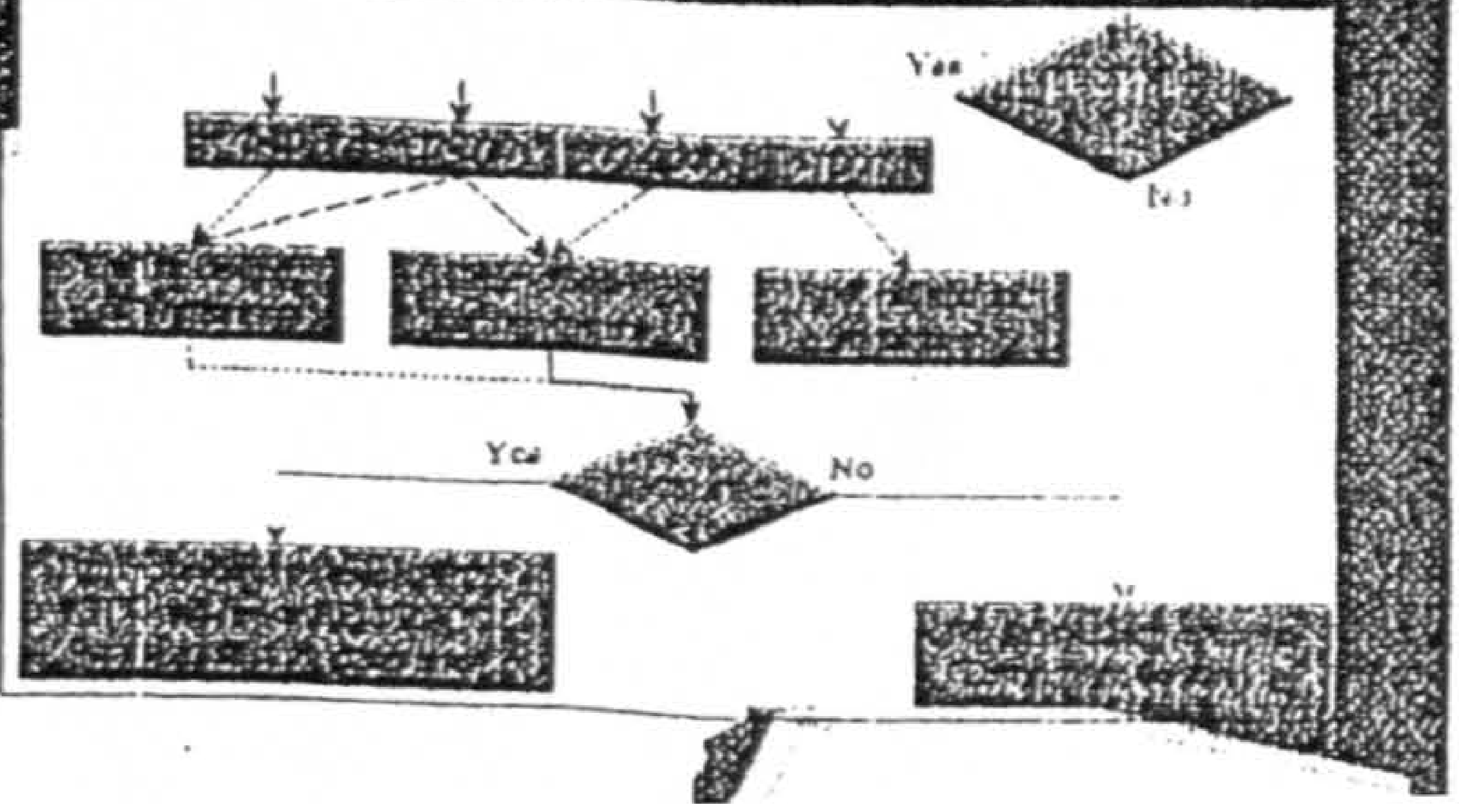

Decision Process In
Risk Characterisation

3.15 Literature Review – To Date

There follows a table of references that I have used, read or ear marked as useful during my first six months at the Environment Agency.

Selenium toxicity to aquatic life: an argument for sediment-based water quality criteria		Environmental toxicology and chemistry	Canton S.P. and Van Derveer W.D., 1997, Vol.16, No.6, pp1255-1259		
Fugacity-based model of PCB bioaccumulation in complex aquatic food webs		Environmental Science and . Technology	Campfens J. and MacKay D., 1997, Vol.31, No.2, pp.577-583		
Fugacity Analysis and Model Of Organic-Chemial Fate in a Sewage-Treatment Plant		Environmental Science and Technology	Clark B., Henry J.G. and Mackay D., 1995, Vol.29, No.6, pp.1488-1494		
A Fugacity Model Of Pesticide Runoff To Surface-Water – Development And Validation		Chemosphere	Diguardo A., Calamari D., Zanin G., Consalter A. and Mackay D., 1994, Vol.28, No.3, pp.511-531		
A Modeling Procedure To Evaluate The Coherence Of Independently Derived Environmental-Quality Objectives For Air, Water And Soil		Environmental Toxicology And Chemistry	Van de Meent D. and De Bruijn J.H.M., 1995, Vol.14, No.1, pp.177-186		
Modeling Intercompartment Transfer Of Pollutants - The Case Of Lead		Science Of The Total Environment	Van de Meent D., 1990, Vol.90, Jan., pp 41-54		
Deriving Quality Criteria For Water And Sediment From The Results Of Aquatic Toxicity Tests And Product Standards - Application Of The Equilibrium Partitioning Method		Water Research	Van der Kooij L.A., Van de Meent D., Van Leeuwen C.J. and Bruggeman W.A., 1991, Vol.25, No.6, pp.697-705		
A Spreadsheet-Based Box Model To Predict The Fate Of Xenobiotics In A Municipal Waste-Water Treatment-Plant		Water Research	Struijs J., Stoltenkamp J. and Van de Meent D., 1991, Vol.25, No.7, pp.891-900		
Uniform System For The Evaluation Of Substances: 4. Distribution And Intake		Chemosphere	Jager D.T., Visser C.J.M. and Van de Meent D., 1994, Vol.29, No.2, pp.353-369		
Added risk approach to derive maximum permissible concentrations for heavy metals: How to take natural background levels into account		Ecotoxicology And Environmental Safety	Struijs J., Van de Meent D., Peijnenburg W.J.G.M., Van den Hoop M.A.G.T. and Crommentuijn T., 1997, Vol.37, No.2, pp.112-118		
Fate Prediction Of Specific Organic-Compounds In Bioreactors		Water Science And Technology	Jacobsen B.N., Becher G., Jensen B.K., Monarca S., Scholzmuramatsu H. and Struijs J., 1996, Vol.33, No.6, pp.289-296		
A Rationale For The Appropriate Amount Of Inoculum In Ready Biodegradability Tests		Biodegradation	Struijs J., Stoltenkampwouterse M.J. and Dekkers A.L.M., 1995, Vol.6, No.4, pp.319-327	Biodegradation	
Standardized Biodegradability Tests - Extrapolation To Aerobic Environments		Water Research	Struijs J. and Vandenberg R., 1995, Vol.29, No.1, pp.255-262	Biodegradation	
Testing Surfactants For Ultimate Biodegradability		Chemosphere	Struijs J. and Stoltenkamp J., 1994, Vol.28, No.8, pp.1503-1523	Biodegradation	
Headspace Determination Of Evolved Carbon-Dioxide In A Biodegradability Screening-Test		Ecotoxicology And Environmental Safety	Struijs J and Stoltenkamp J., 1990, Vol.19, No.2, pp.204-211	Biodegradation	
Reductive Dehalogenation Of Dichloroanilines By Anaerobic Micro-organisms In Fresh And Dichlorophenol-Acclimated Pond Sediment		Applied And Environmental Microbiology	Struijs _J and Rogers J.E., 1989, Vol.55, No.10, pp.2527-2531	Biodegradation	

Paper Title	Book	Journal	Date, Vol. Etc.	Keywords	Publishers
Risk assessment of four major surfactant groups in the Netherlands		Tenside surfactants Detergents	1997, Vol.34, No.4, pp.242-249	PEC, PNEC, NOEC	
A method for evaluating consumer product ingredient contributions to surface and drinking water: Boron		Environmental toxicology and chemistry	1997, Vol.16, No.10, pp2070-2081	ROUT model	
Indirect measuring of key water quality parameters in sewage treatment plants		Journal of chemometrics	1996, Vol.10, No.5-6, pp.697-706	Phosphorus content	
Assessment of chemical fate in the environment using evaluative, regional and local-scale models		Environmental toxicology and chemistry	1996, Vol.15, No.9, pp.1638-1648	Mackay models	
Evaluation and modification of the simpletreat chemical fate model for activated-sludge sewage-treatment plants		Water science and technology	1996, Vol.33, No.6, pp.279-287	Simpletreat model	
Octamethylcyclotetrasiloxane (OMCTS), a case-study - summary and aquatic risk assessment		Environmental toxicology and chemistry	1995, Vol.14, No.10, pp.1667-1673	low solubility, high Kow and v. high H const.	
Fugacity analysis and model of organic-chemical fate in a sewage-treatment plant		Environmental toxicology and chemistry	1995, Vol.29, No.6, pp.1488-1494	Mackay models	
Simulation of the operating conditions of the municipal waste treatment plant at low- temperatures using a model that includes the IAWPRC activated sludge model		Water science and technology	1994, Vol.30, No.4, pp.105-113	IAWPRC activated sludge model	
Upgrading of existing sewage treatment plants by computer simulation - game or reality		Water science and technology	1994, Vol.29, No.12, pp.97-106	STREAM advanced simulation model	
Prediction of the fate of alcohol ethoxylates in sewage treatment plants		Chemosphere	1997, Vol.34, No.8, pp.1795-1801	Simpletreat model, Mackay level III	
Ecological risk assessment: an imput for decision making		Environmental management	1997, Vol.21, No.6, pp.812-816	RA EUSES	
European Union System for the Evaluation of Substances (EUSES). Principals and structure		Chemosphere	1997, Vol.34, No.8, pp.1823-1836	EUSES	
Environmental risk assessment of chemical substance		Chima	1997, Vol.51, No.5, pp.222-227	Mackay, USES, EUSES, EU TGD	
Comparison of the QSAR models for toxicity and biodegradability of anilines and phenols		Chemosphere	1997, Vol.34, No.2, pp.429-446	QSAR	
A QSAR based biodegradabiity model - A QSBR		Water research	1996, Vol.30, No.9, pp.2206-2214	QSAR	
Estimation of exposure and ecotoxicity related parameters by computer based structure property and structure-activity relationships		Toxicological and environmental chemistry	1993, Vol.40, No.1-4, pp.57-69	QSAR	
Application of experts' judgement to derive structure biodegredation relationships.		Environmental science and pollution research	1996, Vol.3, No.4, pp.224-228	QSAR	
Noncongeneric structure-toxicity correlation using fuzzy adaptive least squares		ACS symposium series	1995, Vol.606, pp141-152	QSARs, FALS	
Standerdized biodegredability tests - extrapolation to aerobic environments		Water research	1995, Vol.29, No.1, pp.255-262	OECD Biodeg.	
Toxicity measurements and their use in treatment strategies		Journal of the institute of water and environmental management	1994, Vol.8, No.2, pp.144-155	QSARs	
Risk assessment of chemicals: An introduction	x	-	1995, Ed. Van Leeuwen C.J. and Hermens J.L.M.		Kluwer Academic Publishers
Ecotoxicology - The study of polutants in ecosystems	x	-	1988, 2nd Ed., Moriarty F.		Academic Press
Risk assessment of chemicals in the environment	x	-	1988, Ed. Richardson M.L.		Royal Society of Chemistry
Toxic hazard assessment of chemicals	x	-	1986, Ed. Richardson M.L.		Royal Society of Chemistry
Predicting modes of toxic action from chemical structure: Acute toxicity of fathead minnow		Environmental toxicology and chemistry	Russom C.L., Bradbury S.P., Broderius S.J., Hammermeister D.E. and Drummond R.A., 1997, Vol.16, No.5, pp948-967	Modes of toxic action	
Introduction: Structural properties for determining mechanisms of toxic action		Env. Health Perspect.	Bradbury S.P. and Lipnick R.L., 1990, No.87, pp181-182	Modes of toxic action	
Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals		Environmental toxicology and chemistry	Broderius S.J., Kahl M.D. and Hoglund M.D., 1995, No.9, pp1591-1605	Modes of toxic action	
Rules for distinguishing toxicants that cause type I and type II narcosis syndrome		Env. Health Perspect.	Veith G.D. and Broderius S.J., 1990, No.87, pp207-211	Modes of toxic action	
Structural-toxicity relationships for the fathead minnow: Narcotic industrial chemicals		Can. J. Fish Aquat. Sci.	Veith G.D., Call D.J. and Brooke L.T., 1983, No.40, pp743-748	Modes of toxic action	
Structural activity relationships for screening organic chemicals for potential ecotoxicity effects		Drug Metab. Rev.	Veith G.D., DeFoe D. and Knuth M., 1984, No.15, pp1295-1303	Modes of toxic action	
A QSAR study of the acute toxicity of some industrial organic chemicals to goldfish		Xenobiotica	Lipnick R.L., Watson K.R. and Strausz A.K., 1987, No.7, pp1011-1025	Modes of toxic action	
Behavioural toxicity syndromes: A promising tool for assessing toxicity mechanism in jeuvenile fathead minnows		Environmental toxicology and chemistry	Drummond R.A. and Russom C.L., 1990, Vol.9, No.1, pp37-46	Modes of toxic action	
Modeling the join toxicity of xenobiotics to aquatic organisms: Basic concepts and approaches	x		Broderius S.J., 1991, pp107-127	Modes of toxic action	In Aquatic toxicology and risk assessment 14th Vol., Ed. Mayers M.A. and Barron M.G.

3.16 Glossary

The following is a glossary of terms that have been used and that have come up during my first six months at the Environment Agency.

AF	Assessment Factor
ALARA	As Low As Reasonably Achievable
ASL	Approved Supply List
BCF	Bio-concentration Factor
CA	Competent Authority
CAU	Chemical Assessment Unit
CNU	Chemical Notification Unit
DoE	Department of the Environment
EA	Environment Agency
EASE	Estimation and Assessment of Substance Exposure
EC	European Community
EC_{50}	Effect Concentration for the median or 50th percentile
ECB	Environmental Chemical Bureau
EEC	European Economic Community
EFTA	European Free Trade Association
EHS	Ecotoxicology and Hazardous Substances
EINECS	European Inventory Existing Chemical Substances
ELINCS	European List of Notified Chemical Substances
ERA	Environmental Risk Assessment
ESR	Existing Substances Regulation
ETU	Environmental Toxicology Unit
EU	European Union
EURAM	European Ranking Method
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HRA	Human Risk Assessment
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IPS	Informal Priority Setting method
IUCLIDS	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
LC_{50}	Lethal Concentration for 50th percentile
LCA	Life Cycle Assessment
LOAEL	Lowest Observable Adverse Effect Level

LOEC	Lowest Observable Effect Concentration
MATC	Maximum Acceptable Toxicant Concentration
NOAEL	No Observable Adverse Effect Level
NOEC	No Observable Effect Concentration
NONS	Notification Of New Substances
OECD	Organisation for Economic Co-operation and Development
PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
PPE	Personal Protective Equipment
(Q)SAR	(Quantitative) Structural Activity Relationship
RA	Risk Assessment
RCR	Risk Characterisation Ratio
RPE	Respiratory Protective Equipment
SETAC	Society of Environmental Toxicology and Chemistry
SNIF	Standard Notification Interchange Format
STP	Sewage Treatment Plant
TGD	Technical Guidance Document
UVCB	Substances of Unknown or Variable Composition, complex reaction products or Biological material
WAF	Water Accommodated Fraction
WWTP	Waste Water Treatment Plant

12 Month Report

ENVIRONMENT
AGENCY

BRUNEL
UNIVERSITY

Engineering Doctorate in Environmental Technology

12 Month Report

1st October 1998

By
Nik Robinson

Contents

Executive Summary

This report is the second six monthly report of my Engineering Doctorate. It contains an introduction and review of my work up to the end of the twelve-month period. An introduction to the Environment Agency and the National Centre for Ecotoxicology and Hazardous Substances (NC EHS) can be found in my first six monthly report. The whole of this period was spent working with the Environmental Toxicology Section (ETS). I have reviewed the aims and objectives that were set for this period and then laid down the new objectives for the next six-month period, as well as looking at more long-term aims. Finally a revised Gantt chart is including planning my next 3-6 months and taking a wider look at how my time might be split later in the research programme, attendance at modules is also shown. There is also a glossary of terms at the end of this report to help explain the many acronyms that are used in the field of ecotoxicology.

1 Introduction

My first six month report introduced my research project and programme and outlined both my long-term aims and those for the first and subsequent six month periods. I also considered the modules I had attended and included some material from these. Here I shall review the aims and objectives set in my first report and my progress towards them and have stated those for the following period.

The only outstanding objective from the first six months was the report on the Chemical Assessment Unit (CAU). This report had been written and was awaiting review by my supervisors before submission to my portfolio. My supervisors have now seen the report, however it is still waiting for comments from Dr. Steve Robertson the CAU Manager. In future I have decided to submit reports to everyone wishing to make comments at the same time and to give a reasonable date for when comments are required. Hopefully this should prevent deadlines slipping again as they have in the case of this report.

Following this section is a review of the work carried out within this second six-month period and my aims and objectives for the future, and in particular the next six months. I have also reviewed my work from the point-of-view of the course objectives and requirements, to indicate how I believe I am fulfilling these criteria. I have not included a review of the modules attended this period other than the conference organisation, project management elective module, which required a considerable commitment of time. The assignments completed for the other modules attended can be found in my portfolio.

2 Review

2.1 Objectives from last period:

In Box 1 below can be seen the objectives that were set and agreed for last time for the next 3 months, however due to a continuing commitment to the Kennet and Avon canal incident and the Engineering Doctorate Conference 1998, these objectives have occupied my last 6 months.

- To review structured methodology of the EQS system
  - How chemicals are chosen for assessment
  - Data collation
  - Data interpretation
  - What happens after the assessment has been carried out
- To analyse and understand the significance of ecotoxicology endpoints
  - EC_{50}/LC_{50}
  - NOEC/LOEC
  - Their meaning, statistical validity and confidence limits
- To write a report on the National Centre's response and handling of the Kennet and Avon incident
  - Involvement in pollution incident
  - Chemical information, used/needed
  - Point at which National Centre should be informed
  - Thought processes
    - what was needed
    - what was used
    - what else would have been useful
- To identify the learning points from the incident and to develop and propose a management system for coping with incidents

Box 1 - Objectives set after 6 months for the next three months in the ETS

I have continued my investigation of the EQS system and identified the ways in which chemicals are chosen for assessment. The data collation and interpretation stages of the EQS process are less proscribed as they are in the European notification system and these areas have taken more time to understand than they did at the CAU. One area that is very vague is the assigning of assessment factors to ecotoxicological data where "good scientific knowledge" is applied. This knowledge is however not always transparent. In an attempt to gain a greater understanding of the process, I intend to follow the setting of an EQS all the way through the system, from the identification of a need for an EQS value for a substance, through to the final setting of an EQS value. My report on the ETS is due before the end of December 1998. As part of the work on the ETS and EQS system I have had to recognise and understand the significance of ecotoxicological endpoints, their meaning, statistical validity and confidence limits. All this work will be included in my report on the ETS.

The other objective, to write a report on the NC EHS's response and handling of the Kennet and Avon canal incident, has also taken longer than anticipated. The incident seminar was postponed a number of times, and the release date of the final draft report on the technical investigation, by WRc, was also delayed. My work has focused on considering the management of the incident by the Area office, the NC EHS, as well as input by WRc and other contractors. I am investigating the strengths and weaknesses in the handling of the incident, examining what data was available, and what data was needed or would have helped. I have looked at the communications involved and how the NC EHS were contacted, at what levels and how in future they could or should deal with enquiries. My report considers the incidents management and the involvement of the NC EHS and makes recommendations on how similar incidents of this level could be handled and dealt with in future. It is intended to highlight areas of the Agency's handling of this incident that might provide lessons for future incident management. It is intended that this report will be completed by the end of November 1998. I intend to submit two reports, firstly one directed towards an internal audience (Agency staff), one that complements the WRc technical report and will therefore not contain expansion or details on the handling of the event, just discussion on the decisions and actions made. I shall then also submit a further report, more applicable to readers of my portfolio, which contains some of the background thinking and information that I worked on in order to produce the first report, the second report being more easily read as a document in its own right.

Another major commitment during this period was to the Project Management elective module that I undertook which involved myself and another Research Engineer organising the 1998 Engineering Doctorate Conference. This required far more time than had originally been appreciated. The Conference that took place in September 1998, had been in the planning stages since March, and the final report on the project management exercise is to be completed by the end of November. Great experience was gained throughout the project, in managing meetings and effective minute taking and agenda setting. Delegation became a necessary skill as did overall clear organisation and communication with students, academic and industrial contacts. The final report will be included in my portfolio, however the general view was that the conference was very successful and continued to show the high level of input that had been seen in previous years.

Longer-term aims that were set last period are outlined overleaf in Box 2, I shall now consider my progress towards these aims. The first two aims, that of understanding toxic modes of action, and direct toxicity assessment will hopefully at least in part be met during my time in the DTA Group, which I shall be joining in January 1999. After spending some time in the DTA Group I believe I will be in a better position to reassess and then move towards reaching some of these aims. Only once I have viewed the three systems can I really make comparisons between control of substances in the CAU vs. ETU, substance specific vs. whole sample and site specific vs. generic risk assessments. However the work I have completed already and the reports which I am producing will help to make the comparisons required in meeting these aims and objectives.

- To understand toxic modes of action

  For aquatic life there are only between 8 and 12, toxic modes of action, and therefore if chemicals mode of action can be assessed, cumulative effects may be able to be considered.

- To become accustomed to the methods of direct toxicity assessment

  This would mean that the toxicity of whole effluent samples would be considered. It would probably take longer and involve more work, but would be more protective of the environment.

- To conduct sensitivity analysis using case studies

  Sensitivity analysis needs to be carried out on all risk assessment processes to see which steps prove to be the sensitive ones and where assessment factors have the greatest effect on the final assessment figures.

- To compare manual vs. EUSES risk assessment calculations

  As was previously mentioned, EUSES has its problems for risk assessment compared with manual assessments, or does this indicate that manual assessments are too site specific.

- To consider site specific vs. generic risk assessment

  Which method of risk assessment leads to greater protection of the environment? Is there a place for both in risk assessment practices?

- To compare risk assessments conducted in the CAU vs. ETU

  Draft assessment documents are available for nonylphenol, acrylomide, tri-/per- chloroethylene and acetonitrile, which have been conducted under each system. What does a comparison of the results suggest? Is either method more protective than the other, and are the results of one as applicable to the customers of the other results?

Box 2 - Longer-term aims for work within the NC EHS

2.2 Objectives Proposed for Next Period:

Below in Box 3 the agreed objectives for next period are outlined.

- Complete report on the Chemical Assessment Unit by end of 1998
  - Get final comments from Steve Robertson on draft copy
  - Amend and produce final copy
- Complete report on the Kennet and Avon incident by end of November
  - Produce final draft
  - Circulate for comments with return date
  - Amend and produce final copy
- Complete report on the Environmental Toxicology Unit and the EQS system by end of 1998
  - Produce final draft
  - Circulate for comments with return date
  - Amend and produce final copy
- Start period working in DTA Group
  - Investigate whole toxicity testing
  - Review work being carried out at Waterlooville Laboratory
  - Write report on direct toxicity assessment

Box 3 - Objectives agreed and set for the next 6 months

2.3 Aims and Objectives of the Engineering Doctorate Program:

Below I have outlined the aims and objectives of the course from the EngD Joint Regulations, (Section 2.1). The table summarises how I feel my research work will demonstrate and meet these required attributes.

Aims and Objectives of EngD Program	How Attributes Will Be Demonstrated
REs should: (i) be equipped as engineering research-designers to plan and lead flexible and innovative R&D programmes that respond to customers' needs.	The Kennet & Avon incident has required a very flexible approach, and good interpersonal skills. Also my proposing of integrated sustainable practices for the risk assessment of substances, mindful of the effects these systems have on chemical industries will help to fulfil this objective.
(ii) be able to work effectively, and to form, work within and where necessary lead teams with a multi-disciplinary background to tight time schedules.	I believe organising the 1998 EngD Conference, demonstrated these attributes, most notably, working to deadlines and working effectively both within and leading teams. My work on risk assessment systems will also require forming and working with multi-disciplinary teams, biologists, ecotoxicologists and business managers all having inputs and constraints on my work.
(iii) possess comprehensive expert knowledge of the field of Environmental Technology, of the techniques needed to balance social and economic benefit against resource utilisation and environmental impact, and of the processes of technology transfer needed to ensure the application of research into practice	Expert knowledge of environmental technology and in particular risk assessment, ecotoxicology and environmental legislation will be of great importance throughout my research. I will also need to balance not only social and economic but also environmental benefits, in all developments my research produces. Finally, methods of technology transfer, particularly in the development of transparent risk assessment methodologies will also be of great importance, to ensure the proper use of risk assessment systems in industry. My reports on the CAU, ETU and the Kennet & Avon incident will at least in part demonstrate achievement of this.

Table 1 - Aims and objectives of the Engineering Doctorate

Aims and Objectives of EngD Program	How Attributes Will Be Demonstrated
(iv) have demonstrated ability for originality and for innovation	In any methodologies and systems I design or develop, I intend to incorporate originality and innovation, creating systems that are tailored towards the needs of both the Environment Agency and industry (their customers).
(v) possess a working knowledge of project management and business methods and their implications for research and development	Through organising the 1998 EngD Conference I have learnt the strength of good project management, and feel I have started to incorporate lessons learnt from this project into the organisation of my research. I shall practice and improve these new skills I have gained during the course of my research and beyond.
(vi) possess and have demonstrated a high level of communication and presentation skills .	I am conscientious about my presentation and feel that it is generally of a high standard. I have continued to develop this skill through the production of reports, an EngD promotional presentation and my conference presentation. I am also working on my ability to communicate complex scientific points in a concise and easily understood manner.

Table 1 - Aims and objectives of the Engineering Doctorate (continued)

The Joint Regulations (Section 4.4.1) also outline criteria that are necessary for eligibility to graduate as a Doctor of Engineering. Many of these are assessed as part of the taught modules, however two criterion of particular note are to be tested in the final *viva voce*, but I feel should be considered here and throughout the degree program, these are to:

- Demonstrate evidence of innovation and a contribution to knowledge via research into either:
  - (i) novel understanding of the environmental consequences of systems for providing or using goods or services, or;
  - (ii) novel methods of improving the environmental performance of systems for providing or using goods or services thereby contributing to more sustainable development.

- Demonstrate an understanding of the context of the research: this must include the scientific context and, where appropriate should include the commercial and social context.

Further to these is the consideration that the work should meet the criterion of environmental technology, which is unique to the Brunel/Surrey Engineering Doctorate program. I feel I will meet these criteria in the following ways:

My innovation and contribution to knowledge shall primarily be in the area of risk assessment, although work such as that which I have undertaken on the Kennet & Avon canal incident will contain novel aspects. Through my initial study of the existing systems their strengths, weaknesses, and possible synergies will be outlined. Novel methodologies will then be researched, devised and documented. The contribution to knowledge clearly being in the generation of newly improved, risk assessment practices, systems and methodologies. These will be transparent to both implementers and users, protective of the target environmental compartments and the environment as a whole. However, they will also endeavour not to over regulate or over protect, causing unnecessary restrictions to industry and loss of faith in risk assessment practices. An understanding of the environmental consequences of risk assessment systems and methodologies will be necessary and demonstrated in throughout my work.

An understanding of the context of the research will be necessary and demonstrated in the transparent nature of the developed systems, due to their use by industry and scientists at different levels. An understanding of the scientific context will be demonstrated in the application of the novel systems to ensure the protection of the environment, with good use of data and knowledgeable interpretation of results. As mentioned earlier, the commercial and social context will also have to be considered, being careful not to over regulate or over protect, as well as constructing transparent methodologies and systems to ensure easy application and use.

Finally, my research is at the core of the NC EHS's activities. As such I believe I shall demonstrate environmental technology through the construction of novel risk assessment practices that while ensuring protection, don't over regulate, practices that are workable in industry and which promote sustainable development in the chemical field.

3 Project Planning Gantt Chart

There follows a table of references that I have used, read or ear marked as useful during my first six months at the Environment Agency.

4 Glossary

The following is a glossary of terms that have been used and that have come up during my first six months at the Environment Agency.

AF	Assessment Factor
ALARA	As Low As Reasonably Achievable
ASL	Approved Supply List
BCF	Bio-concentration Factor
CA	Competent Authority
CAU	Chemical Assessment Unit
CNU	Chemical Notification Unit
DETR	Department of the Environment, Transport and the Regions
DTA	Direct Toxicity Assessment
EA	Environment Agency
EASE	Estimation and Assessment of Substance Exposure
EC	European Community
EC_{50}	Effect Concentration for the median or 50th percentile
ECB	Environmental Chemical Bureau
EEC	European Economic Community
EFTA	European Free Trade Association
EINECS	European Inventory Existing Chemical Substances
ELINCS	European List of Notified Chemical Substances
EQS	Environmental Quality Standard
ERA	Environmental Risk Assessment
ESR	Existing Substances Regulation
ETS	Environmental Toxicology Section
EU	European Union
EURAM	European Ranking Method
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice
HEDSET	Harmonised Electronic Data SET
HRA	Human Risk Assessment
HSE	Health and Safety Executive
IPS	Informal Priority Setting method
IUCLIDS	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
LC_{50}	Lethal Concentration for 50th percentile
LCA	Life Cycle Assessment

LOAEL	Lowest Observable Adverse Effect Level
LOEC	Lowest Observable Effect Concentration
MATC	Maximum Acceptable Toxicant Concentration
NC EHS	National Centre for Ecotoxicology and Hazardous Substances
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(Q)SAR	(Quantitative) Structural Activity Relationship
RA	Risk Assessment
RCR	Risk Characterisation Ratio
RPE	Respiratory Protective Equipment
SETAC	Society of Environmental Toxicology and Chemistry
SNIF	Standard Notification Interchange Format
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TGD	Technical Guidance Document
UVCB	Substances of Unknown or Variable Composition, complex reaction products or Biological material
WAF	Water Accommodated Fraction
WWTP	Waste Water Treatment Plant

18 Month Report

ENVIRONMENT
AGENCY

BRUNEL
UNIVERSITY

Engineering Doctorate in Environmental Technology

18 Months Report

1st April 1999

By
Nik Robinson

Contents

Executive Summary

This report is the third in a series of six monthly reports tracking the author's progress through out the duration of the Engineering Doctorate course. It contains an introduction and review of work up to the end of the eighteen-month period. A more general introduction to the Environment Agency and the National Centre for Ecotoxicology and Hazardous Substances (NCEHS) can be found in the first report.

During this third period of research the author remained with the Environmental Toxicology Section (ETS) in an attempt to bring the work in this section to a close. The aims and objectives from the previous period are reviewed and the new objectives for the next six-month period are outlined. Finally a revised Gantt chart is including showing the proposed timescales for projects with modules and other overlapping commitments indicated. There is also a glossary of terms at the end of this report to help explain the many acronyms that are used in the field of ecotoxicology.

1 Introduction

The objectives agreed for this period are reviewed in detail in the following section, and agreed objectives for the next period are also outlined. This last period has seen further slip in objectives that were agreed at the end of the first six-month period. The second report essentially repeating these objectives and giving time scales for their completion. However, through a lack of clearly defined objectives, too wide a scope and an unfocused approach, progress towards these objectives became slow. For these reasons outstanding work was, where possible, finished within this period with the remaining objective being set aside to allow the research program to move forward.

The report on the Chemical Assessment Unit (CAU) that had remained outstanding from the first six-month period has now been completed. The final draft of the report on the Kennet & Avon Canal Incident has been completed and copies distributed with a three-week deadline for comments. The proposed report on the ETS section has not been written, a review of the system and its methodologies having been completed, but not documented. The research has now moved on to the Direct Toxicity Assessment (DTA) section, and a review of this section's work, the methodology behind DTA and its use as a risk assessment tool will all be considered.

A review of the modules attended this period has not been included, however the completed assignments can be found in the author's portfolio.

2 Review

2.1 Objectives from the Last Period:

The objectives that were agreed at the beginning of this period can be seen below (Box 1). There was further slip in the progress towards these objectives during this period. Although time scales had been agreed for the completion of the outstanding objectives, progress was slow, this being partly due to a lack of focus in the work. Future objectives will be stated clearly, with a clear time scale and a well defined scope, to prevent the aim of the research becoming lost in an attempt to encompass to wide a field.

- Complete report on the Chemical Assessment Unit by end of 1998
  - Get final comments from Steve Robertson on draft copy
  - Amend and produce final copy
- Complete report on the Kennet and Avon incident by end of November
  - Produce final draft
  - Circulate for comments with return date
  - Amend and produce final copy
- Complete report on the Environmental Toxicology Unit and the EQS system by end of 1998
  - Produce final draft
  - Circulate for comments with return date
  - Amend and produce final copy
- Start period working in DTA Group
  - Investigate whole toxicity testing
  - Review work being carried out at Waterlooville Laboratory
  - Write report on direct toxicity assessment

Box 1 - Objectives set after 6 months for the next three months in the ETS

It was decided that in order to forward the research the outstanding work should, where possible, be finished within this period, and the remaining objective set aside.

This helped to ensure that the review of the methods and tools used in the Direct Toxicity Assessment (DTA) section commenced before the end of this period.

The CAU report, overdue from last period, was completed during the early stages of this period. One clear lesson from the completing of this first report was that final draft copies of reports should be submitted to all concerned, clearly stating a sensible date by which comments need to be returned. This will then prevent the iterative process of submitting to each person separately and encourage any comments to be returned promptly. The report on the CAU clearly outlines the European Union's system for notifying new and existing chemicals, a summary of some points raised in this report can be seen below (Box 2).

> The notification system provides a structured system for obtaining information on new chemicals, ensuring this information is expanded and updated if there is concern or the substance is marketed in a greater quantity. However, the system is not an effective approach to retrospectively gaining the information on the large number of chemicals classed as existing substances.
>
> There are problems with the generic assessment that is performed to allow the results to be accepted throughout Europe, with a need for transparency so that the sensitivity and dependability of values can be seen. One possible refinement would be the splitting of the aqueous compartment, (e.g. Freshwaters, Estuaries, Seas).
>
> There is a bias towards the aquatic compartment, with a need for further research on models for the other environmental compartments (soil, sediment and air) to ensure multi-compartment assessments.
>
> There also needs to be a form of review or update to allow the system to learn from the experience of the assessments that have already been processed. A review of old calculations compared to the new ones were further data has been submitted would indicate whether base set calculations are actually representative in light of new data. Also trend in species sensitivity, toxicity by industry, etc. could be investigated.

Box 2 - Summary of some of the key points disscussed in the CAU report

The final draft of the report on the Kennet & Avon Canal Incident was completed and copies distributed to all concerned. Any comments on the report were requested within three weeks. One week has been marked on the Gantt project plan (see section 4) for making any corrections and producing the final report. The report examined the technical investigation and the involvement of the NCEHS in the investigation, a summary of some of the points raised can be found below (Box 3).

A tiered approach to incident investigations is required, most specifically for analysis methods. This tiered system would then help focus and lead incident investigations.

The communication during incidents needs to be streamlined, helping to convey the Agency's control of the incident to the public, media and other stakeholders. And scientific staff are needed in the incident room to understand and convey technical information, along with effective return communications from the incident room to help lead their work.

The awareness of the NCEHS's ETAS information service needs to be increased. Also the hierarchical, tiered contact structure needs to be maintained and adhered to, to reinforce the position's of the Regional Contacts.

Although the same level of information support as provided in this incident would have been possible further afield such a level of involvement by the NCEHS has ramifications on other work and can result in slip of other obligations. For this reason the remit of ETAS and its level of support need to be clarified and communicated to its customers.

Computer processing of data obtained from routine monitoring could search for potential pollution problems and areas of concern and highlight these "hot spot". Also a combination of several existing databases of chemicals and their physical, chemical and ecotoxicological properties, could be used to generate a large database for querying, using known properties in a pollution incident to generate a target list of chemicals to help direct and lead analyses and investigations.

Box 3 - Summary of some of the key points disscussed in the Kennet & Avon Incident report

The proposed report on the ETS section has not been written. Although a review of the system and its methodologies was carried out, the required information was not readily available and a lack of clear focus has caused progress towards this objective to slip considerably. It was decided that the best course of action would be to move on to the next section (DTA) and if necessary and/or possible try to revisit the ETS and produce a report on the EQS system at a later date.

A work program for the time to be spent with the DTA and a proposed set of objectives/deliverables were outlined in draft towards the end of this period. These objectives are yet to be agreed by the author's industrial and academic supervisors, however the work plan suggests a period of just less than six months in the DTA split into three research/review areas:

1. Direct toxicity assessment – current demonstration programme, methodology, strengths and weaknesses
    - Short report/document on DTA its methods and strengths and weaknesses, as well as other similar programs like the US EPA's WET.

2. Ecotoxicology and biological effect measures – Tests, organisms and end-points
    - Short report/document on ecotoxicology, tests, organism and end-points, to ensure understanding.

3. DTA as a risk assessment tool – tiered testing programme, how DTA fits in with LEAPs and as a one in a series of RA tools
    - Full report on DTA as a tool and how it fits in with the other risk assessment tools/processes available in ecotoxicology

It is intended that approximately six weeks will be spent on each of the first two areas of study, and a longer period of about twelve weeks are intended for the final part. This will ensure the work is finished by early September so as not to interfere with the Engineering Doctorate Conference, and also leaves the remainder of September free to embark on new research areas and for identifying further areas of contribution.

2.2 Objectives Proposed for the Next Period:

Below in Box 4 the proposed objectives for the next period are outlined.

- Complete report on Kennet and Avon Canal Incident
  - Final corrections to be made to report
  - Produce and distribute final copies

19 – 23/04/99

- Produce report after stage 1 of DTA programme
  - Produce report on *DTA – methodology, strengths and weaknesses*
  - Circulate for comments with return date
  - Amend and produce final copy

29/03 – 07/05/99

- Produce report after stage 2 of DTA programme
  - Produce report on *Ecotoxicology – tests, organisms and end-points*
  - Circulate for comments with return date
  - Amend and produce final copy

10/05 – 18/06/99

- Produce report after stage 3 of DTA programme
  - Produce report on *DTA as a risk assessment tool*
  - Circulate for comments with return date
  - Amend and produce final copy

21/06 – 10/09/99

- Propose further areas of novel research for remaining stages of research program

Box 4 - Objectives proposed for then next 6 months

2.3 Aims and Objectives of the Engineering Doctorate Program:

Below I have outlined the aims and objectives of the course from the EngD Joint Regulations, (Section 2.1). The table summarises how I feel my research work will demonstrate and meet these required attributes.

Aims and Objectives of EngD Program	**How Attributes Will Be Demonstrated**
REs should:	
(i) be equipped as engineering research-designers to plan and lead flexible and innovative R&D programmes that respond to customers' needs.	I feel my continuing work on the Kennet & Avon incident has demonstrated my flexibility, and good interpersonal skills. Also some of the areas address to needs expressed by those involved in the investigation, developing methods an ideas, such as the decision tree, to express complex situations, and identify areas of strength and weakness.
(ii) be able to work effectively, and to form, work within and where necessary lead teams with a multi-disciplinary background to tight time schedules.	In this last period I have not needed to lead any teams but have continued to work within and as part of many overlapping teams as part of my work on the Kennet and Avon Canal Incident. I also believe my work in the DTA will also require forming and working with multi-disciplinary teams, biologists, ecotoxicologists and business managers all having inputs and constraints on my work.
(iii) possess comprehensive expert knowledge of the field of Environmental Technology, of the techniques needed to balance social and economic benefit against resource utilisation and environmental impact, and of the processes of technology transfer needed to ensure the application of research into practice	Expert knowledge of environmental technology and in particular risk assessment, ecotoxicology and environmental legislation is of great importance in my research. I need to balance not only social and economic but also environmental benefits, in all aspects of my work, in the Kennet and Avon Incident, both economical costs and environmental cost had a pronounced effect on the chosen actions and solutions. Finally, methods of technology transfer, particularly in the development of transparent risk assessment methodologies will also be of great importance, to ensure the proper use of risk assessment systems in industry.

Table 1 - Aims and objectives of the Engineering Doctorate

Aims and Objectives of EngD Program	How Attributes Will Be Demonstrated
(iv) have demonstrated ability for originality and for innovation	In the Kennet and Avon report I developed a decision tree diagram to communicate the actions and reactions of the incident in a novel way tailoring the information towards the needs of both the Agency and outside interested parties.
(v) possess a working knowledge of project management and business methods and their implications for research and development	I have implemented many of the lessons learnt from the conference organisation into the managing of this periods work, and have also learnt new lessons, particularly concerning focusing of objectives. I shall practice and improve these new skills I have gained during the course of my research and beyond.
(vi) possess and have demonstrated a high level of communication and presentation skills	I continue to take pride in my presentation and feel that it is generally of a high standard. I have continued to develop this skill through the production of reports, as well as presenting and lecturing to both peer groups and undergraduates. I am also continuing to work on my ability to communicate complex scientific points in a concise and easily understood manner.

Table 1 - Aims and objectives of the Engineering Doctorate (continued)

The Joint Regulations (Section 4.4.1) also outline criteria that are necessary for eligibility to graduate as a Doctor of Engineering. Many of these are assessed as part of the taught modules, however two criterion of particular note are to be tested in the final *viva voce*, but I feel should be considered here and throughout the degree program, these are to:

- Demonstrate evidence of innovation and a contribution to knowledge via research into either:
  - (i) novel understanding of the environmental consequences of systems for providing or using goods or services, or;
  - (ii) novel methods of improving the environmental performance of systems for providing or using goods or services thereby contributing to more sustainable development.

- Demonstrate an understanding of the context of the research: this must include the scientific context and, where appropriate should include the commercial and social context.

Further to these is the consideration that the work should meet the criterion of environmental technology, which is unique to the Brunel/Surrey Engineering Doctorate program. I feel I will meet these criteria in the following ways:

My innovation and contribution to knowledge shall primarily be in the area of risk assessment, although work such as that which I have undertaken on the Kennet & Avon canal incident will contain novel aspects, such as the decision tree diagram and suggestions of improved data sets and data analysis. Through my initial study of the existing systems their strengths, weaknesses, and possible synergies will be outlined. Novel methodologies will then be researched, devised and documented. The contribution to knowledge clearly being in the generation of newly improved, risk assessment practices, systems and methodologies. These will be transparent to both implementers and users, protective of the target environmental compartments and the environment as a whole. However, they will also endeavour not to over regulate or over protect, causing unnecessary restrictions to industry and loss of faith in risk assessment practices. An understanding of the environmental consequences of risk assessment systems and methodologies will be necessary and demonstrated in throughout my work.

An understanding of the context of the research will be necessary and demonstrated in the transparent nature of the developed systems, due to their use by industry and scientists at different levels. An understanding of the scientific context will be demonstrated in the application of the novel systems to ensure the protection of the environment, with good use of data and knowledgeable interpretation of results. As mentioned earlier, the commercial and social context will also have to be considered, being careful not to over regulate or over protect, as well as constructing transparent methodologies and systems to ensure easy application and use.

Finally, my research is at the core of the NCEHS's activities. As such I believe I shall demonstrate environmental technology through the construction of novel risk assessment practices that while ensuring protection, don't over regulate, practices that are workable in industry and which promote sustainable development in the chemical field.

3 Project Planning Gantt Chart

There follows a table of references that I have used, read or ear marked as useful during my first six months at the Environment Agency.

4 Glossary

The following is a glossary of terms that have been used and that have come up during my first six months at the Environment Agency.

AF	Assessment Factor
ALARA	As Low As Reasonably Achievable
ASL	Approved Supply List
BCF	Bio-concentration Factor
CA	Competent Authority
CAU	Chemical Assessment Unit
CNU	Chemical Notification Unit
DETR	Department of the Environment, Transport and the Regions
DTA	Direct Toxicity Assessment
EA	Environment Agency
EASE	Estimation and Assessment of Substance Exposure
EC	European Community
EC_{50}	Effect Concentration for the median or 50th percentile
ECB	Environmental Chemical Bureau
EEC	European Economic Community
EFTA	European Free Trade Association
EINECS	European Inventory Existing Chemical Substances
ELINCS	European List of Notified Chemical Substances
EQS	Environmental Quality Standard
ERA	Environmental Risk Assessment
ESR	Existing Substances Regulation
ETS	Environmental Toxicology Section
EU	European Union
EURAM	European Ranking Method
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice
HEDSET	Harmonised Electronic Data SET
HRA	Human Risk Assessment
HSE	Health and Safety Executive
IPS	Informal Priority Setting method
IUCLIDS	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
LC_{50}	Lethal Concentration for 50th percentile
LCA	Life Cycle Assessment

LEAPs	Local Environment Action Plans
LOAEL	Lowest Observable Adverse Effect Level
LOEC	Lowest Observable Effect Concentration
MATC	Maximum Acceptable Toxicant Concentration
NC EHS	National Centre for Ecotoxicology and Hazardous Substances
NOAEL	No Observable Adverse Effect Level
NOEC	No Observable Effect Concentration
NONS	Notification Of New Substances
OECD	Organisation for Economic Co-operation and Development
PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
PPE	Personal Protective Equipment
(Q)SAR	(Quantitative) Structural Activity Relationship
RA	Risk Assessment
RCR	Risk Characterisation Ratio
RPE	Respiratory Protective Equipment
SETAC	Society of Environmental Toxicology and Chemistry
SNIF	Standard Notification Interchange Format
STP	Sewage Treatment Plant
TGD	Technical Guidance Document
UVCB	Substances of Unknown or Variable Composition, complex reaction products or Biological material
WAF	Water Accommodated Fraction
WWTP	Waste Water Treatment Plant

24 Month Dissertation

ENVIRONMENT
AGENCY

BRUNEL
UNIVERSITY

Engineering Doctorate in Environmental Technology

24 Months Dissertation

1st October 1999

By
Nik Robinson

Contents

Executive Summary

A two-year review of the industrial research completed in the first half of the author's Engineering Doctorate course is presented.

This dissertation comprises a general introduction to the industrial sponsor for this research: the Environment Agency and the National Centre for Ecotoxicology and Hazardous Substances (NCEHS) where the research is being performed. Also presented is a review of progress and work during the first 24 months of the course. Proposed research and a work plan of for the remaining two years is outlined and considered.

Research Title

The development and harmonisation of risk assessment procedures to help evaluate the marketing, use and environmental impact of toxic substances

Goals and Objectives

Through an understanding of the existing risk assessment systems, the author will propose areas and methods for developing and harmonising existing practices to ensure environmental protection without unnecessary cost to industry.

An initial goal of this research was to gain a full understanding of the existing risk assessment systems and their methodologies. Time was spent with each of the main functions in the NCEHS who perform environmental risk assessments:

Chemical Assessment Unit (CAU) –

Assesses EU Notifications for the UK in which a risk assessment is performed for all "new substances" prior to marketing, "existing substances" being assessed to a similar standard retrospectively on a priority basis.

Environmental Toxicology Section (ETS) –

Provides an ecotoxicological information service and oversees the setting and implementation of Environmental Quality Standards (EQSs): hazard based assessments required by EU for List I and List II substances in the Dangerous Substances Directive.

Direct Toxicity Assessment (DTA) –

Direct Toxicity Assessment (DTA) considers and assesses the toxicity of mixtures and whole effluents rather than on a single substance basis. A demonstration programme is currently running to assess the use and implementation of DTA as a risk assessment tool.

From this comprehensive understanding of the strengths and weaknesses of risk assessment systems there will be an opportunity to highlight overlaps and areas for improved practices.

Contribution to Knowledge

My contribution to knowledge shall primarily be in the area of risk assessment. Novel approaches and methodologies will be researched, detailed and documented. New practices in risk assessment and improved systems and methodologies will be outlined, while ensuring systems and methodologies are:

- Transparent to both implementers and users
- Protective of the environment
- Not over regulating or protective, resulting in excessive cost to industry

An understanding of the context of the research will be necessary and demonstrated in the transparent nature of the developed systems, due to their use by industry and scientists at different levels. Novel systems and methods will be developed, ensuring good use of data and knowledgeable interpretation of results.

This research is at the core of the NCEHS's activities. As such, environmental technology will be demonstrated through the construction of novel risk assessment practices that, while still ensuring protection of the environment, do not over-regulate and are workable for both regulators and industry.

Two projects proposed for the remaining two years of research are:

- *Sensitivity analysis of the Predicted Environmental Concentration (PEC) side of the risk characterisation calculation as part of the EU Notification Process*

By highlighting the most sensitive values in the PEC calculation, further testing can be directed towards the variables which have the greatest effect on the result. These findings will influence the environmental exposure calculations in other risk assessment systems.

- *Desk study to compare the application of existing and DTA controls on a mixed effluent using real discharges of fully characterised effluents for the case study*

The data for this study are available and will help to show where the strengths and weaknesses in the DTA form of control lie in comparison with standard single substance control measures. The results of this work will help to effectively focus the targeting of the DTA tool to discharges.

Methodological Approach

By first analysing and then comparing and contrasting the different systems and methodologies employed in the risk assessment of substances, areas of overlap and synergy will be emphasised. In the event of overlaps, possible options for harmonising and rationalising these systems will be examined and subsequently the most applicable solution will be investigated and proposed.

Sensitivity analysis will be used to assess the variables used in risk assessment calculations, and will allow refinement inorder to reduce uncertainty, to be targeted towards the most sensitive values in a calculation.

The various control systems and methods will be compared for real effluents and discharges in real situations by analysing case studies and direct comparisons based on both literature and field data.

Peer Reviewed Papers

Both project proposals outlined above will produce results and findings that can be published in academic, peer reviewed journals. It is likely that both papers would be aimed at the Society for Environmental Toxicology and Chemistry's (SETAC) journal 'Environmental Toxicology and Chemistry'.

There are publishable findings in the work completed on the Kennet & Avon Canal Incident. The possibility of publishing areas of this work will be considered. However the sensitivity of the information, whether it must remain internal to the Agency and which publications would be suitable for these findings, is unknown at this stage.

1 Introduction

This report is a two-year review of the industrial research completed in the first half of the author's Engineering Doctorate course. This dissertation replaces the six-monthly report for this period, but also stands as a complete document, with a general introduction to the industrial sponsor for this research, the Environment Agency and the National Centre for Ecotoxicology and Hazardous Substances (NCEHS) where the research is being carried out.

1.1 The Environment Agency

The Agency is a non-departmental public body established by the Environment Act 1995. The Agency became operational on the 1st April 1996 from which point it took over the functions of its predecessors – the National Rivers Authorities, Her Majesty's Inspectorate of Pollution, Waste Regulation Authorities and associated sections of the former Department of the Environment. The Agency's approach is a holistic, multi-media approach. This is the first of its kind in Europe with operations being divided into seven main functions:

- Pollution Control
- Water Resources
- Flood Defence
- Fisheries
- Navigation
- Recreation
- Conservation

The Agency's overall aim is to protect and enhance the whole environment and contributes to the worldwide environmental goal of Sustainable Development, which is defined as (Brundtland, 1987):

"Development that meets the needs of the present without compromising the ability of future generations to meet their own needs".

The Agency has head offices in London and Bristol and eight Regional offices across England and Wales. The Regions are then sub-divided into Areas. This structure resulted in expertise being dispersed and in order to counteract this, national "Centres of Excellence" were set up, one of which is the National Centre for Ecotoxicology and Hazardous Substances (NCEHS), with whom this research project is based.

The NCEHS comprises of a business group and five scientific groups:

- Chemical Assessment Unit
- Direct Toxicity Assessment
- Environmental Toxicology
- Nutrients
- Pesticides

Appendix 7.1 shows an organisational structure for the NCEHS.

1.2 The Research

1.2.1 Title

The development and harmonisation of risk assessment procedures to help evaluate the marketing, use and environmental impact of toxic substances

1.2.2 Goals and Objectives

Before considering the development and harmonisation of existing environmental risk assessment systems, a full understanding of these systems and their methodologies was required. The purpose of the first half of this research program was to investigate and understand the existing systems for risk assessment of toxic substances in the environment. This results focus on three of the main functions within the NCEHS,

- The Chemical Assessment Unit (CAU)
- The Environmental Toxicology Section (ETS)
- The Direct Toxicity Assessment Section (DTA).

The main business areas of each of these groups are outlined below together with the environmental risk assessment systems, which are implemented. In developing a comprehensive understanding of these risk assessment systems the strengths and weaknesses can be highlighted, and areas where there are overlaps and opportunities for improved practices identified.

CAU

The CAU is part of the joint UK Competent Authority (CA) along with the Health and Safety Executive (HSE). The EU Notification Process requires any company marketing a chemical in the EU to indicate this intention to the local CA and supply basic physical, chemical and toxicological data prior to marketing.

Using the data supplied as part of the notification, the CAU perform an environmental risk assessment to assess whether there is a cause for concern.

ETS

This Section provides an ecotoxicological information service to support the Agency and its customers and helps develop Environmental Quality Standards (EQSs). In addition to these two areas the section also works on various ecotoxicology projects and policy guidance (e.g. endocrine disrupting substances and the Groundwater Regulations).

The Environmental Toxicology Advice Service (ETAS) is utilised by the Areas and Regions within the Agency mainly on an operational basis, with support and information being requested in the case of pollution incidents etc. It was through this service that the NCEHS originally became involved in the Kennet & Avon pollution incident where large fish mortalities was caused by an unidentified pollutant.

The EQS system sets limits for the concentration of chemicals in receiving waters based on water quality standards. The system requires a complete review of all available ecotoxicological data on the substances. From this data a hazard-based assessment of the chemical is made.

DTA

The DTA group primarily develops methods, tests and guidance for direct toxicity assessment. The DTA approach to risk assessment is to measure the whole toxicity of mixtures and effluents, thus implicitly measuring any additive or synergistic effects in the mixture. The DTA Demonstration Program, a collaborative project, is intended to test and demonstrate the use of the DTA method and proposed protocol as developed by the DTA Steering Group (Tinsley 1998).

These risk assessment systems can be broadly divided into two groups: substance-specific and whole-effluent assessments.

Substance Specific Assessments:

There is the EU Notification system, which is predominantly a pre-marketing assessment system, which considers the risk of chemicals before they reach the market. The EQS system is also a substance-specific control system, although it is more a hazard-based assessment (fate, behaviour etc. are not explicitly considered). Discharge consents and IPC (soon to be superseded by IPPC[†]) authorisations are also substance-specific controls, the latter targeting emissions on a process basis. Discharge consents as outlined in the Water Resources Act 1991 are directed solely towards water emissions. Although the effects of these Regulations are taken into consideration they will not be studied in-depth.

Whole Effluent Toxicity Assessments:
Instead of measuring single substance effects (it being rare for substances to be discharged singly), the whole effluent, or whole sample is assessed. Problems arise here with the temporal heterogeneity of effluents, and therefore depending on the discharge, profiled testing and assessment needs to be performed.

There is little comparative work on the various risk assessment systems, and although there is much work carried out on developing new bioassays and Quantitative Structure Activity Relationships (QSARs[‡]), the comparative assessment of models and systems and sensitivity analyses of the variables used in these seems to be poorly reported. This research aims to compare the various assessment systems and models and to highlight and suggest methods for their improvement.

1.2.3 Contribution to Knowledge

My innovation and contribution to knowledge shall primarily be in the area of risk assessment. Through the initial study of the existing systems, their strengths, weaknesses and possible synergies will be outlined. Novel approaches and methodologies will be researched, and proposed, generating newly improved, risk assessment practices, systems and methodologies. In the proposal of these new risk assessment practices, particular consideration will be made to ensure systems and methodologies are:

- Transparent to both implementers and users
- Protective of the environment
- Not over regulating or protective, resulting in excessive cost to industry

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[†] IPPC authorisations are required on all new processes covered by the regulations from 31st October 1999, all existing processes must have completed IPPC authorisations by the same date in 2005.

[‡] Relationships used to predict physicochemical and ecotoxicological parameters for substances from their chemical structure in the absence of primary data.

There is a necessity to understand the context of the research and this will be demonstrated in the transparent nature of the developed systems, due to their use by industry and scientists at different levels. An understanding of the scientific context will be demonstrated in the application of the novel systems to ensure the protection of the environment, through good use of data and knowledgeable interpretation of results. Also, the commercial and social context will be considered; being careful not to over regulate, or over protect, as well as constructing transparent methodologies and systems to ensure easy application and use.

This research is at the core of the National Centre for Ecotoxicology and Hazardous Substances' activities. As such, environmental technology will be demonstrated in the construction of novel risk assessment practices that, while ensuring protection of the environment, do not over regulate and are workable in industry.

Two projects that are proposed for the 2-years of remaining research are:

- *Sensitivity analysis of the Predicted Environmental Concentration (PEC) side of the risk characterisation calculation as part of the EU Notification Process*

By highlighting the most sensitive values in the PEC calculation, further testing can be directed towards variables and parameters that have the greatest effect on the result. These findings will influence the environmental exposure calculations in other risk assessment systems.

- *Desk study to compare the application of existing and DTA controls on a mixed effluent using real discharges of fully characterised effluents for the case study*

The data for this study is available and will help to show where the strengths and weaknesses in the DTA form of control lie in comparison with standard single substance control measures. The results of this work will help to most effectively focus the targeting of the DTA tool to discharges.

1.2.4 Methodological Approach

By first analysing and then comparing and contrasting the different systems and methodologies employed in the risk assessment of substances, areas of overlap and synergy will be highlighted. Where there are overlaps, examination of the possible options for harmonising and rationalising these systems will be made, and through detailed consideration the most applicable solution proposed.

Sensitivity analysis will be used to assess the variables used in risk assessment calculations, and will allow uncertainty refinement to be targeted towards the most sensitive values in a calculation.

Through case studies and direct comparisons based on both literature and field data the various control systems and methods will be compared for real effluents and discharges in real situations.

1.2.5 Reports and Papers

Various reports have been completed during the course of this research to date, most notably the report on the CAU and the report on the NCEHS Involvement in the Kennet & Avon Canal Incident. These pieces of work are mentioned in later sections where relevant and can be found in the author's Engineering Doctorate portfolio.

Both of the areas of work proposed above for the last half of this research should produce results and finding that can be published in academic, peer reviewed journals. It is likely that both papers would be targeted at the Society for Environmental Toxicology and Chemistry's (SETAC) journal 'Environmental Toxicology and Chemistry'. There are also publishable findings in the work completed on the Kennet & Avon Canal Incident. The possibility of publishing areas of this work will be considered. However, the sensitivity of the information, whether it would have to remain internal to the Agency and which publications would be suitable for these findings, is unknown at this stage.

In line with the Agency's policy on printing and reports, this dissertation and all assignments and reports have been printed on paper produced from one hundred percent recycled and chlorine-free pulp, and most recently, where possible are printed double-sided.

2 Review

This section reviews and considers the work completed in the first two years of this research programme. A retrospective Gantt chart showing how the time was split in the first two years can be found in Appendix 7.2. A Gantt chart outlining the proposed work plan for the remaining two years can be found in section 4.

2.1 Objectives and Goals

Box 1 (page 13) outlines agreed long-term aims and overall objectives.

The comparison of manual vs. EUSES risk assessments was examined while with the CAU and this was documented in the report on that section. The methodology and implementation of DTA is currently being considered and some areas of this work were presented in the author's poster presentation at the following:

- SETAC UK National Annual Conference 7-9th September 1999, Cardiff
- Engineering Doctorate Conference 14-15th September 1999, University of Surrey

Proposals for work on conducting sensitivity analyses on risk assessment calculations and models have been made for the next period, as well as the comparison of different risk assessment systems through the use of case studies.

- To understand toxic modes of action

  For aquatic life there are only between 8 and 12, toxic modes of action, and therefore if chemicals' mode of action can be assessed, cumulative effects may be able to be considered.

- To become accustomed to the methods of direct toxicity assessment

  This would mean that the toxicity of whole effluent samples would be considered. It would probably take longer and involve more work, but would be more protective of the environment.

- To conduct sensitivity analysis using case studies

  Sensitivity analysis needs to be carried out on all risk assessment processes to see which steps prove to be the sensitive ones and where assessment factors have the greatest effect on the final assessment figures.

- To compare manual vs. EUSES risk assessment calculations

  As was previously mentioned, EUSES has its problems for risk assessment compared with manual assessments, which possibly indicates that manual assessments are too site specific.

- To consider site specific vs. generic risk assessment

  Which method of risk assessment leads to greater protection of the environment? Is there a place for both in risk assessment practices?

- To compare risk assessments conducted in the CAU vs. ETS

  Draft assessment documents are available for nonylphenol, acrylomide, tri-/per- chloroethylene and acetonitrile, which have been conducted under each system. What does a comparison of the results suggest? Is either method more protective than the other, and are the results of one as applicable to the customers of the other results?

Box 1 - Long Term Aims and Objectives of Research

2.2 The Chemical Assessment Unit

The first period of this research was spent working within the Chemical Assessment Unit (CAU), who perform risk assessments on new and existing chemicals for the EU Notification system, as part of the joint UK Competent Authority (CA) along with the Health and Safety Executive (HSE). The aims and objectives that were agreed for the time spent within the CAU are outlined in Box 2 (below).

- To develop an understanding of the current EU Notification system
  - To understand the methodology
  - To understand the models applied
- To become accustomed to the workings of the computer programme EUSES
- To select the necessary data from notification dossiers for use in comparative risk assessments
- To compare the results of manual and (EUSES) computer-conducted risk assessments
- To complete a preliminary report on the activities of the Chemical Assessment Unit

Box 2 - Aims and Objectives for Work Within the CAU

The EU Notification Process as outlined in the 1967 Dangerous Substances Directive, (67/548/EEC) and most recently it's 7th Amendment, requires any company marketing a chemical in the EU to indicate this intention and supply basic physical, chemical and toxicological data prior to marketing under the following classifications:

- New substances
- Existing substances

A new substance is defined as any chemical marketed in the EC after 18th September 1971 (EEC, 1994).

There are then two categories of regulation, and respective lists for substances depending on how the substance is classified:

NONS - Notification Of New Substances regulations
ELINCS – European List of Notified Chemical Substances
ESRs - Notification of Existing Substances Regulations
EINECS – European Inventory of Existing Chemical Substances

Existing chemicals are assessed on a priority basis and of the approximately 100,000 chemicals on the EINECS list only 110 of them are currently being considered.

Any company wishing to market a new chemical substance in the EU for the first time must notify the local country's CA of this intention and supply the required information, including physical and chemical data as well as human and ecological toxicity results. From these data a Risk Assessment (RA) is produced resulting in one of the four conclusions outlined below:

(i) *The substance is of no immediate concern for man or the environment.*

(ii) *The substance is of concern, further information required at next tonnage threshold.*

(iii) *The substance is of concern, further information required immediately.*

(iv) *The substance is of concern, risk reduction recommendations required.*

The approach used to perform these RAs is to calculate Predicted Environmental Concentrations (PECs) and Predicted No Effect Concentrations (PNECs) and then calculate the ratio of these two values (PEC/PNEC) which is termed as the Risk Characterisation Ratio (RCR) for each environmental compartment. If the RCR is greater than 1 that is to say that the predicted concentration in the environment is greater than the predicted no-effect concentration, then further research or risk reduction may be required, as outlined in the conclusions above.

Further research aims to reduce the magnitude of uncertainty inherent in the calculations, which stems from:

- Intra- inter-laboratory variation of physical, chemical and toxicity data.
- Simplicity of and assumptions within exposure models.
- Intra- inter-species variations (biological variance).
- Short-term to long-term toxicity extrapolation.
- Laboratory data to field impact extrapolation.
- Additive, synergistic and antagonistic effects arising from the presence of other substances (not directly accounted for).

The costs of some of the processes required in a notification are outlined below. From this it can be seen that further testing (chronic daphnia or fish test etc.) entails a significant cost to industry:

Process	Approx. Cost
Notification fee	£6,000
Physical-chemical analysis	£5,000
Mammalian toxicity testing	£50,000
Acute aquatic toxicity tests	£3,000 to 5,000
Chronic tests (daphnia)	£12,000
Chronic tests (fish)	£70,000
Pond field test	>£100,000

Table 1 - Cost to Industry of Prossesses Required in a EU Notification

The methodologies involved in the calculation of the PEC and PNEC values are complex and for this reason considerable time was spent in gaining an understanding of them. Each shall now be considered in turn.

2.2.1 Notification System Exposure Assessment

The environment is potentially at risk from exposure to chemical substances at all stages of the substance's lifecycle. For new substances, no measured levels of the chemical in the environment will be available for obvious reasons, therefore the concentration of a substance that is likely to enter the environment must be estimated. A Predicted Environmental Concentration (PEC) is calculated, primarily using data supplied by the producers and importers of a substance in the 'base set' (see Table 2 page 17 for 'base set' information) of physical-chemical and ecotoxicological data. Data from emission scenario documents (data on generic emission properties by industry type) are also used. The following lifecycle stages are principally considered in the assessment procedure:

- Production
- Processing
- Formulation
- Use (industry/trade/consumer)
- Transport and storage
- Disposal, (inc. waste treatment)

Base Set Information	
0	Manufacturer and notifier identity and location of production site
1	Identity of the substance 1.1 Name 1.2 Molecular and structural formula 1.3 Composition of substance 1.4 Methods of detection and determination
2	Information on the substance 2.0 Production 2.1 Purpose of use 2.2 Estimated production/imports 2.3 Recommended precautions 2.4 Emergency action in case of spillage 2.5 Emergency action in case of injury 2.6 Packaging
3	Physiochemical properties 3.0 Standard state 3.1 Melting point 3.2 Boiling point 3.3 Relative density 3.4 Vapour pressure 3.5 Surface Tension 3.6 Water solubility 3.8 Partition Coefficient o/w 3.9 Flash point 3.10 Flammability 3.11 Explosive properties 3.12 Self-ignition temperature 3.13 Oxidising properties 3.15 Granulometry
4	Toxicological studies 4.1 Acute toxicity 4.2 Repeated dose 4.3 Other effects
5	Ecotoxicological studies 5.1 Effects on organisms 5.2 Degradation 5.3 Sorption tests
6	Possibility of rendering substance harmless 6.1 For industry/skilled trades 6.2 For the public at large
7	Risk Assessment
9.1	Declaration of unfavourable effects on man and environment
9.2.1	Proposed classification and labelling
9.2.3	Proposed safety data sheet

Table 2 – Structure of base set information (EEC, 1994)

For the purpose of calculating local and regional scale PEC values a standardised generic environment has been defined to allow risk characterisation at the EU level. For this environment, default values have been set for properties such as the density of the solid and water phases and air; temperature (12°C); and various other characteristics of the soil, sediment and other environmental compartments. The model used to describe the environment is called a 'multimedia compartment model' such as in the diagram below (Van Leeuwen and Hermens, 1995). These models represent the environment as a set of spatially homogenous (zero dimensional) boxes, one box for each compartment, and the degradation and transfer of chemicals between these boxes is modelled. Most models use six compartments to describe the environment (Air, Land, Water, Sediment, Groundwater and biota).

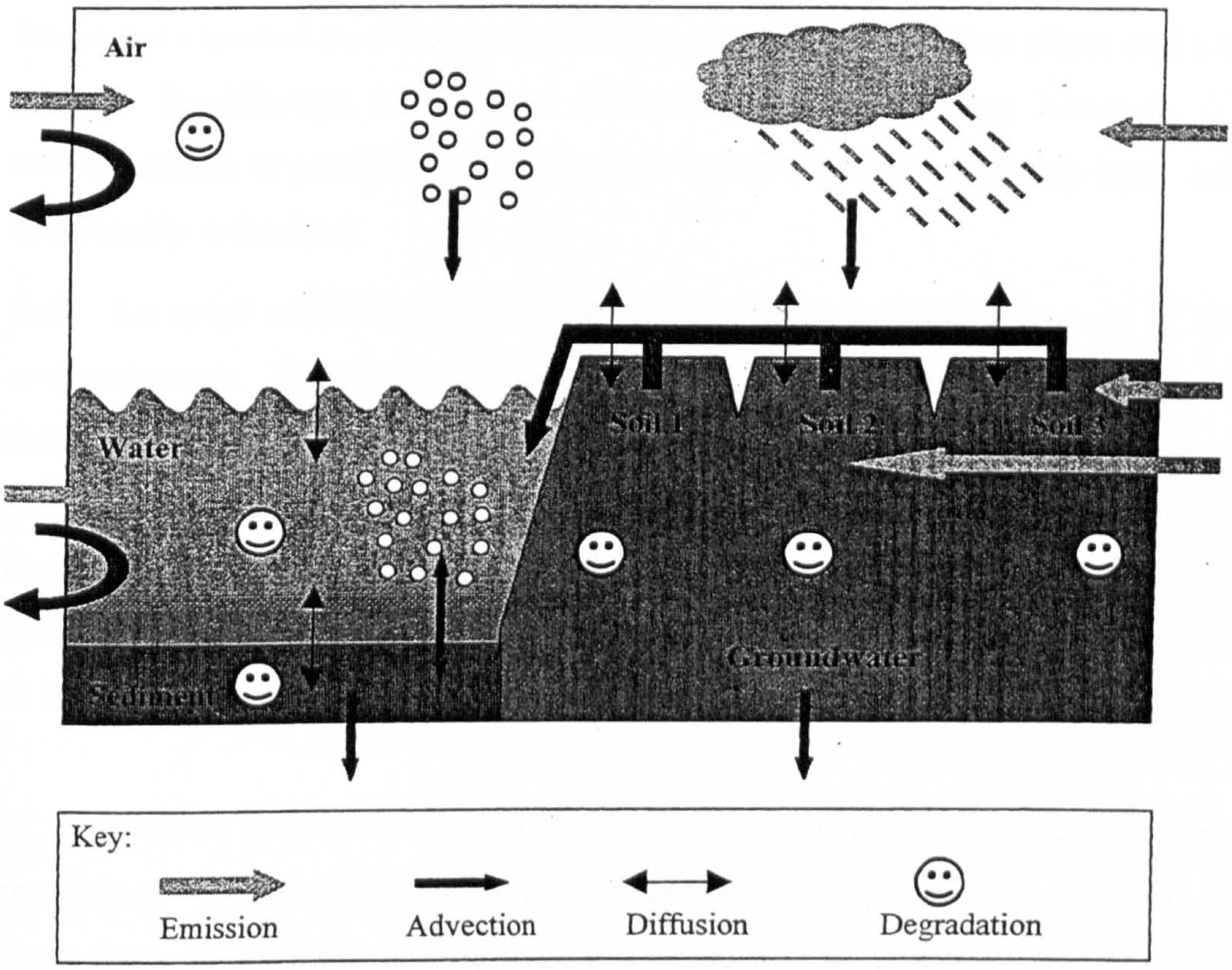

Figure 1 - Regional environmental compartment model (as EEC, 1994)

The six environmental compartments are defined in more detail below:

1) Air - is a bulk compartment, consisting of a gas phase, an aerosol and a rainwater phase. Airflow (wind), evaporation (from soil and water), wet and dry deposition, and degradation all influence the concentration of substances in air.

2) Aquatic - the truly dissolved state of a substance. Colloidal or macromolecular materials are considered to be part of the compartment's suspended matter and biota. These phases influence the fate of chemicals by binding the substance and preventing mass transfer and degradation processes in the aquatic phase. Suspended matter acts as a physical carrier across the sediment-water interface.

3) Suspended matter - all abiotic colloidal or macromolecular materials that are not truly dissolved. There is a continual flux across the sediment-water interface through sedimentation and re-suspension.

4) Aquatic Biota - This compartment refers to all living organisms in the aquatic compartment, from bacteria to mammals. The compartment is small and usually plays an insignificant role with regard to the overall fate of a chemical.

5) Sediment - treated as a bulk compartment, consisting of a water phase and a solid phase. Equilibrium is assumed between these two phases, however, if the sedimentation of particles is greater than the re-suspension this top layer will be continually refreshed.

6) Soil - the most stationary, and therefore most spatially inhomogeneous of all the compartments. The fate of chemicals is largely dependent on the characteristics that vary so widely between soil types. Soil use also affects chemical loading. A single compartment is not usually sufficient in multimedia chemical fate models, therefore soil is subdivided into natural soil (Soil 1), agricultural soil (Soil 2) and industrial soil (Soil 3). Usually only the topsoil layer is considered, and assumed to be homogeneous in as far as there is no variation in concentration with depth.

These multimedia models are based on the concept of partitioning and the relative concentrations of chemicals in each compartment at equilibrium. Fugacity (the tendency for a chemical to escape from the phase it is in) is also used to model this partitioning (Campfens & MacKay, 1997; Clark *et al.* 1995; Diguardo *et al.* 1994). The results from the multimedia model are steady-state concentrations, which can be regarded as estimates of long term, average exposure levels.

The following equations outline the calculation of the $PEC_{aquatic}$ and are an area where sensitivity analysis and further work can be focused, see section on Proposed Future Research for details.

$$PEClocal_{aquatic} = Clocal_{water} + PECregional_{aquatic}$$

Equation 1

$PEClocal_{aquatic}$	Predicted environmental concentration during episode	$(mg.l^{-1})$	
$Clocal_{water}$	Local conc. in surface water during emission episode	$(mg.l^{-1})$	Eq. 2
$PECregional_{aquatic}$	Regional concentration in surface water	$(mg.l^{-1})$	*

* regional PEC value calculated from tonnage production/imported and use category.

$$Clocal_{water} = \frac{Clocal_{eff}}{\left[1+\left(Kp_{susp} \times SUSP_{water} \times 10^{-6}\right)\right] DILUTION}$$

Equation 2

$Clocal_{water}$	Local conc. in surface water during emission episode	$(mg.l^{-1})$	
$Clocal_{eff}$	Concentration of chemical in STP effluent	$(mg.l^{-1})$	STP data
Kp_{susp}	Solid-water partition coefficient of suspended matter	$(l.kg^{-1})$	Eq. 3
$SUSP_{water}$	Concentration of suspended matter in river	$(mg.l^{-1})$	15 default
DILUTION	Dilution factor (from river flow)	(-)	10 default

$$Kp_{susp} = Foc_{susp} \times Koc$$

Equation 3

Kp_{susp}	Partition coefficient solid-water in suspended matter	$(l.kg^{-1})$	
Koc	Organic carbon-water partition coefficient	$(l.kg^{-1})$	base set/QSAR
Foc_{susp}	Weight fraction of organic carbon in compartment	$(kg.kg^{-1})$	0.1

By taking an in-depth look at these equations and considering the relationship between various parameters and variables i.e. vapour pressure, Koc, Kow and other partition coefficients, multivariate analysis can be used to test the sensitivity of default values and those supplied as part of the base set. This information will help direct efforts and expenditure in refining the PEC calculation values.

2.2.2 Notification System Effect Assessment

The notification system aims to protect the aquatic and terrestrial ecosystems, top predators, microbial activity in a STP, and the atmosphere. Ideally for each system a Predicted No Effect Concentration (PNEC) would be directly calculated. A PNEC being the predicted concentration below which an unacceptable environmental effect will not occur. The PNEC is calculated by dividing the lowest short term (LC_{50}, median lethal concentration; EC_{50}, median effect concentration) or long term (NOEC, no observed effect concentration) value by an assessment factor (AF). The AF is used to reflect the degree of uncertainty in extrapolation from a laboratory test on a limited number of species to the "real" environment, the AF used for long term data being less than that for short term due to the reduced uncertainty.

At the 'base set' acute (short-term) ecotoxicological tests are required on three species and trophic levels, algae, daphnia and fish. Below examples are shown of AFs used in the calculation of various PNEC values.

Data Available	Assessment Factor
At least one short-term $L(E)C_{50}$ from each of three trophic levels of the base-set (fish, daphnia and algae)	1000
One long-term NOEC (either fish or daphnia)	100
Two long-term NOECs from species representing two trophic levels (fish and/or daphnia and/or algae)	50
Long-term NOECs from at least three species (normally fish, daphnia and algae)	10
Field data or model ecosystems	Reviewed on a case-by-case basis

Table 3 – Assessment Factors for Aquatic PNEC Derivation (EEC, 1994)

Data Available	Assessment Factor
$L(E)C_{50}$ short-term toxicity tests, (e.g. plants, earthworms, or micro-organisms)	1000
NOEC for one long-term toxicity test (e.g. plants)	100
NOECs for additional long-term toxicity tests of two trophic levels	50
NOECs for additional long-term toxicity tests for three species of three trophic levels	10
Field data or model ecosystems	Reviewed case-by-case

Table 4 - Assessment factors for soil PNEC derivation (EEC, 1994)

The actual PNEC value is then calculated as shown in Equation 4 (below):

$$PNEC_{comp} = L(E)C_{50\,min} \times AF$$

Equation 4

$PNEC_{comp}$	Predicted No Effect Concentration by compartment	($mg.kg^{-1}$)	
$L(E)C_{50\,min}$	Organic carbon-water partition coefficient	($mg.kg^{-1}$)	base set/QSAR
AF	Weight fraction of organic carbon in compartment	(-)	Table 3-4

The situation is even more complex for sediment PNEC calculation, with ecotoxicity data not always being available for sediment dwelling organisms, in which case the sediment PNEC is extrapolated from the aquatic PNEC value.

$$PNEC_{sed} = \frac{K_{sed-water}}{\rho_{sed}} \times PNEC_{aquatic} \times 1000$$

Equation 5

Where:

$PNEC_{sed}$	Predicted no effect concentration in sediment	($mg.kg^{-1}$)
$K_{sed-water}$	Sediment-water partitioning coefficient	($m^3.m^{-3}$)
ρ_{sed}	Bulk density of suspended matter	($kg.m^{-3}$)
$PNEC_{aquatic}$	Predicted no effect concentration in water	($mg.l^{-1}$)

2.2.3 Notification System Risk Characterisation

Having calculated PEC and PNEC values as part of the exposure assessment and the dose-response assessment, risk characterisation is then conducted. This process involves the calculating of PEC/PNEC ratios or risk characterisation ratios (RCRs as termed in EUSES). The evaluation procedures linked with the testing for the aquatic environment has resulted in a highly structured decision scheme for the aquatic compartment as detailed overleaf (page 23).

One major concern over this system is that initial assessments need to be sufficiently conservative so as to highlight all substances that may be of concern for the environment. This is because once the risk characterisation ratio falls below the level of concern (<1) the substance will not be considered further until its production/import reaches another tonnage level. If a chemical with chronic effects, that is only to be marketed in low quantities, is brought onto the market, having passed the assessment at base set, it is unlikely to be reassessed under the notification system, even though there might actually be cause for concern.

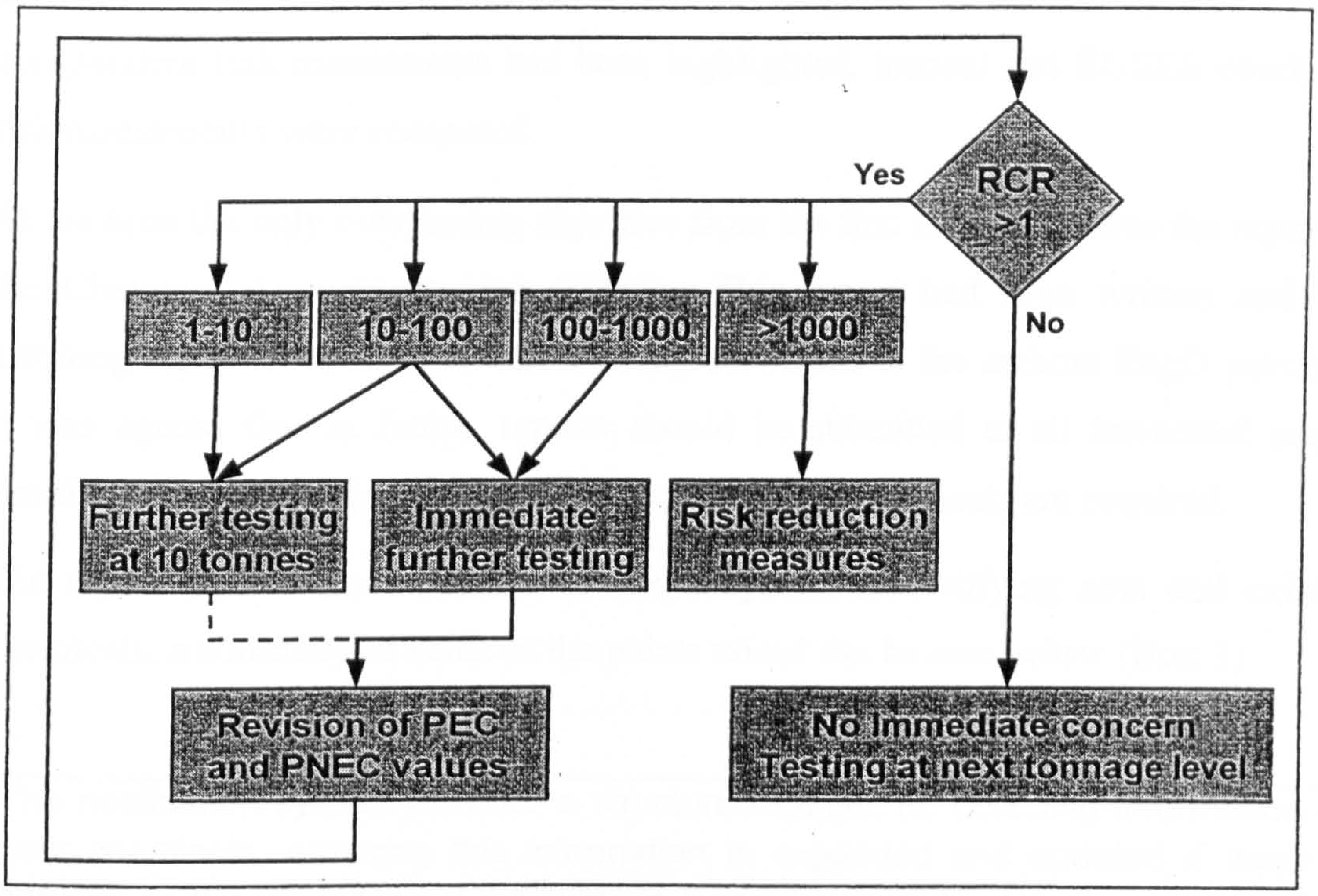

Figure 2 - Risk Characterisation Decision Diagram for the Aquatic Compartment (as Van Leeuwen & Hermens, 1995)

2.2.4 European Union System for the Evaluation of Substances

Considerable time was also spent reviewing the computer system called EUSES, (European Union System for the Evaluation of Substances). The program is intended to be an automated version of the technical guidance documents that accompany the regulations. This computer system contains the necessary models needed to perform the risk assessment of chemicals. However as a result of poor documentation, generic modelling and a lack of transparency in its use, results obtained from the program rarely concur with those produced manually by risk assessors.

The sensitivity analyses as outlined earlier could be performed using the EUSES program. However the lack of access to source code and the lack of transparency of the calculations being performed would make this complicated and findings possibly hard to attribute.

2.2.5 Discussion

A report was prepared documenting work within the CAU and an in-depth look at the risk assessment as part of the EU notification system. The strengths and weaknesses of the system were also discussed. With reference to the agreed aims and objectives, a comprehensive understanding of the EU Notification system was gained and the computer program EUSES investigated. After the required data for comparative risk assessments had been highlighted, manual and EUSES conducted risk assessments were compared.

At the time the only outstanding objective from the first six months was the report on the Chemical Assessment Unit (CAU). This report had been written and was awaiting supervisors' review before being submitted to the authors EngD portfolio. It was agreed that in future, reports should be submitted to all interested parties simultaneously including a reasonable date for when comments are required.

The report on the CAU outlines the EU's system for notifying new and existing chemicals; a summary of some of the points raised can be seen below (Box 3).

> The notification system provides a structured system for obtaining information on new chemicals, ensuring this information is expanded and updated if there is concern or the substance is marketed in a greater quantity. However, the system is not an effective approach to retrospectively gaining the information on the large number of chemicals classed as existing substances.
>
> There are problems with the generic assessment that is performed to allow the results to be accepted throughout Europe, with a need for transparency so that the sensitivity and dependability of values can be seen. One possible refinement would be the splitting of the aqueous compartment, (e.g. Freshwaters, Estuaries, Seas).
>
> There is a bias towards the aquatic compartment, with a need for further research on models for the other environmental compartments (soil, sediment and air) to ensure multi-compartment assessments.
>
> There also needs to be a form of review or update to allow the system to learn from the experience of the assessments that have already been processed. A review of old calculations compared to the new ones where further data has been submitted would indicate whether 'base set' calculations are actually representative in the light of new data. Also trend in species sensitivity, toxicity by industry, etc. could be investigated.

Box 3 - Summary of some of the Key Points Disscussed in the CAU Report

2.3 The Environmental Toxicology Section

The second period of work was spent within the Environmental Toxicology Section (ETS) which provides and runs an Environmental Toxicology Advice Service (ETAS). ETAS supplies information and advice on the impact of chemicals on the environment, including physical and chemical properties, and any EQS, WHO or other limit values that are applicable, to both internal operational staff and external customers. The ETS also co-ordinates the development of EQSs for the Agency. The agreed aims and objectives for the time spent with the ETS are shown in Box 4 (below).

- To familiarise myself with the operations and activities of the Environmental Toxicology Section
- To ascertain the background to and method of producing Environmental Quality Standards
- To review reports on completed Environmental Quality Standards

After the first three months these aims and objectives were refined and added to, to reflect the work that was being carried out on the Kennet and Avon Incident

- Review structured methodology of the EQS system
    - How chemicals are chosen for assessment
    - Data collation
    - Data interpretation
    - What happens after the assessment has been carried out
- To analyse and understand the significance of ecotoxicology endpoints
    - EC_{50}/LC_{50} (mean effect/lethal concentration)
    - NOEC/LOEC (no/lowest observable effect concentration)
    - Their meaning, statistical validity and confidence limits
- To write a report on the National Centre's response and handling of the Kennet and Avon incident
    - Involvement in pollution incident
    - Chemical information, used/needed
    - Point at which National Centre should be informed
    - Thought processes
        - what was needed
        - what was used
        - what else would have been useful
- To identify the learning points from the incident and to develop and propose a management system for coping with incidents

Box 4 - Aims and Objectives for Work Within the ETS

2.3.1 Environmental Quality Standards

On arrival at the ETS the initial aim was to review the structure and methodology of the EQS system and to analyse and understand the significance of ecotoxicology endpoints, including their meaning, statistical validity and confidence limits. In the longer term, strengths and weaknesses were to be identified and comparisons and contrasts made with the CAU's notification system. However the EQS system proved to be less prescribed than the notification system, with many decisions and the interpretation of data being left to "good scientific judgement". The process is far from transparent and it is not always possible to see how the assessment factors used have been derived.

Under the EC Dangerous Substances Directive 76/464/EEC the UK has various obligations to set EQSs. An EQSs being defined as,

> "the concentration of a substance which should not be exceeded in the receiving water in order to protect the use of the water." (Whitehouse & Fawell, 1997)

The EQS for the protection of aquatic life is derived to protect all aquatic species from the available data. All forms of data are consulted and considered in the setting of EQSs, with the lowest reliable and relevant adverse effect concentrations being identified and appropriate extrapolation factors applied.

The available data is critically assessed in terms of reliability and relevance with the emphasis being on experimental test procedures and species used. Primary data (relevant and reliable tests) are used to set the EQS value with secondary data (tests with inadequate detail) being used to support the derived value. Figure 3 (overleaf) details the hazard assessment scheme for the derivation of EQSs.

During the course of this research the possibility of following the process of setting an EQS from the identification of a need for a standard for a substance, through to the final setting of a value, has been highlighted as an area where further time could be spent. The examination of this process would allow the transparency of the decisions made to be assessed and critiqued. The proposed report on the ETS section has not been written, although a review of the system and its methodologies have been completed they have not been documented. It was felt that the slip in this objective had become too great and that it was better to get back on track with the research and revisit this area at a later date.

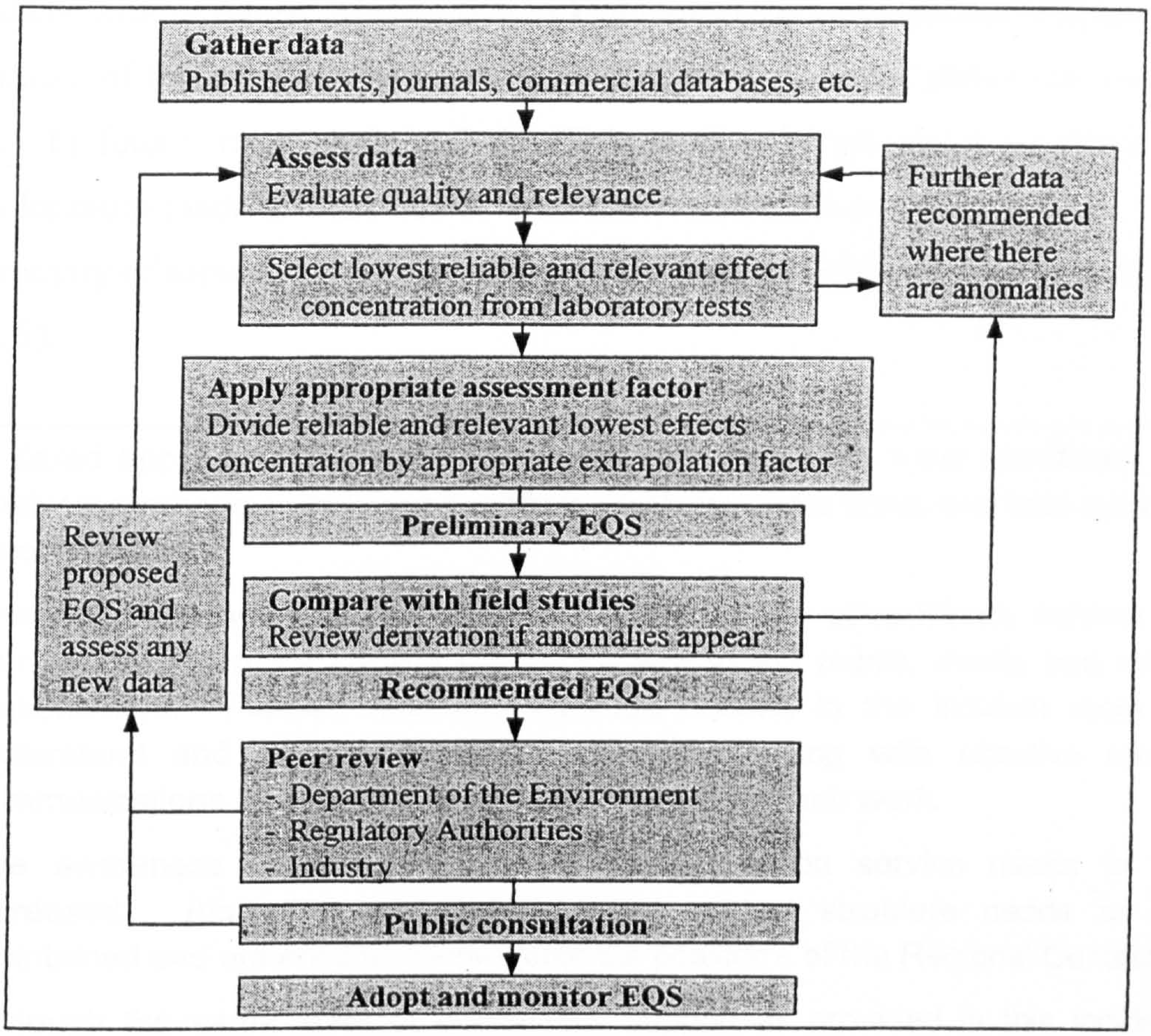

Figure 3 - Hazard Assessment Scheme for the Derivation of EQSs (Whitehouse & Fawell, 1997)

2.3.2 The Kennet & Avon Incident

While with ETS, the group aided a large pollution incident through ETAS. An objective was set for the author to assess the National Centre's contribution to the incident management and to look at how and what could be done in the future.

Originally it was anticipated that one to two months would be spent on this project, however the event which lasted for four weeks on the ground entailed a greater commitment than expected. This extended commitment resulted in slippage of the work on the EQS system and the report on the Kennet and Avon went through much iteration, some points of which are still being disputed within the Agency.

The Kennet and Avon report focused on the management of the incident by the Area office, the NCEHS, as well as input by WRc and other contractors; examining what data was available, and what data was needed and would have helped. The communications and how the NCEHS were contacted, at what levels and how in future they could or should deal with enquiries were all considered. Recommendations are made on how similar incidents of this level could be handled and dealt with in future. However a lack of clear focus and selective analysis at the beginning of this project was partly to blame for the extended period that the work took. In future, clear goals and deadlines need to be set and more importantly considerations made of what will be done if the work starts to overrun.

A summary of some of the key conclusions and recommendations are outlined below (Box 5).

A tiered approach to incident investigations is required, most specifically for analysis methods. This tiered system would then help focus and lead incident investigations.

The communication during incidents needs to be streamlined, helping to convey the Agency's control of the incident to the public, media and other stakeholders. Further, scientific staff are needed in the incident room to understand and convey technical information, along with effective return communications from the incident room to help lead their work.

The awareness of the NCEHS's ETAS information service needs to be increased. Also the hierarchical, tiered contact structure needs to be maintained and adhered to, to reinforce the position's of the Regional Contacts.

Although the same level of information support as provided in this incident would have been possible further afield such a level of involvement by the NCEHS has ramifications on other work and can result in slippage of other obligations. For this reason the remit of ETAS and its level of support need to be clarified and communicated to its customers.

Computer processing of data obtained from routine monitoring could search for potential pollution problems and areas of concern and highlight these "hot spots". Also a combination of several existing databases of chemicals and their physical, chemical and ecotoxicological properties, could be used to generate a large database for querying, using known properties in a pollution incident to generate a target list of chemicals to help direct and lead analyses and investigations.

Box 5 - Key Conclusions and Recommendations from the Kennet and Avon Incident Report

2.4 The Direct Toxicity Assessment Section

Direct Toxicity Assessment (DTA) involves an assessment of the potential harm of whole samples. The effects of all substances present together in a sample are examined, providing a more holistic assessment than substance specific measures. Such an approach implicitly considers the additive, antagonistic and synergistic effects of chemicals in a mixture. Although DTA has not been used to any extent in the UK to date, there has been extensive use of similar principles, Whole Effluent Toxicity (WET), used in the US by the US EPA. Agreed aims and objectives for work within the DTA are shown in Box 6 (below).

- Direct toxicity assessment – current demonstration programme, methodology, strengths and weaknesses
    - Short report/document on DTA its methods and strengths and weaknesses, as well as other similar programs like the US EPA's WET.
- Ecotoxicology and biological effect measures – Tests, organisms and end-points
    - Short report/document on ecotoxicology, tests, organism and end-points, to ensure understanding.
- DTA as a risk assessment tool – tiered testing programme, how DTA fits in with LEAPs and as a one in a series of RA tools
    - Full report on DTA as a tool and how it fits in with the other risk assessment tools/processes available in ecotoxicology

Box 6 - Aims and Objectives for Work within the DTA

It was agreed that approximately six weeks would be spent on each of the first two areas of study and a longer period of about twelve weeks on the final area of research.

2.4.1 The DTA Method

The DTA method aims to target river catchments, those showing greatest effect, or those showing effects that cannot be explained through chemical analysis alone. The discharges entering the targeted catchment will then be screened to identify those of concern and contributing to the in-stream effects. Then through the use of in-situ bioassays, and through field measurements risk assessments will be made and where necessary Toxicity Reduction Evaluation (TRE) required. Figure 4 (below) details the proposed scheme for risk assessments using DTA.

As already mentioned, DTA implicitly considers any synergistic, additive, antagonistic, etc. effects in the toxic mixture being tested. However, Smith *et al.* (1998) mention Van Loon and Hermens (1995) findings for various chemical mixtures in aquatic systems that, even where toxic synergy or antagonism was present the toxicity of the mixture was generally additive. This would suggest that controlling mixed effluents by single substance controls would attain similar toxicity controls. However DTA does allow effluents that haven't been characterised to be assessed and controlled, and if synergistic effects that were greater than additive were present the DTA approach would ensure the most efficient control of these effluents.

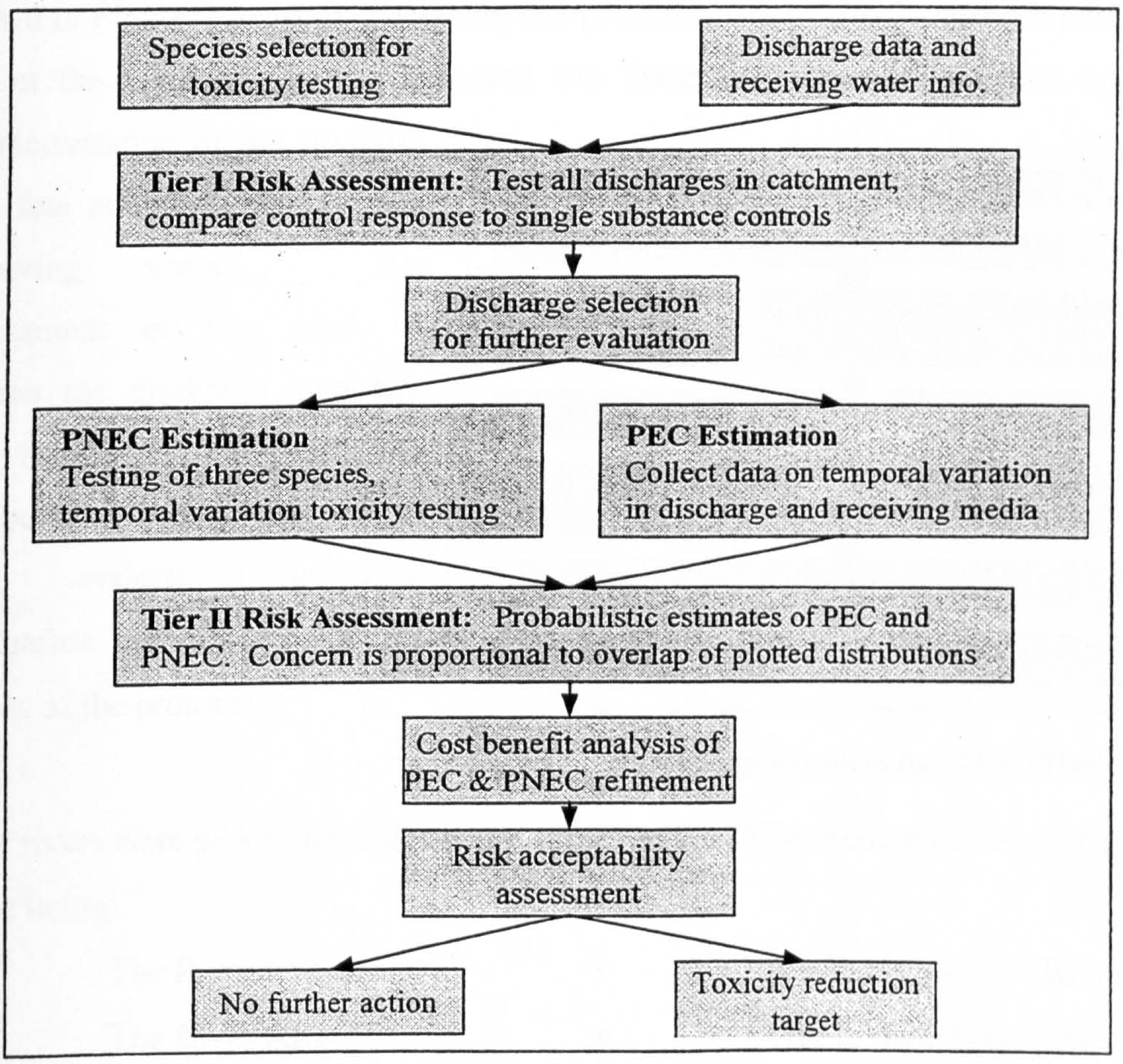

Figure 4 - Proposed Risk Assessment Scheme for DTA (Forrow *et al.* 1998)

2.4.2 The DTA Demonstration Programme

In 1996 a group formed from the Environment Agency, the Scottish Environmental Protection Agency (SEPA) and the Department of Environment Northern Ireland (DENI) produced a consultation document and set up a steering group to demonstrate the use of DTA as a ecotoxicological tool for assessing polluting effluents. The fundamental questions that were to be addressed by the group were:

- How sensitive are the ecotoxicology tests and endpoints used?
- What relevance do these tests and endpoints have to ecological harm?

The group also set out a protocol for the use of the DTA approach, which originally resembled the following steps:

1. DTA used to identify toxicity sources and assess their impact
2. DTA used on a priority basis
3. DTA used to determine reduction in toxic load required

This then progressed into a four-stage and more recently a seven-stage protocol as shown in Figure 5 (below). Selection and prioritisation of discharges are still carried out at the beginning of the protocol, but there are separate steps to cover the characterisation of the toxicity, and fate and dispersion in the receiving waters. An assessment of the need to reduce the discharge step has now been incorporated into the protocol, before moving on to the toxicity reduction evaluation and implementation stages of the protocol.

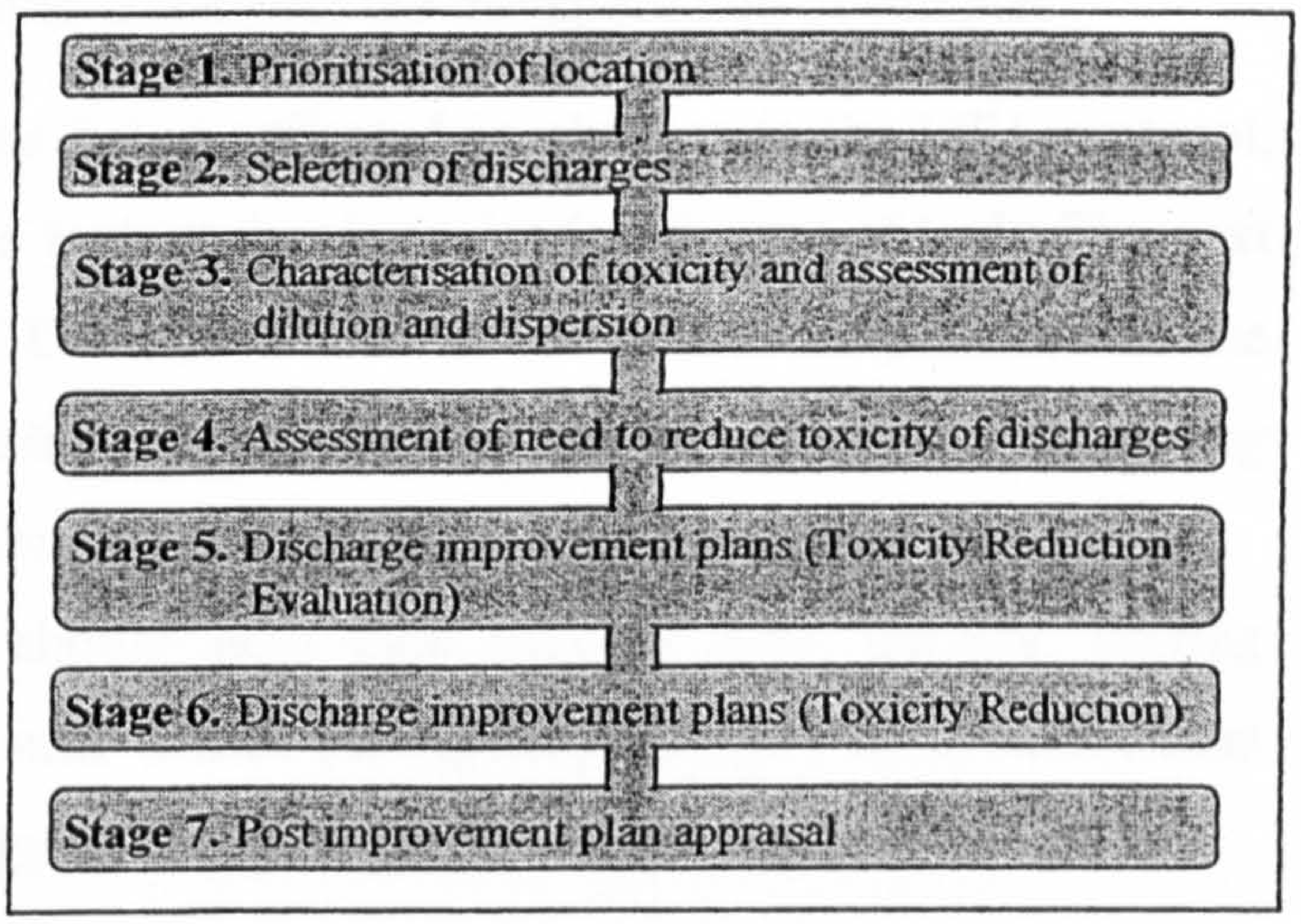

Figure 5 - Seven-Stage Protocol for DTA (Tinsley, 1998)

Four rivers were picked for assessment as part of the DTA demonstration programme these being:

- The River Esk
- The River Aire
- A tributary of the River Spey
- The Lower Tees Estuary

The first two stages of the protocol were completed for the Aire and Esk projects first. The Aire project was closed however in late '98 - early 1999 due to a lack of toxicity being found in the initial assessments. The Spey project was postponed and further work is unlikely in the light of the other projects. The Tees project commenced late '98 - early 1999 with 12 discharges being screened for the magnitude and distribution of toxicity.

The lessons that the group feel have been learnt already in the demonstration program are as follows:

- Early screening of discharges is vital to ensure efficient use of resources
- There is a need for synchronised testing of chemistry, biology and fisheries to ensure the data is current
- Culturing difficulties are experienced with some levels of water hardness
- There is a poor correlation between daphnia test results and chemical and biological luminescence test results, possibly requiring a larger test battery
- Inter laboratory variation has been low using the rapid daphnia tests showing good accuracy
- Courier services are variable and affect the transportation of samples

These along with other points are being reflected in changes in the DTA protocol, Figure 4 addresses DTA from the factors that have lead to the use of tool. The next step towards implementation of DTA as a tool in the control of pollution in the environment will involve demonstrating how the tool can be integrated into existing control systems and educating industry and regulators in is use and value.

The demonstration programme should help gain support from industry, leaving education of Area and Regional staff within the Agency, along with Environmental Protection Officers (EPOs) as a significant goal towards future implementation.

2.4.3 The DTA Demonstration Programme

The first short report was completed and submitted for comments. The second short report is in-progress, and the final report on DTA is to be completed soon. Many of the findings and thoughts from the work in the DTA section were reported in the poster presented at the SETAC and EngD conferences in September 1999. A copy of this poster can be found in Appendix 7.3.

2.5 Conference

Although not strictly part of this research a major commitment during the first twelve-month period was to the Project Management elective module undertaken, involving two Research Engineers organising the 1998 Engineering Doctorate Conference. This required far more time than was suggested or appreciated. The Conference that took place in September 1998 had been in the planning stages since March, and the final report on the project management exercise was completed for the end of November. Great experience was gained throughout the project, in managing meetings and effective minute taking and agenda setting. Delegation became a necessary skill as did overall clear organisation and communication with students, academic and industrial contacts. In Box 7 (below) a brief outline of the main recommendations can be found.

- From feed back forms the general view was that the conference was above average. Delegates noted in particular the conference facilities and the quality of oral presentations and panel discussions as good to excellent.

  "High standard of presentation, posters good but could be improved"
- Poster presentations were a little cramped and presenters should be by their posters at appropriate times. Colour coding of poster presentations by subject area was also though to be a good idea.
- The possibility of 2nd or 3rd year Research Engineers making oral presentations was also discussed, and would lead to the presentation of more detailed research.
- The introduction of keynote addresses was received well, although keynote speakers need to be fully briefed on the requirement upon them.

Box 7 - Summary of Recommendations from 1998 Conference Report

2.6 Progress Towards EngD Aims and Objectives

The aims and objectives of the Engineering Doctorate course, as taken from the EngD Joint Regulations (Section 2.1) are summarised in two tables in this section. Tables 5 outlines the attributes required to be demonstrated and progress towards these to date, while Table 6 indicates how it is thought that these attributes will be demonstrated in the remaining two years of research.

Aims and Objectives of EngD Programme	How Attributes Have Been Demonstrated
REs should:	
(i) be equipped as engineering research-designers to plan and lead flexible and innovative R&D programmes that respond to customers' needs.	The work on the Kennet & Avon incident demonstrated flexibility, and good interpersonal skills, particularly evident in the continuing discussions. A consideration of customers' needs has been demonstrated in the clear way in which complex issues were expressed.
(ii) be able to work effectively, and to form, work within and where necessary lead teams with a multi-disciplinary background to tight time schedules.	Work on the 1998 EngD Conference required good leadership and teamwork skills while considering real time and budgetary constraints. Also the research in the DTA section has involved working with multi-disciplinary teams including ecotoxicologists, biologists and section and business managers, all having inputs and constraints on the work.
(iii) possess comprehensive expert knowledge of the field of Environmental Technology, of techniques needed to balance social and economic benefit against resource utilisation and environmental impact, and of the processes of technology transfer needed to ensure the application of research into practice	Expert knowledge of environmental technology and in particular risk assessment, ecotoxicology and environmental legislation is of great importance in my research. I need to balance not only social and economic but also environmental benefits, in all aspects of my work, in the Kennet and Avon Incident, both economical costs and environmental cost had a pronounced effect on the chosen actions and solutions. Finally, methods of technology transfer, have been demonstrated in the clear and concise way in which my findings, and conclusions have been presented both in the CAU and Kennet and Avon Incident reports.
(iv) have demonstrated ability for originality and for innovation	A decision tree diagram was used in the Kennet and Avon report to communicate the actions and reactions of the incident in a novel way.
(v) possess a working knowledge of project management and business methods and their implications for research and development	Many lessons have been learnt in the first two years of this research. The organising of the conference required the rapid learning of effective project management, learning points from which have since been demonstrated in the approach to the organisation of the author's research.
(vi) possess and have demonstrated a high level of communication and presentation skills	The presentation of all work has continued to be of a high standard. Many good constructive points were gained from presenting a poster at the National SETAC conference

Table 5 – Progress to Date Towards Aims and Objectives of the Engineering Doctorate

Aims and Objectives of EngD Programme	How Attributes Have Been Demonstrated
REs should:	
(i) be equipped as engineering research-designers to plan and lead flexible and innovative R&D programmes that respond to customers' needs.	The work on the proposed projects will require the demonstration of flexibility and innovation in their approach. Where possible risks and constraints have been highlighted at the proposal stage in order that the research programme may more readily adapt to changing situations e.g. availability of primary data.
(ii) be able to work effectively, and to form, work within and where necessary lead teams with a multi-disciplinary background to tight time schedules.	The proposed CAU sensitivity analysis project will entail dealing with groups internal and external to the Agency. While the EQS/DTA comparative risk assessment project will require close ties to both the ETS and the DTA as well as members of the collaborative DTA steering group.
(iii) possess comprehensive expert knowledge of the field of Environmental Technology, of techniques needed to balance social and economic benefit against resource utilisation and environmental impact, and of the processes of technology transfer needed to ensure the application of research into practice	An appreciation of the social and economic aspects relating to the risk assessment of chemicals will be demonstrated in both proposed projects. Sensitivity analysis of the EU notification PEC calculation, allowing greater understanding and more informed decisions to be made when further testing is required. While a compare and contrast study on the DTA and EQS risk assessment systems for real effluents will help to strength and support the use of the most effective system for given circumstances. Technology transfer will also be of great importance, to ensure the proper use of risk assessment systems and models in industry.
(iv) have demonstrated ability for originality and for innovation	The sensitivity analysis project will require the creation and use of effective analysis methods, the results from these studies being presented clearly and in detail.
(v) possess a working knowledge of project management and business methods and their implications for research and development	The project proposals and the remaining two-year Gantt chart contained in this document are examples of the way in which the time required for and constraints upon various projects are being budgeted and how both research and course work are being effectively considered and managed.
(vi) possess and have demonstrated a high level of communication and presentation skills	A poster presentation of results from the first project is planned for the May 2000 SETAC conference. Also, two peer reviewed papers, the 2000 EngD Conference and final dissertation will demonstrate these skills.

Table 6 – How the Aims and Objectives of the Engineering Doctorate will be Achieved

The Joint Regulations (Section 4.4.1) also outline criteria that are necessary for eligibility to graduate as a Doctor of Engineering. Many of these are assessed as part of the taught modules, however two criterion of particular note are to be tested in the final *viva voce*, but are worth considering here and throughout the degree program, these are to:

- Demonstrate evidence of innovation and a contribution to knowledge via research into either:
  - (i) novel understanding of the environmental consequences of systems for providing or using goods or services, or;
  - (ii) novel methods of improving the environmental performance of systems for providing or using goods or services thereby contributing to more sustainable development.
- Demonstrate an understanding of the context of the research: this must include the scientific context and, where appropriate should include the commercial and social context.

Further to these is the consideration that the work should meet the criterion of environmental technology, which is unique to the Brunel/Surrey Engineering Doctorate program. It is believed that this research will meet these criteria in the following ways:

The innovation and contribution to knowledge in this research shall primarily be in the area of risk assessment, although work on the Kennet & Avon canal incident also contains novel aspects and publications from this work are to be investigated. From the initial study of existing systems further areas of work have been outlined. Novel methodologies will then be researched, devised and documented. Contributions to knowledge will come from both the proposed projects for the second half of this research. An understanding of the environmental consequences of risk assessment systems and methodologies will be demonstrated throughout this work.

An understanding of the context of the research will be necessary and demonstrated in the transparent nature of the developed systems, due to their use by industry and scientists at different levels. An understanding of the scientific context will be demonstrated in the application of the novel systems to ensure the protection of the environment, with good use of data and knowledgeable interpretation of results. The sensitivity analysis of current exposure models ensuring the proper interpretation and use of the supplied data, the findings of this work also informing other risk assessment systems.

This research is at the core of the activities of the NCEHS. As such environmental technology will be demonstrated through the construction and refinement of novel risk assessment practices that while ensuring protection, don't over regulate, practices that are workable in industry and which promote sustainable development in the chemical field.

3 Proposed Further Research

This section reviews proposed projects for the final two years of research. The projects have been set out in a similar form to that which is required by the Agency in "Form A" research and development proposal applications. Presenting the proposed work in this fashion has ensured that timescales, risk and constraints and other key areas of project planning have been considered.

3.1 Introduction

While working for the three functions mentioned in earlier sections, various areas and opportunities for further work have become apparent. These are outlined in the form of project proposals in the following sections and are to in the process of being discussed and agreed with both the industrial and academic supervisors, as well as the heads of sections that the work would be conducted within.

The proposed projects are of real and significant worth, producing results and findings that can be published in the peer reviewed literature.

3.2 Project Proposal 1

3.2.1 Project Title:

Sensitivity analysis of values in the environmental exposure section of the European Notification risk assessment system as performed in the EUSES system.

3.2.2 Project Area/Group:

Chemical Assessment Unit

3.2.3 Background:

As part of the notification system a standard base set of information has to be supplied from which a risk assessment is made. The UK Competent Authority (the CAU and HSE) has approximately 1200 such notification records, and the New Chemical Database (NCD) has approximately 6500 records at the European Chemical Bureau (ECB). By conducting a detailed sensitivity analysis on the data variables that are used, it can be determined which values are of greatest importance and have the greatest effect on the calculation. This would mean in the case where an assessment highlights a cause for concern, the costs and benefits of refining the PEC or the PNEC values would be better understood.

3.2.4 Objectives:

Overall objective: To carry out a sensitivity analysis on the variables supplied in a notification in order to relate their effect on the calculated PEC value.

Specific objectives (i): To analyse and study the interrelation of various variables e.g. solubility, vapour pressure and partition coefficients in order to inform the multivariate sensitivity analysis.

Specific objectives (ii): To carry out single and multivariate sensitivity analysis on the PEC calculation of the EU notification process, in order to highlight critical and sensitive variables.

Specific objectives (iii): To report findings, including those variables with the most significant effect on the PEC value in order to allow these factors to be considered when planning further testing to refine assessments.

3.2.5 Methodology:

From the 1200 records held by the CAU, those with full base sets of data can be found and an initial trial sample selected and analysed.

A fuller analysis could then be made using all records that satisfy the base set and any other requirements.

Once the sensitive values have been highlighted, these findings could then be confirmed through the analysis of the full NCD data set at the ECB.

3.2.6 Risks and Constraints:

Initially methods for sensitivity analysis will need to be investigated, to see whether a standard spreadsheet can be used or whether some form of MATLAB or C++ program is required. Also the CAU's New Chemicals data set needs to be checked to highlight those suitable for study.

In-depth sensitivity analysis of available and suitable UK data set records, with a view to highlighting the key variables in the PEC calculation, those having the greatest effect on the resulting PEC value. Reporting and publishing of sensitivity findings.

The larger EU data set could then be analysed in light of findings from UK sensitivity analysis to confirm these finding in the larger, EU database. Reporting and publishing of results will ensue.

Some form of blind labelling system may be required to protect the 'commercial in confidence' nature of some of the data. The further analysis of the EU database would help to strengthen previous findings but would not be essential.

3.2.7 Targets and Timescales:

Task	Total Time
(i) Understanding of target variables for sensitivity analysis and their interrelationship. (ii) Outline and understanding of the methods (particularly statistical) to be employed including any database, spreadsheet or programs required.	2 months
Initial, early findings and confirmation of analysis method	3 months
Suitable records from UK data set fully analysed and report and possible paper on findings from these analyses.	4-5 months

Table 6 - Targets and Timescales for the Proposed CAU Project

3.2.8 Required Resources:

Access to CAU new chemical SNIF data.

Processing/computing facilities to deal with large computations.

Support and advice on statistics issues (WRc, Tony Walm - Anglian Region)

Access to ECB NCD if EU data set to be used

3.3 Project Proposal 2

3.3.1 Project Title:

Comparative study of single substance and whole sample toxicity risk assessments on selected discharges

3.3.2 Project Area/Group:

Direct Toxicity Assessment and Environmental Toxicology Sections

3.3.3 Background:

The DTA Demonstration Programme (EA National R&D Project P2-094) targeted four catchments for the trial of the proposed DTA seven-stage protocol. The work on the Tees Estuary has produced by far the best results with some discharges now being assessed for toxicity reduction. A comparative study of the control of discharges using either substance specific or whole sample toxicity assessment tools would highlight the strengths and weaknesses in each approach for such situations.

3.3.4 Objectives:

Overall objective: To carry out a comparison of the DTA and EQS risk assessment and control systems in order to highlight the strengths and weaknesses.

Specific objectives (i): To identify suitable discharges for which a comparative study of controls could feasibly be performed.

Specific objectives (ii): To carry out assessments using both single substance and whole sample toxicity controls in order to make comparisons.

Specific objectives (iii): To report findings and indicate where decisions and controls would differ under the two different assessment regimes.

3.3.5 Methodology:

The DTA Demonstration Programme investigated at four different sites; the available data from each of these would need to be assessed to see if enough data is available (i.e. characterisation of effluent) to perform a desk based comparative study.

Where full characterisations have not been performed these could be submitted for characterisation, or a laboratory based piece of research carried out, to characterise the required effluents.

Where characterisations are not available, process mechanisms could be reviewed to allow an approximation of the effluents content to be made.

Andy Girling and Dave Forrow to be contacted regarding DTA Demonstration Programme and EA research programme on DTA/EQS comparison.

3.3.6 Risks and Constraints:

Initial data collation from the test catchments and effluent discharges. Evaluate data sets for suitability for comparative assessment.

Discussion with DTA group regarding research programme comparison and proposed desk study.

Re-assess feasibility of study.

Actual comparison of assessment systems and resulting limits and/or controls. If sites with most data are assessed first, those with incomplete or small data sets will soon be identified as feasible or not for the comparison.

If required data is unavailable this should be apparent in the first month at which point the work can be shelved possibly reporting the data that would be needed to carryout the work at a later date.

By making comparisons on the larger data sets first, data sets with insufficient information can be highlighted earlier without entering into too much depth on the comparative analysis. Also, if enough data has already been gained, further smaller studies do not have to be considered.

Not all identified chemicals may have EQSs set for them, a quick search can be made for any limits set by other organisations or bodies (WHO, US EPA etc.) to allow some consideration of what values the UK might apply if required.

3.3.7 Targets and Timescales:

Task	Total Time
Review of data available and which discharges and catchments are applicable for the comparative analysis to be made.	1 month
If feasible comparative analysis can be carried out duration dependent on number of discharges with sufficient data for analysis.	3-4 months
Reporting and publishing of findings from comparative assessments	4-5 months

Table 7 - Targets and Timescales for the Proposed DTA/ETS Project

3.3.8 Required Resources:

The data from the demonstration will be required, preferably the assessment data rather than the raw test data. Chemical characterisations and composition of the effluents being considered will be needed to allow single substance assessments to be made.

Access to EQSs, WHO and other limit value data will be required to make single substance assessments.

3.4 Further Project Proposals

Two further areas of work that are to be considered, which have not been proposed as formal project proposals to date are:

- Further work resulting in publishable findings on the Kennet and Avon Incident.
- The tracking and following of an EQS through the complete process from a requirement for a standard being highlighted through to the setting of provisional and agreed values.

4 Project Plan and Gantt Chart

ID	Task Name	Start
1	Engineering Doctorate Program	Mon 15/09/97
2	Time in DTA	Mon 29/03/99
3	24 Month Dissertation	Fri 01/10/99
4	Supervisors Meeting	Thu 13/01/00
5	Supervisors Meeting	Mon 13/03/00
6	Module - Finance (dist. Learn.)	Mon 04/10/99
7	HOLIDAY	Mon 11/10/99
8	DTA Report Work	Fri 22/10/99
9	EngD Viva	Mon 25/10/99
10	Project Proposal 1	Mon 08/11/99
11	Xmas 99 HOLIDAY	Thu 23/12/99
12	30 Month Report	Mon 20/03/00
13	30 Month Report - Deadline	Sat 01/04/00
14	Supervisors Meeting	Sat 13/05/00
15	PP1 - Write-up and papers	Mon 03/04/00
16	Write PP1 poster for conf	Fri 28/04/00
17	Module - Env. Man. Systems	Mon 08/05/00
18	SETAC Conference 2000	Tue 23/05/00
19	Supervisors Meeting	Thu 13/07/00
20	36 Month Report - Deadline	Sun 01/10/00
21	Project Proposal 2	Mon 29/05/00
22	PP2 - Write-up and papers	Mon 30/10/00
23	Module - Economic Approaches	Mon 05/06/00
24	Conference 2000 - paper	Fri 30/06/00
25	Conference 2000 - pres	Mon 31/07/00
26	Conference - 2000	Tue 12/09/00
27	36 Month Report	Thu 14/09/00
28	Risk Assessment & Managemer	Mon 02/10/00
29	Module - Talking to the media	Mon 23/10/00
30	Xmas 2000 HOLIDAY	Mon 25/12/00
31	30 Month Report	Tue 20/03/01
32	30 Month Report - Deadline	Sun 01/04/01
33	Critical analysis and review - fina	Mon 28/05/01

Project: EngD-99-2001
Date: Wed 26/09/01

5 Literature Review

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6 Glossary

The following is a glossary of terms that have been used in this report and that have arisen during the course of this research at the Environment Agency.

AF	Assessment Factor
ALARA	As Low As Reasonably Achievable
ASL	Approved Supply List
BCF	Bio-concentration Factor
CA	Competent Authority
CAU	Chemical Assessment Unit
CNU	Chemical Notification Unit
DENI	Department of Environment Northern Ireland
DETR	Department of the Environment, Transport and the Regions
DTA	Direct Toxicity Assessment
EA	Environment Agency
EASE	Estimation and Assessment of Substance Exposure
EC	European Community
EC_{50}	Effect Concentration for the median or 50th percentile
ECB	Environmental Chemical Bureau
EEC	European Economic Community
EFTA	European Free Trade Association
EINECS	European Inventory Existing Chemical Substances
ELINCS	European List of Notified Chemical Substances
EngD	Engineering Doctorate
EPO	Environmental Protection Officer
EQS	Environmental Quality Standard
ERA	Environmental Risk Assessment
ESR	Existing Substances Regulation
ETAS	Environmental Toxicology Advice Service
ETS	Environmental Toxicology Section

EU	European Union
EURAM	European Ranking Method
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice
HEDSET	Harmonised Electronic Data SET
HRA	Human Risk Assessment
HSE	Health and Safety Executive
IPC	Integrated Pollution Control
IPPC	Integrated Pollution Prevention and Control
IPS	Informal Priority Setting method
IUCLIDS	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
Koc	Organic carbon – water partition coefficient
Kow	Octanol – water partition coefficient
LC_{50}	Lethal Concentration for 50th percentile
LCA	Life Cycle Assessment
LEAPs	Local Environment Action Plans
LOAEL	Lowest Observable Adverse Effect Level
LOEC	Lowest Observable Effect Concentration
MATC	Maximum Acceptable Toxicant Concentration
NCD	New Chemical Database
NCEHS	National Centre for Ecotoxicology and Hazardous Substances
NOAEL	No Observable Adverse Effect Level
NOEC	No Observable Effect Concentration
NONS	Notification Of New Substances

OECD	Organisation for Economic Co-operation and Development
PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
PPE	Personal Protective Equipment
(Q)SAR	(Quantitative) Structural Activity Relationship
RA	Risk Assessment
RCR	Risk Characterisation Ratio
RPE	Respiratory Protective Equipment
SEPA	Scottish Environmental Protection Agency
SETAC	Society of Environmental Toxicology and Chemistry
SNIF	Standard Notification Interchange Format
STP	Sewage Treatment Plant
TGD	Technical Guidance Document
TRE	Toxicity Reduction Evaluation
USEPA	United States Environment Protection Agency
UVCB	Substances of Unknown or Variable Composition, complex reaction products or Biological material
WAF	Water Accommodated Fraction
WET	Whole Effluent Toxicity
WHO	World Health Organisation
WWTP	Waste Water Treatment Plant

7 Appendix

The following documents are included in the following sections:

Section	Documentation
7.1	Diagram of NCEHS Organisational Structure
7.2	Gantt Chart for the First Two Years of Research
7.3	Poster Presentation for SETAC and EngD Conferences

7.1 Diagram of NCEHS Organisational Structure

7.2 Gantt Chart for the First Two Years of Research

7.3 Poster Presentation for SETAC and EngD Conferences

BRUNEL UNIVERSITY

THE INTEGRATION OF DIRECT TOXICITY ASSESSMENT INTO THE CONTROL OF POINT SOURCE DISCHARGES TO CONTROLLED WATERS

ENVIRONMENT AGENCY

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Introduction

A number of approaches are currently used in England and Wales to control point source discharges of hazardous chemicals to controlled waters throughout a chemical's life cycle. The control systems considered here all involve the collation of data and its assessment for the hazards or risks associated with that chemical. Direct toxicity assessment (DTA) which considers the toxicity of whole effluents may be used in future to assess some discharges, particularly mixtures of substances.

Existing control systems

Existing controls are currently in place to control exposure to hazardous chemicals for:

- Chemical production
- Transportation
- Health and safety
- Storage
- Pollution control
- Waste disposal

Pre-release controls - Aimed at reducing point and diffuse source discharges particularly during the use phase, the EU Notification Process requires the risk assessment of new chemicals prior to marketing. A Predicted Environmental Concentration is (PEC) compared to Predicted No Effect Concentration (PNEC). If the risk characterisation ratio (RCR = PEC/PNEC) is greater than one there is cause for concern (see Figure 1). Assessments are made using a "base set" of physical, chemical and ecotoxicological data. If risks are identified further information is required to refine the assessment or risk reduction may be required. Assessments tend to be generic, applicable Europe-wide.

Emission controls - The Integrated Pollution Control, (IPC) authorisation process of the EPA90, aims to "prevent, minimise or render harmless releases of prescribed substances" and ensure processes are undertaken to Best Available Technology Not Entailing Excessive Cost (BATNEEC) and are the Best Practicable Environmental Option (BPEO). There is a requirement for authorisation of any prescribed processes, listed in Part I, EPA90. Authorisations require BATNEEC and may also set emission limits, to be met. Risk assessments are performed on a case-by-case basis for each type of industrial process and do not consider the quality or type of receiving waters. IPPC (Integrated Pollution Prevention and Control) is intended to supersede IPC in the period up to October 2007 and has a wider scope under its permit scheme.

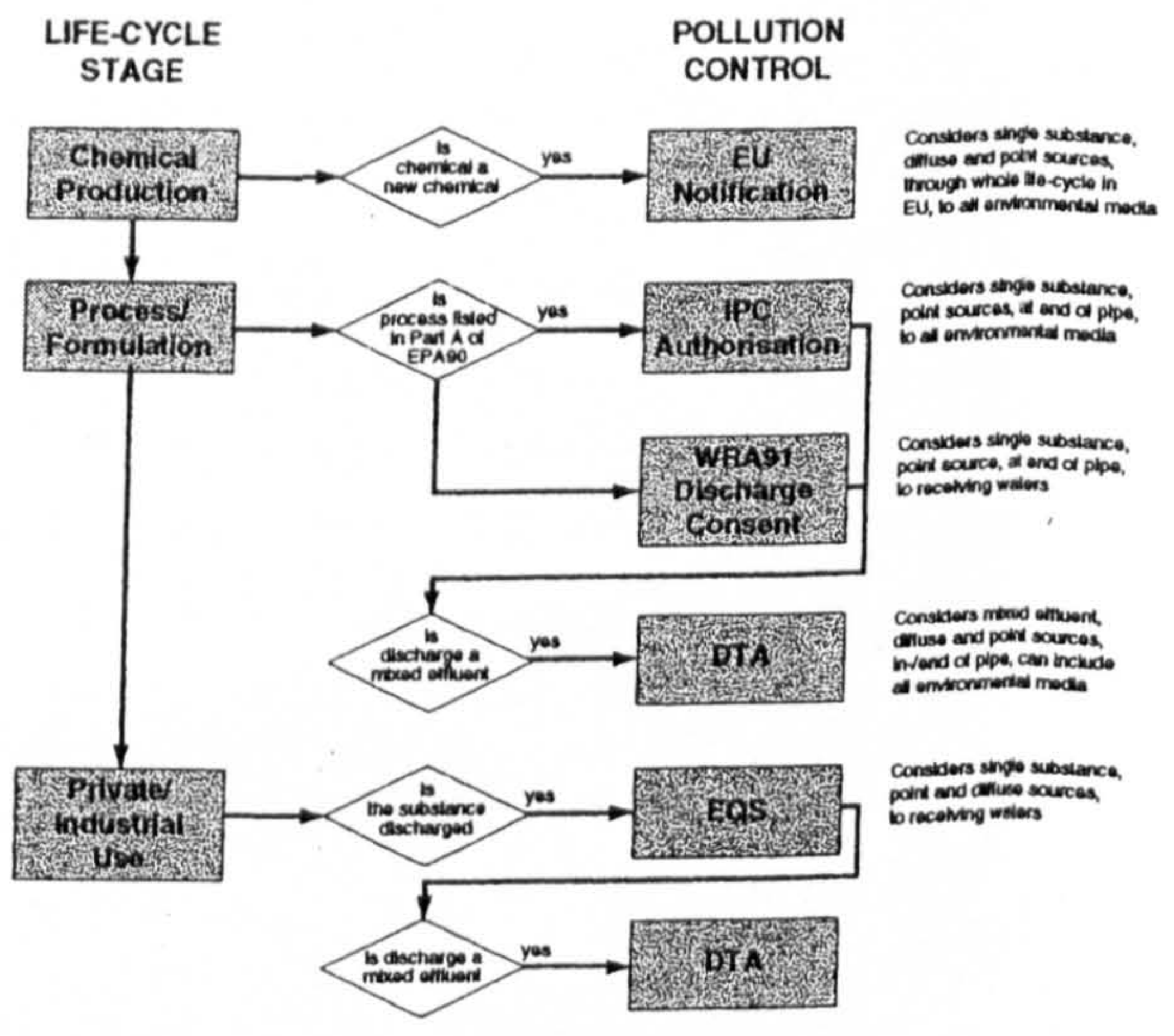


Figure 6 - Implementation of Control System Assessments

The discharge consenting process (WRA91) sets allowable limits on discharges not covered by IPC, legitimising specific discharges of chemicals to controlled waters. These consents are set on a site-by-site basis to meet the required quality objectives for receiving waters. Risk assessments are made on the basis of existing, available data, and after consideration and consultation (see Figure 2), limits to the concentration and flow of discharges are made.

Environmental controls - Environmental Quality Standards (EQSs), are set as maximum and average concentrations that are permissible in watercourses. These apply to single substances and are hazard-based assessments of chemicals in the environment, aiming to control point source discharges to the aqueous environment. EQSs are set through the assessment and consideration of all available ecotoxicological information and the application of a suitable assessment factors (AF) to the lowest reliable effect concentration (see Figure 3).

Direct Toxicity Assessment

DTA is not currently used to control pollution in the UK, however the Environment Agency's R&D Research Project - the DTA demonstration programme, is currently testing a 7 stage protocol for the using the DTA methodology. The concept of DTA is to measure the hazardous nature of an effluent by measuring biological effects on the whole of a sample, which can be extrapolated to the biota of the receiving water. The effluents most suitable for controls using a DTA approach contain many different substances that may interact causing toxic effects not measured using single substance controls, as well as substances whose toxicity is not well understood. The DTA approach seeks to identify areas of concern in the environment, and then works back to the discharges entering the watercourse to identify problem effluents. Whole toxicity measures are then made on these discharges and highlight those that require toxicity reduction. A theoretical risk assessment framework has been proposed (see Figure 4), involving two tiers of assessment with a probabilistic comparison of the PEC and PNEC distributions used to measure the risk.

Integration of Pollution Control Systems

Pollution control systems must be integrated; any one system cannot alone adequately control chemicals and their discharge into the environment. The various systems need to be used together in an integrated manner, to cover both point and diffuse sources of pollution throughout a chemical's life cycle. There is also currently little interaction between the control systems each using separately complied data sets, only EQS risk assessments collating all available data and judging it for quality and applicability. The systems needs to be protective of the environment, without being prohibitive or entailing excessive cost to industry, a wider use of available data would reduce the cost of analysis and toxicity testing for industry.

Discussion

Chemical discharges into controlled waters can only be effectively controlled through integrated control methods. This includes data sharing between systems where appropriate. Through Notification, a basic set of data is collated for every new substance; this data is of high quality and may be relevant for use in other assessments. Notification fate and behaviour data could be of use in IPC authorisations and discharge consenting. EQSs already consider all available ecotoxicological data, however further use of fate, behaviour and PEC data could help to inform decisions on the magnitude of AFs. However, data sharing between companies and industries is scarce, mainly due to commercial confidentiality. A system similar to the notification systems 'data-sharing' could be arranged to facilitate and protect data in these instances. For Notifications, companies are required to "take all reasonable steps to share data". Cross-references to previous data being made in new notifications, companies negotiating directly to share the costs.

Data sharing reduces duplication of effort and unnecessary extra testing (particularly of organisms). One drawback though is that the breadth of available data is reduced, with fewer repeat tests to confirm previous results. This means the ability to judge uncertainty is reduced.

The implementation of DTA requires careful targeting and prioritisation of catchments. The method being applied where impacted biology cannot be explained by chemical analysis, the existing control systems possibly highlighting such areas of concern. Single substance assessments and controls would then be superseded by whole toxicity measures, implicitly considering interactions within the mixtures. The proposed DTA two-tier risk assessment system requires that the first tier of testing identifies all discharges of concern within a catchment without entailing excessive costly testing for industry. Therefore an effective first tier of assessment is critical, to ensure all problem discharges are considered at the second tier of assessment.

The probabilistic assessment at the second tier of assessment accounts for, and represents the variations in the PEC and PNEC estimations rather than, as is the case for notifications, generating a "worse-case" deterministic assessment. The cost benefit assessment of refining these estimations is also critical to the DTA method and may be applicable in other systems also.

Control	Scope	Data used	Assessment	Review
Notification System	Single substance, diffuse and point source, to all env. media	Base-set of physical, chemical and ecotoxicological data carried out for assessment	RCR = PEC / PNEC If RCR > 1 there is cause for concern	If RCR > 1 further data or testing may be required
IPC	Prescribed processes or substances, point source discharges to all env. media	Company must submit application for authorisation including an EIA.	Process specific assessment requiring BATNEEC and BPEO	If process is changed the authorisation must be reviewed
Discharge consents	Single substance, point source, to receiving waters	Company must supply data on quantities of chemicals in process and discharge and their effects on receiving waters	Limits applied to concentration and flow rate of discharge related to full dilution capacity of receiving waters	Modification or variations to conditions may be made by the Authority "from time to time".
EQSs	Single substances, point and diffuse discharges to receiving waters	All available public, industrial data considered and weighted on quality and relevance	Hazard assessment based on lowest ecotoxicological test value and a suitable assessment factor PNEC / AF	Peer review of proposed value, assessment of any new data and monitoring of applied value
DTA	Whole effluents and mixtures, point source discharges to all media	Whole effluent ecotoxicology test data and site specific dispersion data	Tier I - targeting of problem discharges, Tier II - probabilistic PEC, PNEC comparison	Comparison with single substance controls and monitoring of discharges

Figure 5 - Comparison of Control System Assessments

Considerations:
- What other discharge selection criteria could be used in the Tier I assessments in DTA?
- Could cost/benefit analysis of the risk assessment refinement be applied to other systems effectively?
- How can data sharing between systems and companies be facilitated, what frameworks are there for quality assessing existing data?
- Where a DTA assessment supersedes other controls what procedures and support are needed for the adoption of the new controls?
- How can the proposed risk assessment framework for DTA be refined?

Acknowledgement - This research has been jointly funded by the EPSRC and the National Centre for Ecotoxicology and Hazardous Substances of the Environment Agency. Particularly thanks go to D. Forrow and O. Warwick of the Direct Toxicity Assessment Group at the Environment Agency for their help and guidance.

Figure 1 - Risk Assessment Scheme for the EU Notification Process

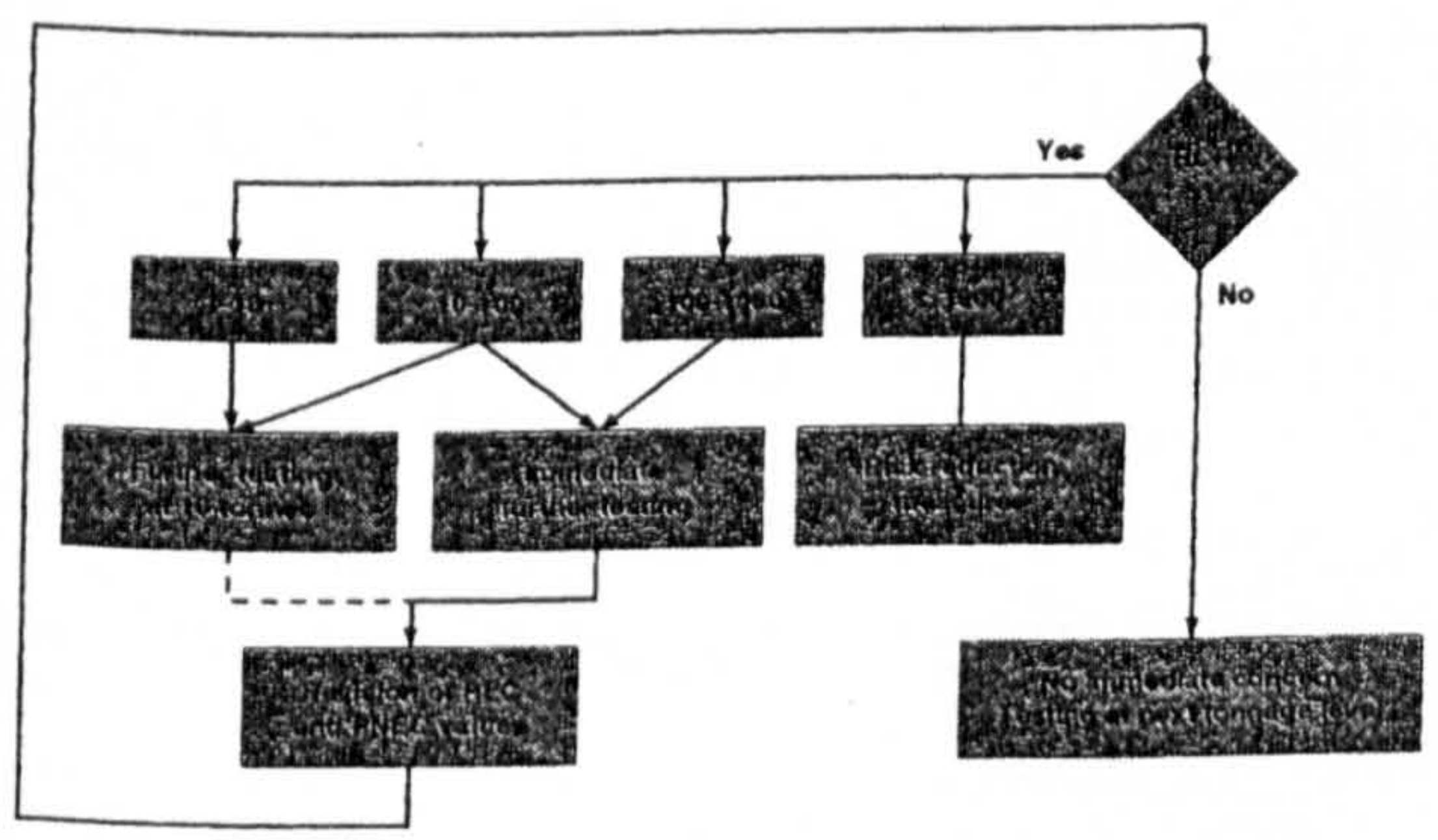


Figure 2 - Risk Assessment Scheme for the WRA91 Discharge Consents Scheme

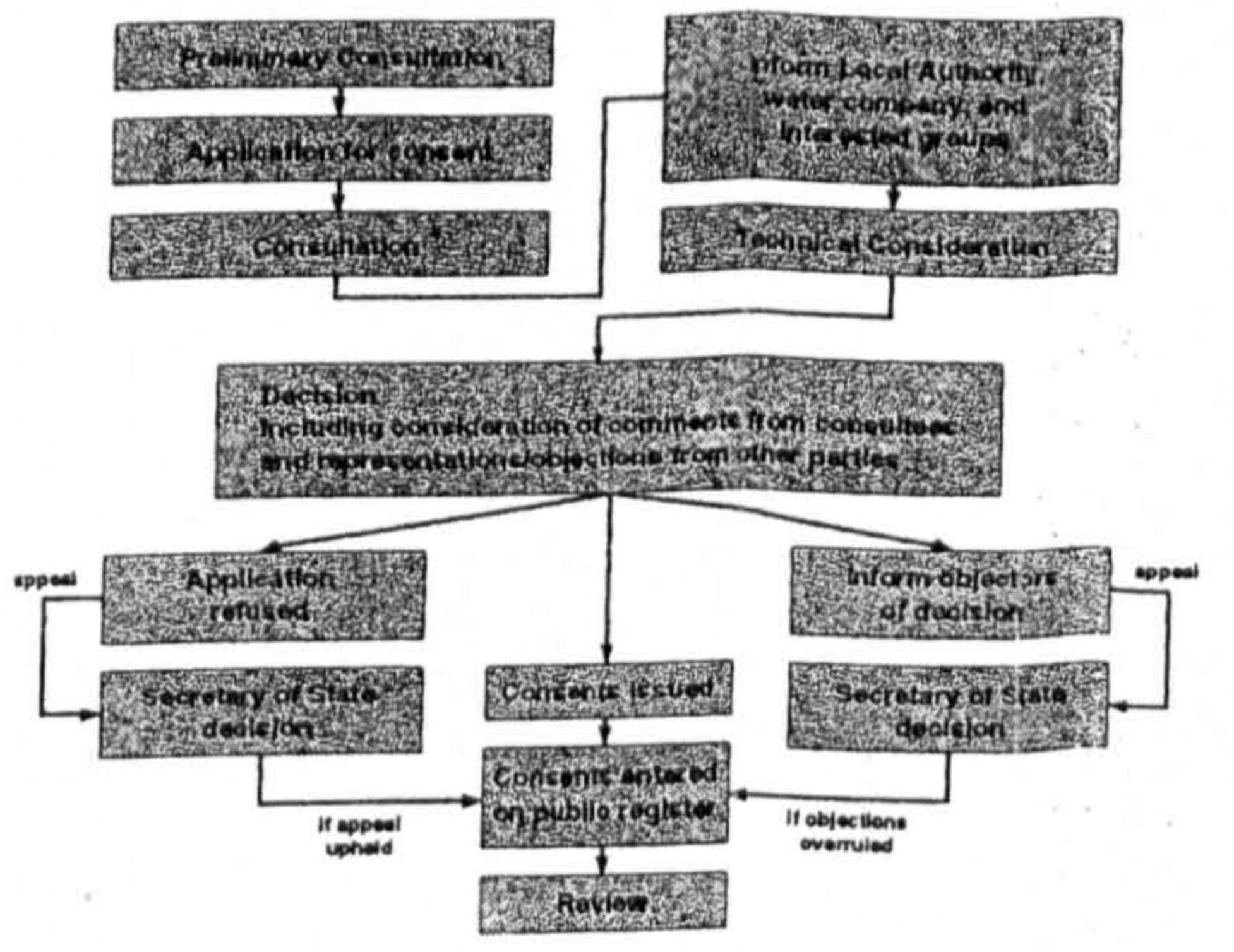


Figure 3 - Hazard Assessment Scheme for the Derivation of Environmental Quality Standards

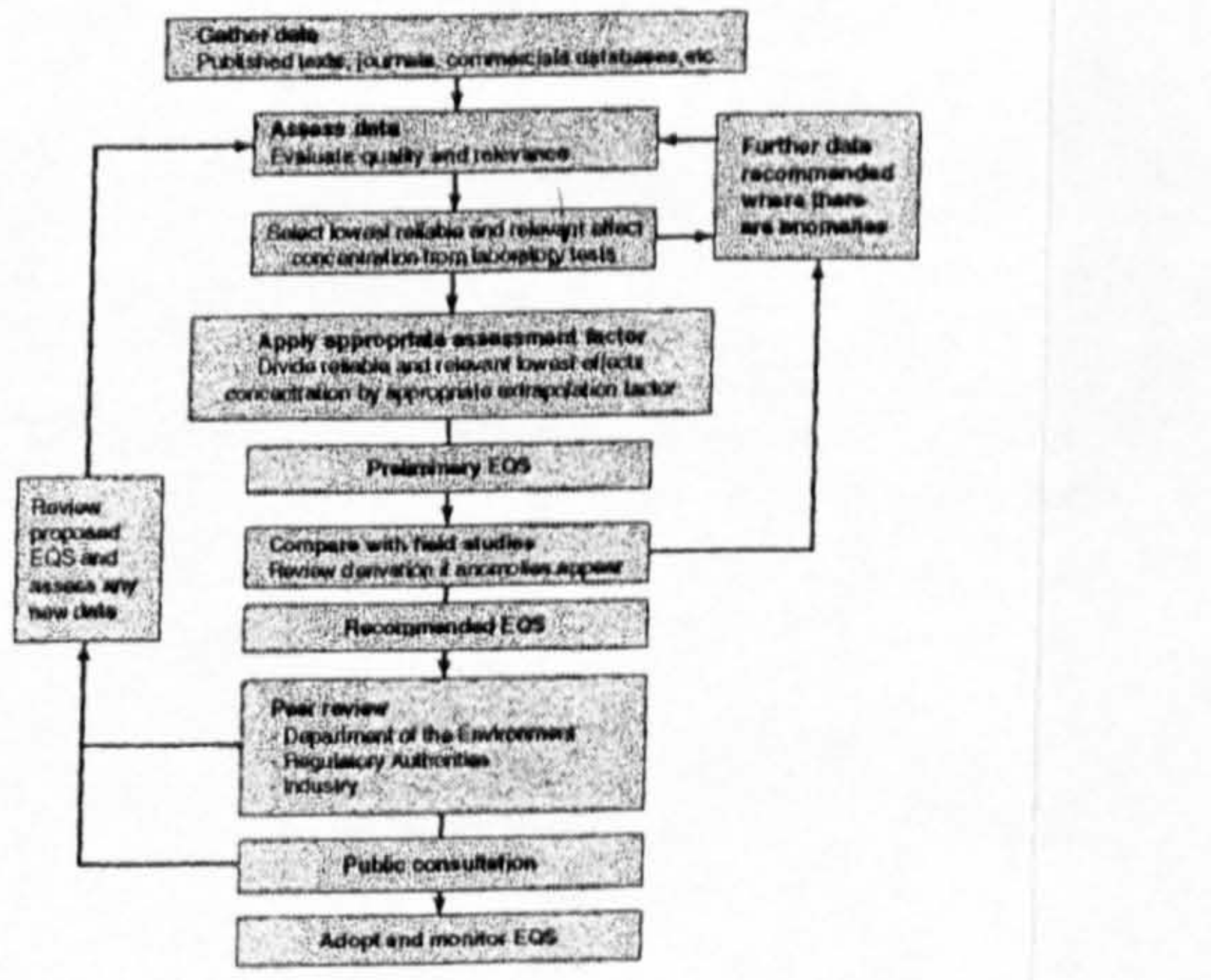
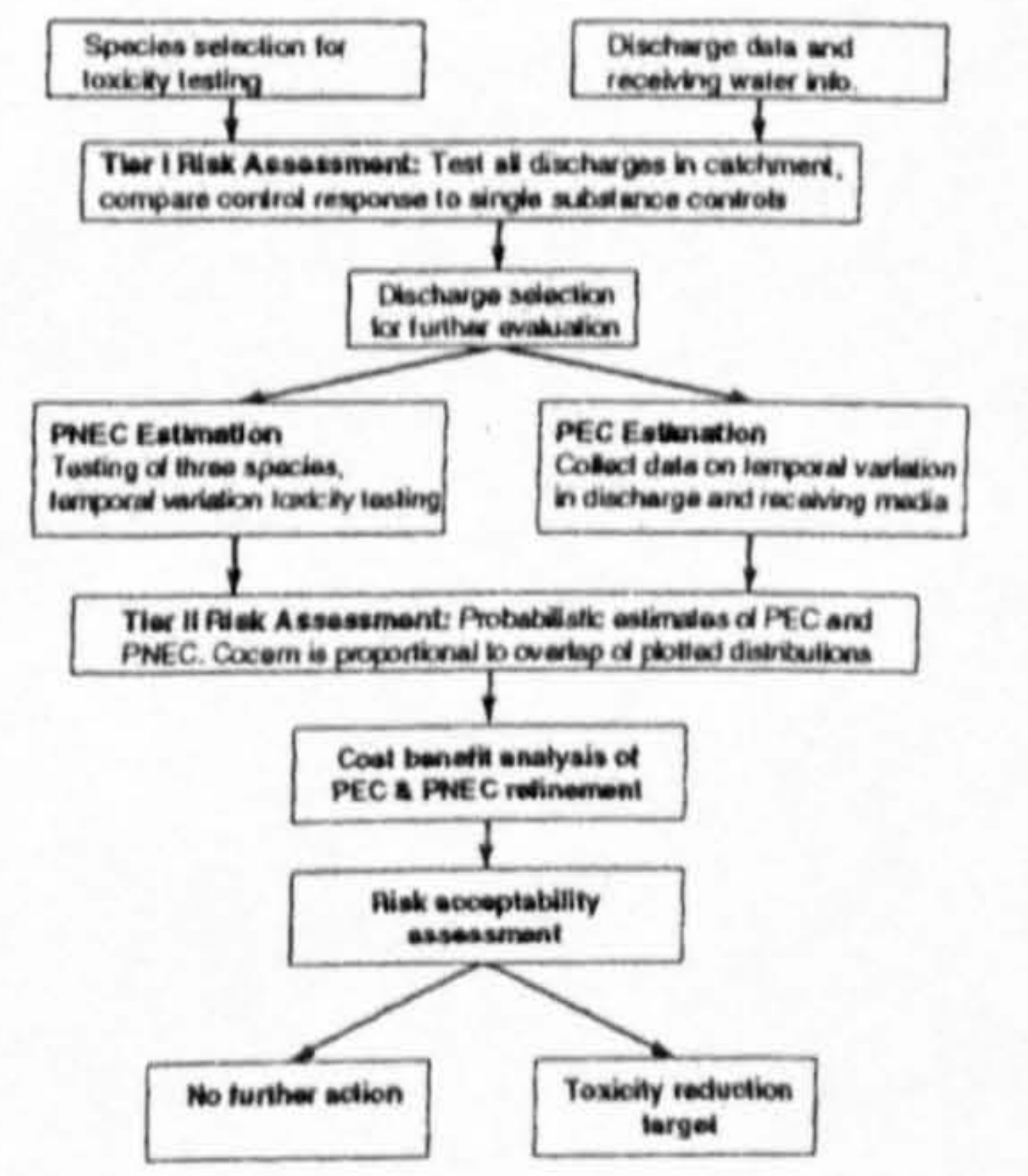


Figure 4 - Proposed Risk Assessment Scheme for the Implementation of Direct Toxicity Assessment



30 Month Report

ENVIRONMENT
AGENCY

BRUNEL
UNIVERSITY

Engineering Doctorate in Environmental Technology

30 Months Report

1st April 2000

By
Nik Robinson

Contents

Executive Summary

This report is the fifth in the series of six monthly reports that track the progress of my research work throughout the duration of the Engineering Doctorate course. It contains an introduction to, and review of, the work undertaken during this period. For a more general introduction to the Environment Agency and the National Centre for Ecotoxicology and Hazardous Substances (NCEHS), I refer the reader to the first six-month report in this portfolio.

This period saw the completion of work with the Direct Toxicity Assessment (DTA) Section, in addition, minor amendments to the time plan and Gantt chart as proposed in the 24-Month Dissertation took place. Additionally work began on the first of the two proposed further projects, the PEC (Predicted Environmental Concentration) calculation sensitivity analysis. The aims and objectives from the previous period have been reviewed and new objectives for the next six-month period are outlined. Finally a revised Gantt chart is included, showing the proposed timescales for projects with modules and other overlapping commitments indicated. There is also a glossary of terms at the end of this report.

1 Introduction

The main objective for this period was the PEC calculation sensitivity analysis project, however, as part of the amendments from the 24 month viva and due to continuing pressures brought about by the distance learning Finance and Marketing module a revised Gantt chart was produced in October. The start of the PEC sensitivity analysis project was moved to the beginning of February to allow time for other constraints and completion of the report on the work in the DTA Section. This work is reviewed in detail in the following sections, and agreed objectives for the next period are outlined.

Some issues remain with regard to the Kennet & Avon Canal Incident and Geoff Brighty is keen for some further work with Helen Wilkinson with respect to emergency response. The report on the DTA Section took longer than expected to complete and comments on the first draft are being collated. Other than minor corrections some consideration will need to be given to the structure to ensure the flow of the report.

The distance learning finance and marketing module was completed during this period. The completed assignments can be found in the portfolio.

2 Review

2.1 Objectives from the Last Period:

The objectives outlined in the 24 month dissertation Gantt chart at the beginning of this period can be seen below (Box 1). These were then reassessed at the supervisors meeting on 13th January 2000.

- Complete report on the Direct Toxicity Assessment Section by end of 1999
    - Get final comments on draft copy
    - Amend and produce final copy
- Complete further work on the Kennet & Avon Canal Incident and emergency response by end of 1999
    - Complete final amendments to Kennet & Avon Canal Incident Report
    - Liase with Helen Wilkinson on emergency response issues with view to training programme for Regional Contacts
- Start PEC sensitivity analysis project (mid Nov. 1999 – end March 2000)
    - Investigate and understand target variables for sensitivity analysis and their interrelationship
    - Gain understanding of uncertainty analysis methods and develop necessary model(s)
    - Carry out initial investigations with a view to poster presentation of initial results at SETAC 2000 conference (May 2000)
    - Continue further analyses and prepare and submit paper for peer review journal.
    - Complete final report on project.

Box 1 - Objectives set from previous 6 month period

The main revisions to the time-scales shown in Box 1 can be seen on the revised Gantt chart in Section 3, and include:

- Completion of DTA Section report, by end of January 2000
- Start PEC sensitivity analysis project, February 2000 – mid June 2000

No time was explicitly allocated for further work on the Kennet & Avon Canal Incident report and further emergency response work.

Work within the DTA Section:

There were two distinct areas of work completed within this Section. Firstly, the author's background knowledge of ecotoxicology and of the tests and data used and produced was highlighted as an area requiring further consideration. Secondly, a comprehensive investigation of the DTA approach to the control of substances was undertaken. This included a review of the DTA Demonstration Programme (EA National R&D Project P2-094) and initial findings from this project, as well as examination and consideration of the proposed DTA protocol and risk assessment framework. A summary of some of the points raised in this report can be seen in Box 2.

- Ecotoxicology
  - The process of ecotoxicological testing was followed, and an idea of the problems and variability within these tests was gained.
  - The manipulation of raw laboratory test data was also investigated and how these data are presented in the form of summary statistics, and what these values represent.

- Direct Toxicity Assessment
  - DTA attempts to measure the toxicity of whole effluents, the nature of such target discharges being complex, and mixtures of known and unknown substances.
  - DTA requires careful and effective prioritisation of catchments and targeting of discharges. These stages being key to the integration of DTA into existing chemical control systems.
  - A two-stage risk assessment process has been proposed as a framework for making ecological decisions, including an initial preliminary risk assessment using acute toxicity testing, with further testing and more in-depth assessment being undertaken at the second stage.
  - The use of probabilistic risk assessment has been outlined. These probabilistic assessments represent the variations in the PEC and PNEC estimations rather than generating a "worst-case" deterministic assessment.
  - An effective first tier of assessment is critical, to ensure all potentially problematic discharges are considered at the second stage of assessment.

Box 2 - Summary of some of the key points disscussed in the DTA report

Sensitivity analysis of the PEC calculation:

This project is based on the calculation of the Predicted Environmental Concentration of a substance as outlined as part of the Notification Process (EC, 1996) under the Dangerous Substances Directive 93/67/EEC. The European Union has developed a computer programme which automates the risk assessment process as outlined in this directive, called EUSES (European Union System for the Evaluation of Substances), (Vermeire *et al.*, 1997).

The model used in EUSES was reproduced in a spreadsheet format, the sensitivity of various physico-chemical property values, model defaults and internal calculations and models will be investigated.

The revised work program for the PEC calculation sensitivity analysis was set as follows:

1. Initial investigation and model construction:
   beginning February – beginning of March
2. Collation and analysis of data:
   beginning March – end of April
3. Write report, papers and poster on results:
   late April – mid June

The production and development of the spreadsheet model has been completed and early trial analyses have been performed. Before further work, HSE will be contacted with respect to the sensitivity of the data being used and what results and data can be presented. Further and more detailed investigations of the sensitivity of parameters and values used in the model will follow. It is hoped from this work that an understanding of the most important and sensitive values can be found which can then be used to direct and aid further research and model development.

The spreadsheet model produced already incorporates many "bug-fixes" and model selection parameters that have been highlighted but not fixed in the European Unions EUSES programme. The spreadsheet format also allows many 100s of simultaneous PEC calculations to be run, thus aiding and speeding up the sensitivity analysis process.

It is intended that a poster of the initial result will be presented at the SETAC 2000 Conference in Brighton at the end of May, this poster being entered into the Student Forum Poster competition. Also a paper will be prepared for submission to a peer reviewed journal, possibly Environmental Toxicology and Chemistry. It is envisaged that the initial work on this paper will be completed by mid June as outlined above (point 3) and then amendments and corrections made as found during the submission process.

2.2 Objectives Proposed for the Next Period:

Below in Box 3 the proposed objectives for the next period are outlined.

- PEC Calculation Sensitivity Analysis
  - Continue sensitivity analysis of Notification data, including production of poster presentation of initial results for SETAC conference (end May)

    – 27/04/2000
  - Write up project report, and papers

    01/05/2000 – 16/06/2000

- Proposed Period of work at Head Office (further details to follow)

  19/06/2000 – 08/09/2000

- EngD Conferenece 2000
  - Decide on paper title and abstract

    05/2000
  - Produce conference paper

    03/07/2000 – 07/07/2000
  - Produce conference presentation

    31/07/2000 – 04/08/2000
  - Conference

    ....

Box 3 - Objectives proposed for then next 6 months

2.3 Aims and Objectives of the Engineering Doctorate Program:

Aims and Objectives of EngD Programme	How Attributes Have Been Demonstrated
REs should:	
(i) be equipped as engineering research-designers to plan and lead flexible and innovative R&D programmes that respond to customers' needs.	Flexibility, and good interpersonal skills have again been demonstrated in the PEC sensitivity analysis project where the areas of sensitivity are being addressed with respect to industry's and regulator's needs the spreadsheet model already incorporates many fixes for bugs highlighted in the EUSES programme.
(ii) be able to work effectively, and to form, work within and where necessary lead teams with a multi-disciplinary background to tight time schedules.	Work on the PEC sensitivity analysis project is requiring communication with many groups including the HSE and possibly the ECB. There are data, confidentiality and time constraints on this project which are continually reviewed and considered.
(iii) possess comprehensive expert knowledge of the field of Environmental Technology, of techniques needed to balance social and economic benefit against resource utilisation and environmental impact, and of the processes of technology transfer needed to ensure the application of research into practice	Expert knowledge of environmental technology and in particular risk assessment, ecotoxicology and environmental legislation continues as the main focus of my research. There is a need to balance social, economic and environmental issues, in all aspects of my work. In the PEC sensitivity analysis project a consideration of the most sensitive values can help to lead and direct further research, analysis and model development producing more efficient and economic assessments. Technology transfer, has been and will continue to be demonstrated through clear and concise presentation of research work and the results and findings obtained.
(iv) have demonstrated ability for originality and for innovation	The spreadsheet model of the PEC calculation allows swift comparison of many variations in data. Further development could include a more user friendly "front-end" to enable wider use in the National Centre.
(v) possess a working knowledge of project management and business methods and their implications for research and development	Many of the lessons learnt in the first two years of this research have enabled better planning and time management of further research work. The PEC sensitivity analysis project, from initial proposal through to planning and conducting has further exhibited these developing skills.
(vi) possess and have demonstrated a high level of communication and presentation skills	All work continues to be presented in a clear manner. The presentation of a poster at the SETAC 2000 conference will allow lessons learned from last year to be demonstrated.

Table 1 – Progress to Date Towards Aims and Objectives of the Engineering Doctorate

The Joint Regulations (Section 4.4.1) also outline criteria that are necessary for eligibility to graduate as a Doctor of Engineering. Many of these are assessed as part of the taught modules, however two criteria of particular note are to be tested in the final *viva voce*, but are worth considering here and throughout the degree programme, these are to:

- Demonstrate evidence of innovation and a contribution to knowledge via research into either:
  (i) novel understanding of the environmental consequences of systems for providing or using goods or services, or;
  (ii) novel methods of improving the environmental performance of systems for providing or using goods or services thereby contributing to more sustainable development.
- Demonstrate an understanding of the context of the research: this must include the scientific context and, where appropriate should include the commercial and social context.

Further to these is the consideration that the work should meet the criterion of environmental technology, which is unique to the Brunel/Surrey Engineering Doctorate program. It is believed that this research will meet these criteria in the following ways:

The innovation and contribution to knowledge in this research shall primarily be in the area of risk assessment. The work on the Kennet & Avon Canal incident, although pollution management in a wider sense, did result in the production of some novel work including an analysis of the National Centre's contribution to the emergency response, and what expectations and requirements there were.

From the initial study of existing risk assessment systems further areas of work have been outlined. The PEC sensitivity analysis project examines the sensitivities within the Notification System's calculation of predicted concentration in the environment. However the findings from this work can be applied more broadly to all environmental risk assessment systems, all of which must make some estimate of the concentration of a substance (or substances) in the environment.

An understanding of the context of the research will be necessary and demonstrated in the transparent nature of the developed systems, due to their use by industry and scientists at different levels. The value of a sensitivity analysis on a calculation like this is that it can help to inform and direct further data requirements, research and model development.

This research is at the core of the activities of the NCEHS. As such environmental technology will be demonstrated through the development of risk assessment practices that while ensuring protection, don't over regulate, and where the main areas of variability an uncertainty are transparent. Such practices allow the regulators and environmental managers to make more informed decisions and help to promote sustainable development in the chemical field.

3 Project Planning Gantt Chart

The following insert is the current Gantt chart for this research work, showing all commitments and proposed periods of work up to October 2001, the end of registration for this course.

4 Glossary

The following is a glossary of terms that have been used and that have come up during this and other work at the Environment Agency.

AF	Assessment Factor
ALARA	As Low As Reasonably Achievable
ASL	Approved Supply List
BCF	Bio-concentration Factor
CA	Competent Authority
CAU	Chemical Assessment Unit
CNU	Chemical Notification Unit
DETR	Department of the Environment, Transport and the Regions
DTA	Direct Toxicity Assessment
EA	Environment Agency
EASE	Estimation and Assessment of Substance Exposure
EC	European Community
EC_{50}	Effect Concentration for the median or 50th percentile
ECB	Environmental Chemical Bureau
EEC	European Economic Community
EFTA	European Free Trade Association
EINECS	European Inventory Existing Chemical Substances
ELINCS	European List of Notified Chemical Substances
EQS	Environmental Quality Standard
ERA	Environmental Risk Assessment
ESR	Existing Substances Regulation
ETS	Environmental Toxicology Section
EU	European Union
EURAM	European Ranking Method
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice
HEDSET	Harmonised Electronic Data SET
HRA	Human Risk Assessment
HSE	Health and Safety Executive
IPS	Informal Priority Setting method

IUCLIDS	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
LC_{50}	Lethal Concentration for 50th percentile
LCA	Life Cycle Assessment
LEAPs	Local Environment Action Plans
LOAEL	Lowest Observable Adverse Effect Level
LOEC	Lowest Observable Effect Concentration
MATC	Maximum Acceptable Toxicant Concentration
NC EHS	National Centre for Ecotoxicology and Hazardous Substances
NOAEL	No Observable Adverse Effect Level
NOEC	No Observable Effect Concentration
NONS	Notification Of New Substances
OECD	Organisation for Economic Co-operation and Development
PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
PPE	Personal Protective Equipment
(Q)SAR	(Quantitative) Structural Activity Relationship
RA	Risk Assessment
RCR	Risk Characterisation Ratio
RPE	Respiratory Protective Equipment
SETAC	Society of Environmental Toxicology and Chemistry
SNIF	Standard Notification Interchange Format
STP	Sewage Treatment Plant
TGD	Technical Guidance Document
UVCB	Substances of Unknown or Variable Composition, complex reaction products or Biological material
WAF	Water Accommodated Fraction
WWTP	Waste Water Treatment Plant

5 References

EC; 1996; Technical Guidance Document In Support Of Commission Directive 93/67/EEC On Risk Assessment For New Notified Substances And Commission Regulation (EC) No 1488/94 On Risk Assessment For Existing Substances

Vermeire T.G., Jager D.T., Bussian B., Devillers J., denHaan K., Hansen B., Lundberg I., Niessen H., Robertson S., Tyle H. and Van der Zandt P.T.J.; 1997; European Union System for the Evaluation of Substances (EUSES) - Principles and Structure; Chemosphere; Vol.34, No.8, pp.1823-1836

36 Month Report

ENVIRONMENT
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BRUNEL
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Engineering Doctorate in Environmental Technology

36 Months Report

1st October 2000

By
Nik Robinson

Contents

Executive Summary

This report is the sixth six-monthly report tracking the progress of my research work throughout the duration of the Engineering Doctorate course. It contains an introduction to, and review of the work undertaken during this period as well as updated time-plans and a Gantt chart of the remaining period of registration on the Engineering Doctorate. For a more general introduction to the Environment Agency and the National Centre for Ecotoxicology and Hazardous Substances (NCEHS), I refer the reader to the first six-month report in this portfolio.

During this period the report on the work with the Direct Toxicity Assessment (DTA) Section was finally completed and research on the first of the two proposed projects (see 24-month report) commenced. The work on the sensitivity analysis of the PEC (Predicted Environmental Concentration) calculation has been significant and resulted in many new opportunities for further work. This six-month period also includes the author's attendance at the SETAC World Congress Conference in Brighton, where a poster presentation was made. Further more the author participated in the 2-week, EuroLabsCourse in Ravenna, Italy, on Environmental Risk Assessment: Advanced Laboratory Techniques.

The aims and objectives from the previous period have been reviewed and new objectives for the next six-month period are outlined. Finally, a revised Gantt chart is included, showing the proposed timescales for the remaining research, with modules and other overlapping commitments indicated. There is also a glossary of terms at the end of this report.

1 Introduction

This period has seen much progress with the research and more specifically on the sensitivity analysis of the Predicted Environmental Concentration (PEC) calculation. This was one of the projects proposed for further research in the 24-month dissertation. The progress on this project is detailed as well as the further work this project has led on to.

Also during this period the progress of the current research has been presented at various forums including:

- An internal Cascade Brief meeting
- The Brunel University Graduate School poster presentation
- And the SETAC World Congress at Brighton

Two modules were also completed during this period, Environmental Management Systems, and Economic Approaches. A third module, Materials, was missed due to overlap with the EuroLabsCourse. The assignments for the modules completed can be found in the author's portfolio.

During this period the author also applied for and was accepted on a EuroLabCourse under the European 5th Framework. The course was entitled Environmental Risk Assessment: Advance Laboratory Techniques, and covered the entire process from sample collection to extraction and then final analyses and testing. The course was based in Ravenna, Italy and there were 24 students from all over Europe including Spain, Hungary, Bulgaria, Finland, Germany and Portugal.

Finally this period included the annual Engineering Doctorate Conference, at which the author gave a 20 minute oral presentation on the PEC sensitivity research work.

2 Review

2.1 Objectives from the Last Period:

The objectives outlined in the 30-month report at the beginning of this period can be seen repeated below (Box 1).

- PEC Calculation Sensitivity Analysis
  - Continue sensitivity analysis of Notification data, including production of poster presentation of initial results for SETAC conference (end May)

    – 27/04/2000
  - Write up project report, and papers

    01/05/2000 – 16/06/2000
- Proposed Period of work at Head Office (further details to follow)

  19/06/2000 – 08/09/2000
- EngD Conference 2000
  - Decide on paper title and abstract

    05/2000
  - Produce conference paper

    03/07/2000 – 07/07/2000
  - Produce conference presentation

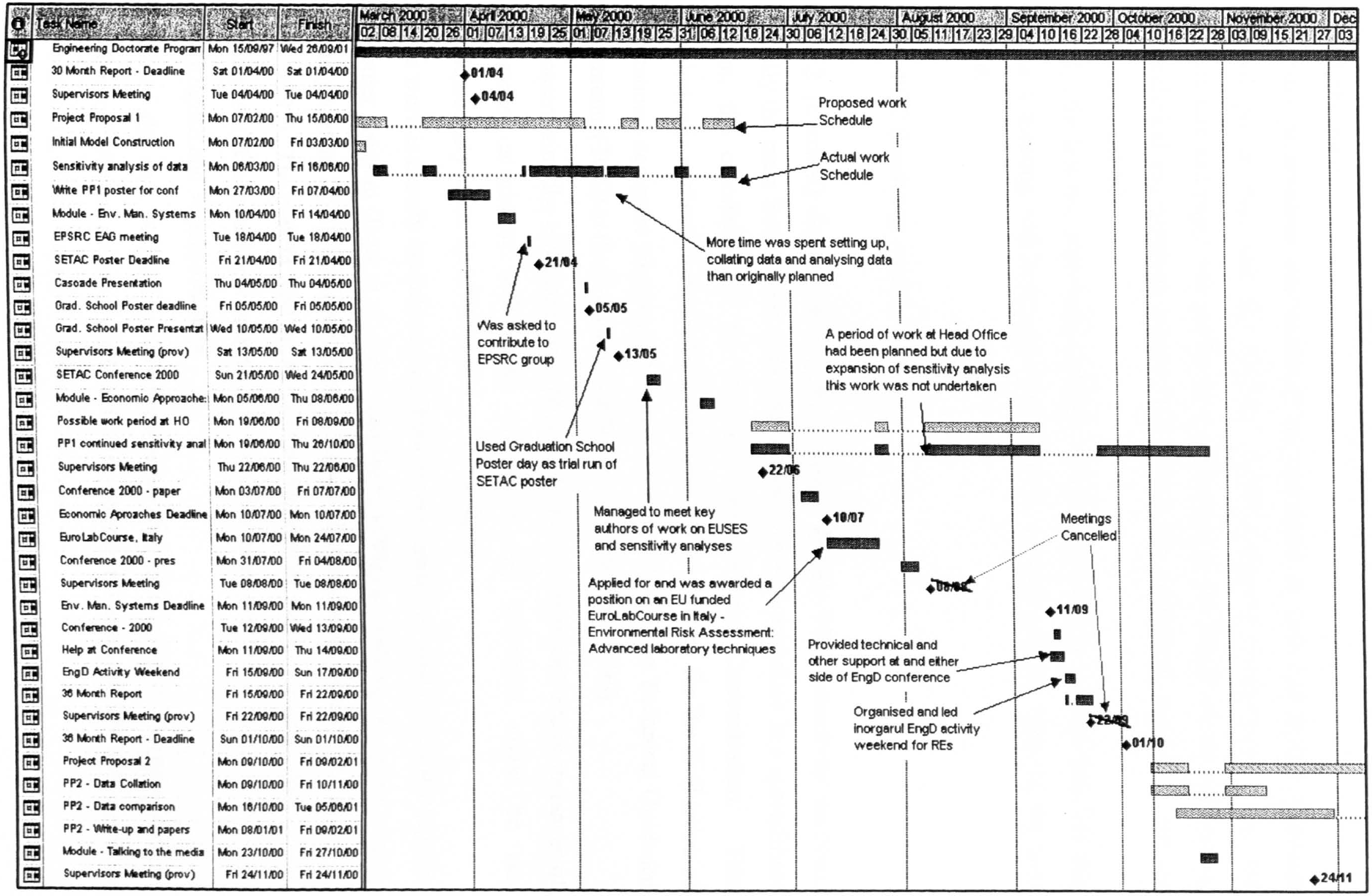
    31/07/2000 – 04/08/2000
  - Conference

    12/09/2000 – 13/09/2000

Box 1 - Objectives set from previous 6-month period

A copy of the Gantt chart for this six-month period can be found on the following page, detailing where significant variations from the proposed times have been made. It can be seen that the time spent on the PEC sensitivity analysis, has been more than originally anticipated. There are two reasons for this, firstly that the creation of the spreadsheet to perform the calculations along with the necessary external inputs and "black box" models took longer to obtain than expected. Secondly, the scope of the project has broadened and further work has continued along new lines of investigation, not outlined in the original project proposal.

Gantt Chart from Previous Period, with Actual Time Spent and Comments



Task Name	Start	Finish
Engineering Doctorate Program	Mon 15/09/97	Wed 26/09/01
30 Month Report - Deadline	Sat 01/04/00	Sat 01/04/00
Supervisors Meeting	Tue 04/04/00	Tue 04/04/00
Project Proposal 1	Mon 07/02/00	Thu 15/06/00
Initial Model Construction	Mon 07/02/00	Fri 03/03/00
Sensitivity analysis of data	Mon 06/03/00	Fri 16/06/00
Write PP1 poster for conf	Mon 27/03/00	Fri 07/04/00
Module - Env. Man. Systems	Mon 10/04/00	Fri 14/04/00
EPSRC EAG meeting	Tue 18/04/00	Tue 18/04/00
SETAC Poster Deadline	Fri 21/04/00	Fri 21/04/00
Casoade Presentation	Thu 04/05/00	Thu 04/05/00
Grad. School Poster deadline	Fri 05/05/00	Fri 05/05/00
Grad. School Poster Presentat	Wed 10/05/00	Wed 10/05/00
Supervisors Meeting (prov)	Sat 13/05/00	Sat 13/05/00
SETAC Conference 2000	Sun 21/05/00	Wed 24/05/00
Module - Economio Approache:	Mon 05/06/00	Thu 08/06/00
Possible work period at HO	Mon 19/06/00	Fri 08/09/00
PP1 continued sensitivity anal	Mon 19/06/00	Thu 26/10/00
Supervisors Meeting	Thu 22/06/00	Thu 22/06/00
Conference 2000 - paper	Mon 03/07/00	Fri 07/07/00
Economic Aproaches Deadline	Mon 10/07/00	Mon 10/07/00
EuroLabCourse, Italy	Mon 10/07/00	Mon 24/07/00
Conference 2000 - pres	Mon 31/07/00	Fri 04/08/00
Supervisors Meeting	Tue 08/08/00	Tue 08/08/00
Env. Man. Systems Deadline	Mon 11/09/00	Mon 11/09/00
Conference - 2000	Tue 12/09/00	Wed 13/09/00
Help at Conference	Mon 11/09/00	Thu 14/09/00
EngD Activity Weekend	Fri 15/09/00	Sun 17/09/00
36 Month Report	Fri 15/09/00	Fri 22/09/00
Supervisors Meeting (prov)	Fri 22/09/00	Fri 22/09/00
36 Month Report - Deadline	Sun 01/10/00	Sun 01/10/00
Project Proposal 2	Mon 09/10/00	Fri 09/02/01
PP2 - Data Collation	Mon 09/10/00	Fri 10/11/00
PP2 - Data comparison	Mon 16/10/00	Tue 05/06/01
PP2 - Write-up and papers	Mon 08/01/01	Fri 09/02/01
Module - Talking to the media	Mon 23/10/00	Fri 27/10/00
Supervisors Meeting (prov)	Fri 24/11/00	Fri 24/11/00

Proposed work Schedule

Actual work Schedule

More time was spent setting up, collating data and analysing data than originally planned

Was asked to contribute to EPSRC group

Used Graduation School Poster day as trial run of SETAC poster

Managed to meet key authors of work on EUSES and sensitivity analyses

Applied for and was awarded a position on an EU funded EuroLabCourse in Italy - Environmental Risk Assessment: Advanced laboratory techniques

A period of work at Head Office had been planned but due to expansion of sensitivity analysis this work was not undertaken

Meetings Cancelled

Provided technical and other support at and either side of EngD conference

Organised and led inorgarul EngD activity weekend for REs

Other points to notice in this review of the Gantt chart are that the period of work at Head Office did not take place. Also, two weeks were spent in Italy at the EuroLabCourse.

A poster presentation was produced and presented at both the Brunel Graduate School poster day, and the SETAC World Congress conference. An oral presentation and paper was produced and presented at the EngD annual conference, and technical and computer support was given to the conference organisers over the conference period.

Finally, the last two supervisor meetings of this period had to be cancelled, for this reason a meeting with both supervisors will be of high priority early in the next period.

2.2 PEC Sensitivity Analysis Project:

Box 2 (overleaf) details the original proposal for the PEC sensitivity analysis. Initially the main focus of the work was to elucidate and reproduce in a spreadsheet format, the calculation for the Predicted Environmental Concentration. This calculation is outlined in the EUSES (European Union System for the Evaluation of Substances) computer program (Vermeire *et al.*, 1997), and the Technical Guidance Documents (TGD) to the European Notification System (EC, 1996).

By constructing the calculation in a Microsoft Excel spreadsheet, many instances of the same calculation with small differences and variances could be run simultaneously to see the effect on the resulting figures.

Some work is already available in the literature on sensitivity analyses of the EUSES computer program (Jager *et al.*, 1997, and Jager, 1998a) as well as an earlier version of the program USES (Uniform System for the Evaluation of Substance) (Jager & Slob, 1995). The present work however is intended to be particular to the situation in England and Wales and how representative the European generic assessment is of the UK (English and Welsh) situation.

Some of the data supplied in Notification dossiers is classed as "commercial in confidence", for this reason a confidentiality agreement with the CAU was signed at the beginning of this work (see Appendix 6.1).

Project Proposal 1

Sensitivity analysis of values in the environmental exposure section of the European Notification risk assessment system as performed in the EUSES computer program.

Project Area/Group: Chemical Assessment Unit

Background:

As part of the notification system a standard base set of information has to be supplied from which a risk assessment is made. The UK Competent Authority (the CAU and HSE) has approximately 1200 such notification records, and the New Chemical Database (NCD) has approximately 6500 records at the European Chemical Bureau (ECB). By conducting a detailed sensitivity analysis on the data variables that are used, it can be determined which values are of greatest importance and have the greatest effect on the calculation. This would mean in the case where an assessment highlights a cause for concern, the costs and benefits of refining the PEC or the PNEC values would be better understood.

Objectives:

Overall objective: To carry out a sensitivity analysis on the variables supplied in a notification in order to relate their effect on the calculated PEC value.

Specific objectives (i): To analyse and study the interrelation of various variables e.g. solubility, vapour pressure and partition coefficients in order to inform the multivariate sensitivity analysis.

Specific objectives (ii): To carry out single and multivariate sensitivity analysis on the PEC calculation of the EU notification process, in order to highlight critical and sensitive variables.

Specific objectives (iii): To report findings, including those variables with the most significant effect on the PEC value in order to allow these factors to be considered when planning further testing to refine assessments.

Methodology:

From the 1200 records held by the CAU, those with full base sets of data can be found and an initial trial sample selected and analysed.

A fuller analysis could then be made using all records that satisfy the base set and any other requirements.

Once the sensitive values have been highlighted, these findings could then be confirmed through the analysis of the full NCD data set at the ECB.

Risks and Constraints:

Initially methods for sensitivity analysis will need to be investigated, to see whether a standard spreadsheet can be used or whether some form of MATLAB or C++ program is required. Also the CAU's New Chemicals data set needs to be checked to highlight those suitable for study.

In-depth sensitivity analysis of available and suitable UK data set records, with a view to highlighting the key variables in the PEC calculation, those having the greatest effect on the resulting PEC value. Reporting and publishing of sensitivity findings.

The larger EU data set could then be analysed in light of findings from UK sensitivity analysis to confirm these finding in the larger, EU database. Reporting and publishing of results will ensue.

Some form of blind labelling system may be required to protect the 'commercial in confidence' nature of some of the data. The further analysis of the EU database would help to strengthen previous findings but would not be essential.

Box 2 – Project Proposal 1 from 24-Month Dissertation

The initial task was to construct the calculations as detailed in the TGD and EUSES in a Microsoft Excel spreadsheet. This done, the calculation had to be validated by entering known data into both EUSES and the Excel spreadsheet (see Appendix 6.2) to ensure both gave the same values and answers.

Having confirmed agreement between the Excel spreadsheet calculation system (henceforth termed as NEXCES) and EUSES, work commenced on correcting some of the more important problems that have been highlighted with the EUSES software. The European Chemical Board (ECB) holds a Black List of bugs that users have found in the program EUSES that it publishes on the Internet (http:/ecb.ei.jrc.it/Euses/blacklst.htm, see Appendix 6.3). Any bugs pertinent to NEXCES were fixed in the spreadsheet these include:

- Concentration in effluent is sometimes calculated as greater than solubility in water – fix: if $Clocal_{eff} > SOL$ then $Clocal_{eff} = SOL$
- Estimation of Koc from Kow uses default QSAR for "predominantly hydrophobic" chemical class, not possible to choose any of other QSARs available and detailed in TGD – fix: Lookup box to allow choice of available QSARs
- TGD outlines two options for calculating Dilution value, 10th-percentile of low-flow or 1/3 of average flow, only former available in EUSES – fix: Dilution is entered as default or changed manually to investigate sensitivity
- The TGD uses SimpleTreat 1.0 to model a Sewage Treatment Plant (STP), only using integers to calculating values, EUSES uses an early version of SimpleTreat 3.0 but gives different results to the current SimpleTreat 3.0 debugged (Stuijs, 1996) – fix: SimpleTreat 3.0 debugged obtained and used for calculating STP emission values

Data Used in PEC Calculation

The physico-chemical data supplied under the base set that are used in the PEC calculation, and the values used in this initial analysis are as shown in Table 1 (overleaf).

Description	Symbol	Example	Units
Molecular weight	*MOLW*	197.28	(g/mol)
Vapour pressure at 25°C	*VP*	0.043	(Pa)
Octanol-water partition coefficient	*Kow*	10000	(-)
Water solubility	*SOL*	7.5	(mg/l)

Table 1 - Base-Set Physical-Chemical Data Used

Further information and assumptions:

Biodegradability - Substance assumed to be non-biodegradable (initially)

Chemical class - In EUSES this is assumed to be "predominantly hydrophobics" for the purpose of selecting a Koc from Kow QSAR. However in NEXCES it is possible to select any of the QSARs. The "predominantly hydrophobics" QSAR value is still used as a default.

E.local.water - Local emission rate to water assumed to be: 0.5 (kg/d) allows use category and A&B tables to be ignored at this initial stage.

PEC.regional.water - Regional PEC assumed to be: 0.0 (mg/l) this is a fair assumption due to low tonnage at base set and results in ease of subsequent calculations.

Description	Symbol	Example	Units
Local emission rate to waste water during episode	*E.local.water*	0.5	(kg/d)
Regional conc. in surface water	*PEC.regional.water*	0	(mg/l)

Table 2 – Assumption for Data Values Used

Default values taken from the EU model and EUSES calculation:

Description	Symbol	Example	Units
Capacity of the STP	*CAPACITY.stp*	10000	(eq)
Sewage flow per inhabitant	*WASTE.inhab*	200	(l/d/eq)
Weight fraction of organic carbon in suspended solids	*Foc.susp*	0.1	(kg/kg)
Dilution Factor	*DILUTION*	10	(-)
Concentration of suspended matter in river	*SUSP.water*	15	(mg/l)

Table 3 - Default Data Values Used

Early Sensitivity Analyses

The European Notification System and risk assessment calculations are intended to produce generic, European wide assessments, however in this work the sensitivities of the PEC calculation and how representative it is of the UK situation were investigated. The measured and default values in the calculation were varied and the effects of these variations on the PEC and the resulting risk assessment were examined. Initially the following investigations were made:

- The sensitivity of the PEC value to the estimated organic carbon partition coefficient (Koc) value
- The effect and applicability of the default dilution factor for receiving waters in the UK

Sensitivity within PEC calculation to organic carbon partition coefficient (Koc):

The adsorption/desorption properties of a substance indicate the tendency for that substance to partition or migrate between the air, water, soil and sediment compartments of the environment. The organic carbon normalised sorption coefficient (Koc) is not always available as a measured value in the base set of data submitted for new chemicals. Analytical measurement of the Koc value can be problematic, therefore there are three options available:

1. Measured Kow value (octanol-water partition coefficient) and QSARs (Quantitative Structural Activity Relationships) (Binten & Devillers, 1994; Sabljic & Güsten, 1995) are used to obtain an estimated value of the Koc
2. HPLC (High Performance Liquid Chromatography) analysis method (OECD Test Guideline 121, 1999) used to obtain an estimate of Koc
3. Batch equilibrium method (OECD Test Guideline 106, 1998) using three standard soil types used to measure Koc

Both the soil and sediment sorption coefficients, and the SimpleTreat model are among the values dependent upon the carbon normalised partition coefficient (Koc). A measured Koc value has now become a requirement at base set, however, if major concerns are not highlighted in the initial risk assessment, this value can be supplied post notification to the Competent Authority. In cases where a measured value is not supplied the Koc can be approximated from the base set Kow value. Quantitative Structure Activity Relationships (QSARs) are used to make an estimation of the Koc value from the measured Kow value. Table 4 outlines some of the equations presented in the QSARs for the prediction of the organic carbon-water partition coefficient (Koc) from the octanol-water partition coefficient (Kow), based on chemical class/structure.

Some problems arise in the measurement of Kow for substances such as surfactants, where the Kow is experimentally hard to determine, and may not properly describe the substances surface activity for these substances a measured Koc value may prove more realistic.

Chemical Class	**Equation**
Predominantly hydrophobics	log Koc = 0.81 log Kow + 0.10
Non-hydrophobics	log Koc = 0.52 log Kow + 1.02
Alcohols	log Koc = 0.39 log Kow + 0.50
Amides	log Koc = 0.33 log Kow + 1.25
Anilines	log Koc = 0.62 log Kow + 0.85
Esters	log Koc = 0.49 log Kow + 1.05
Nitrobenzenes	log Koc = 0.77 log Kow + 0.55
Organic acids	log Koc = 0.60 log Kow + 0.32

Table 4 - QSARs for the partition coefficient of organic carbon-water

In this study, this first method, the estimation of Koc from Kow using QSARs was used because the notification data available for the chemicals examined did not included measured Koc values.

For the modelling of the Sewage Treatment Plant (STP) the SimpleTreat 3.0 model (Struijs, 1996) is used. This model calculates the fractions of the substance that are degraded and directed to air, water and sludge as a function of the log of Henry's Law constant and log Kow, depending on how degradable (See Table 5), the substance is classed as.

Class	Description
No Biodegradability	k.deg = 0 hr^{-1}
Inherent Biodegradability	k.deg = 0.1 hr^{-1}
Ready Biodegradability (outside window)	k.deg = 0.3 hr^{-1} – fulfilled outside of 10-day window criterion
Ready Biodegradability (within window)	k.deg = 0.3 hr^{-1} – fulfilled within 10-day window criterion

Table 5 - Classes of biodegradeability (EC, 1996)

For a non-biodegradable substance, the fraction of the substance being emitted in the aqueous effluent from the STP, under the TGD calculations is found in the following table (Table 6).

%		log.H									
		-4	-3	-2	-1	0	1	2	3	4	5
log.Kow	0	100	100	100	100	98	85	36	9	5	5
	1	100	100	100	100	98	85	36	9	5	5
	2	99	99	99	99	97	84	36	9	5	5
	3	96	96	96	96	94	82	35	6	5	5
	4	79	79	79	79	77	68	30	6	5	4
	5	39	39	39	39	39	35	19	6	4	4
	6	15	15	15	15	15	14	11	6	4	4

Table 6 – Percentage fraction emitted to water from STP (EC, 1996)

As can be seen, because of the nature of this table only integer values can be looked up. In NEXCES values are calculated using the SimpleTreat 3.0 debugged model and therefore are not restricted to whole integers. The SimpleTreat model is also a Microsoft Excel spreadsheet but is self-contained and read-only in nature. Rather than attempting to re-create the model, a small Microsoft Macro was written to take the required input values from each column in NEXCES run them through the SimpleTreat spreadsheet and then enter the resulting output values back into NEXCES for each column of data. For further details and to see the code used for this macro see Appendix 6.4 and PEC Sensitivity Analysis report.

In the sensitivity calculations as mentioned, the regional PEC value, or background concentration, is assumed to be zero. This means the equation for PEC_{water} can then be stated as shown in Equation 1 (overleaf).

$$PEC_{water} \equiv Clocal_{water} = \frac{Clocal_{eff}}{\left[1+\left(Kp_{susp} \times SUSP_{water} \times 10^{-6}\right)\right]DILUTION}$$

Equation 1 – Predicted Environmental Concentration in Local Water

$Clocal_{water}$	Local concentration in surface water during emission episode	(mg.l^{-1})
$Clocal_{eff}$	Concentration of chemical in sewage treatment plant effluent	(mg.l^{-1})
Kp_{susp}	Solid-water partition coefficient of suspended matter	(l.kg^{-1})
$SUSP_{water}$	Concentration of suspended matter in river	(mg.l^{-1})
$DILUTION$	Dilution factor	(-)

The value $Clocal_{eff}$ is the concentration of the substance in the STP effluent, while the factors in the denominator account for dilution in the receiving water and the partitioning of the substance between the water and suspended matter.

Kp_{susp} is directly proportional to the Koc value, which was derived from the measured Kow. The $Clocal_{eff}$ value is dependent on the fractions of emissions directed to effluent by the STP. This is calculated by the SimpleTreat model and depends upon how biodegradable the substance is, its Henry's law constant and Koc value.

The physical and chemical data for a single chemical were used to initially investigate the theoretical variance of Koc. To do this ranges of values for Koc and fractions of emissions from STP were derived and the resulting risk characterisation ratios (RCR) were calculated. These were then plotted as a surface, Figure 1 (overleaf).

The surface graph allows us to see how the two values effect the resulting RCR value. It has been noted that the use of the RCR value in this graph is misleading, because ecotoxicological values are required to calculate a RCR value. Although actual chemical data were used and the RCRs calculated using this data, in subsequent graphs it was decided to just show the resulting PEC value rather than the RCR it would result in for that specific chemical.

As would be expected we can see that for low values of Koc, the RCR is directly proportional to the fraction of emissions directed to water by the STP (Sewage

Treatment Plant). Low values of Koc indicate that adsorption to soil, sediment or sludge will not be a significant process and the majority of the substance will remain in the water phase.

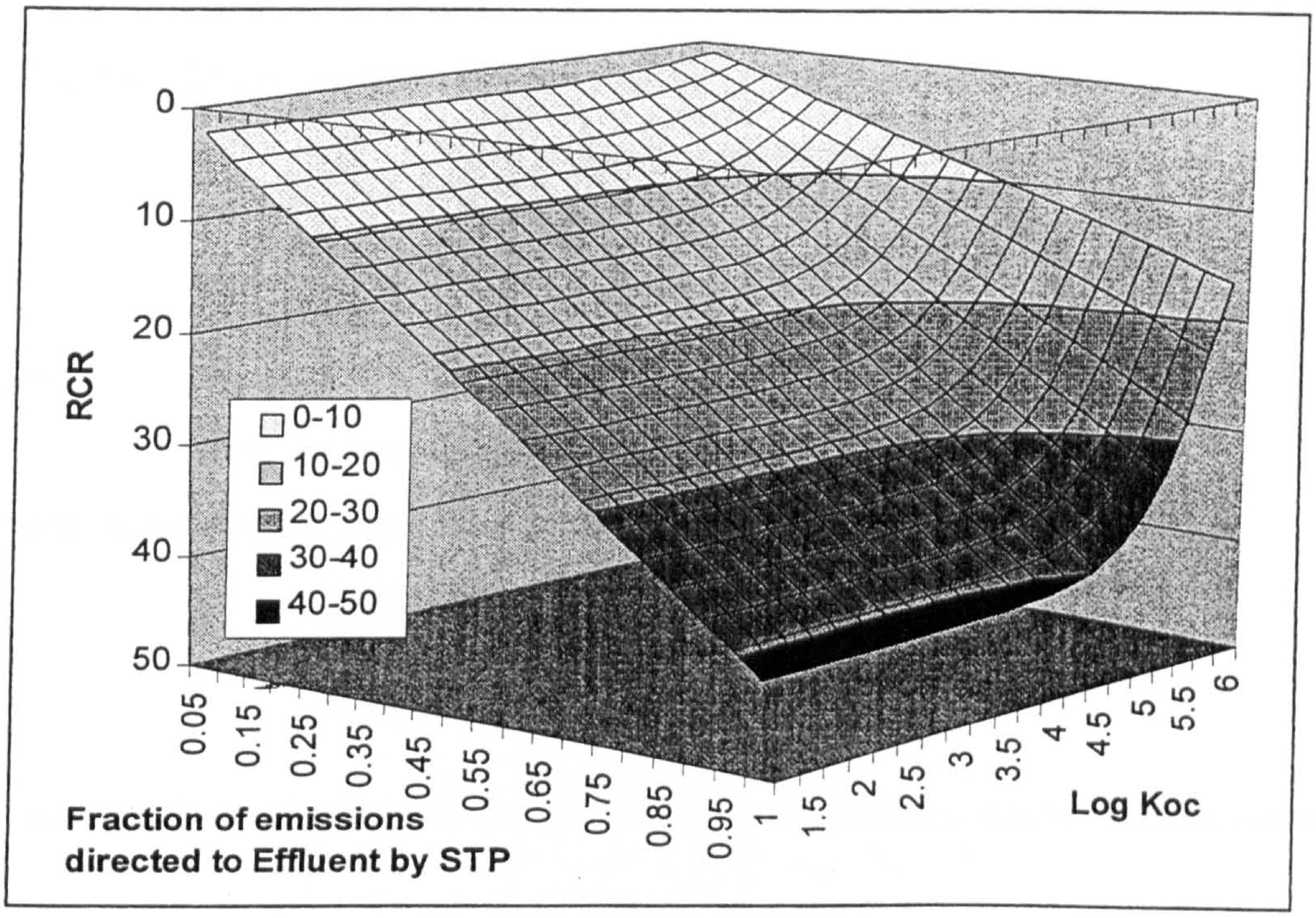


Figure 1 - The Effect of Koc and Fraction of Emission to Water from STP on RCR Value

However, when the value of Koc is high adsorption to suspended solids is high and a significant removal process, therefore the outcome of the risk assessment becomes very sensitive to the Koc value. It is possible to see from the graph that there is a rapid change in Koc between log Koc of 4 and 5.5. The PEC and resulting RCR value are very sensitive to variability in the Koc value in this region. When the Koc values for substances like this fall around this area, the uncertainty in their value will be of greater significance than for lower values of Koc where there is less sensitivity to the value.

Effect of dilution factor used on PEC calculation:

As mentioned the European Notification System aims for a generic European wide assessment; the effect of the default dilution factor used and how representative it is of UK scenarios was examined in this part of the study.

The dilution factor is a measure of how diluted the substance or effluent will become when emitted to a watercourse. The worse case EC default value for the dilution factor is 10, but in site specific assessments a dilution factor can be derived from 1/3 the mean flow or the 10th percentile low flow rate (EC, 1996). The denominator of the PEC calculation (Equation 1) is as follows:

$$\left[1+\left(Kp_{susp}\times SUSP_{water}\times 10^{-6}\right)\right]DILUTION$$

Equation 2 – Denominator of PEC calculation

Where: $Kp_{susp} = 0.1 \times Koc$

$SUSP_{water}$ is a default value, 15 mg/l

The denominator of the equation can therefore be stated as:

$$\left[1+\left(Koc\times 0.1\times 15\times 10^{-6}\right)\right]DILUTION$$

Equation 3 – Denominator of PEC calculation

This means where Koc < $1\text{x}10^5$ the denominator of the PEC equation approximates to:

$$PEC_{water}\equiv Clocal_{water}=\frac{Clocal_{eff}}{DILUTION}$$

Equation 4 – Predicted Environmental Concentration in Local Water, where Koc is Small

In such cases the magnitude of the dilution factor is of a greater importance. An initial investigation into the magnitude of available dilution values found along the River Thames was conducted. The higher the dilution factor, the lower the resulting RCR value. The EU default value is low when compared to some of the dilution factors available at points along the River Thames (see Figure 2 overleaf).

The default value of 10 for the dilution factor used in the PEC calculation may not be representative of all discharges in the UK. Further investigation into the derivation of the default dilution value is needed, and an assessment of where the uncertainties lie. From this data a better examination of how representative or worst case the default EU value for dilution is can be made.

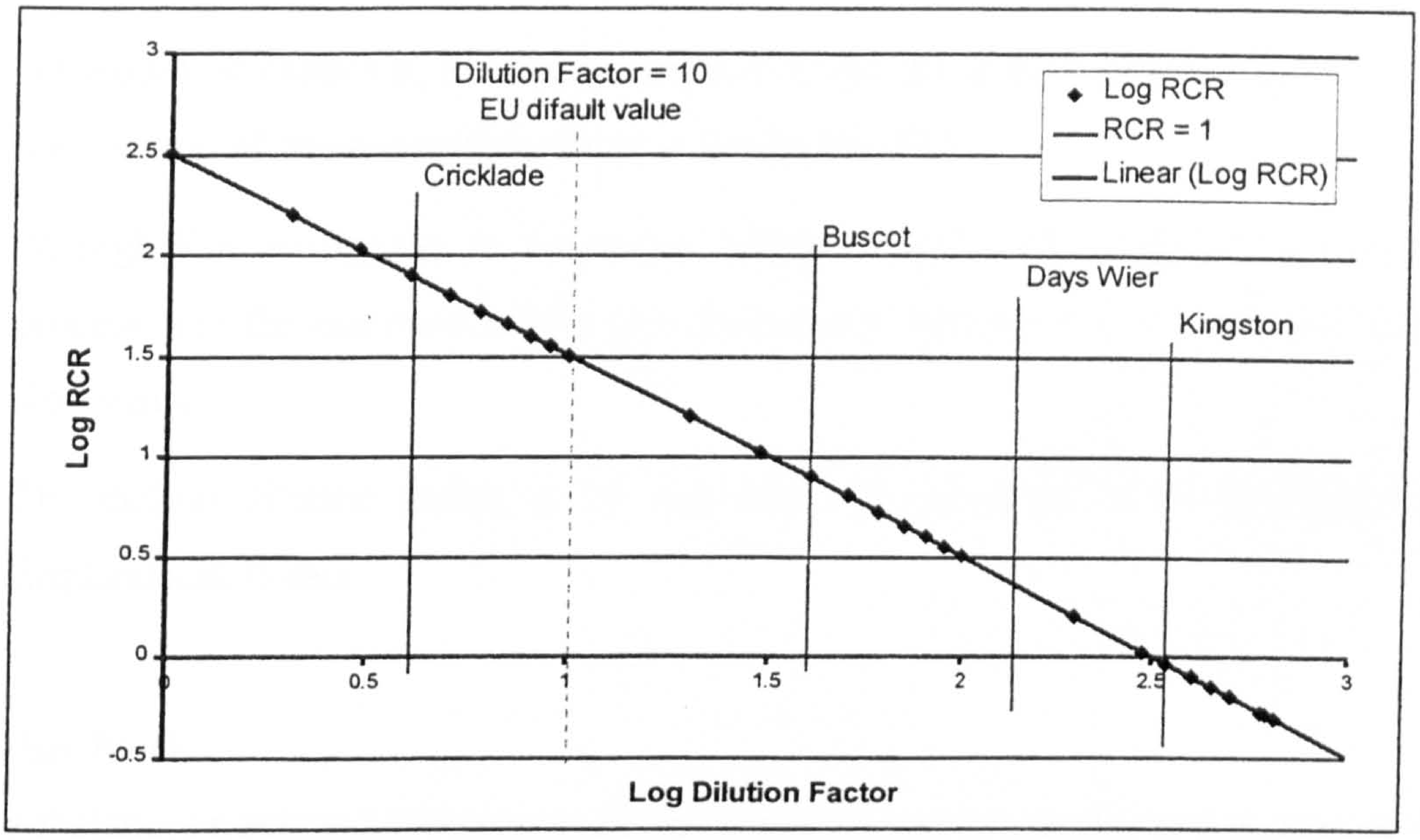


Figure 2 - Log RCR and Log Dilution Factor for the River Thames

From a investigation of dilutions factors available a distribution of values could be created and used to calculate a distribution of resulting PEC values. Then the level of uncertainty acceptable in the risk assessment would become a matter of policy rather than being implicitly considered within the assessment, (Jager *et al.*, 1997) see Figure 3.

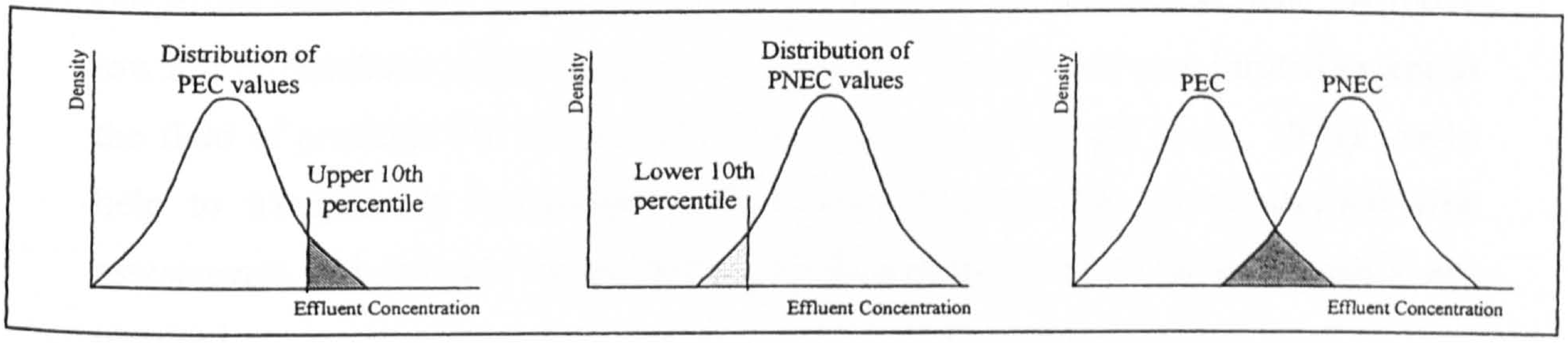


Figure 3 - Probabilistic Estimates of PEC and PNEC values and Risk Assessment Comparing Distributions

Initial Findings

The initial finding of this work show that the NEXCES spreadsheet developed in Microsoft Excel is a valuable and useful tool for modelling a variety of scenarios. The spreadsheet can be used to investigate and assess the sensitivity of the PEC calculation to variations in different parameters.

Initial investigations have also shown that:

- As would be expected, at low values of Koc the RCR is directly proportional to the fraction of emissions directed to water by the STP
- At high Koc adsorption to suspended solids is high and a significant removal process and the outcome of the risk assessment becomes very sensitive to the Koc value
- The default dilution factor of 10 may not representative of all discharges in England and Wales

Further Work

For substances marketed at low tonnage the risk assessments performed as part of the European Notification System often act more as a screening stage to highlight those substances of greater concern so that further data may be obtained. Although the aim of the risk assessment is for generic European-wide assessments, knowledge of the probability distributions for dilution factors and other parameters in the calculation would help to aid risk management decisions.

With a better knowledge and understanding of where the uncertainties in the PEC calculation lie, refinements in data collection and analysis can be made for those properties with the greatest effect on the outcome of the risk assessment. A move towards probabilistic risk assessment, an approach already used to a limited extent in the field of pesticide risk assessments (Solomon, 1996; Maund *et al.*, 1998), could help to transparently communicate the uncertainties within environmental risk assessments and indicate where further development of methods and models are required.

Further work has commenced on the analysis of the distribution of STP size (by population equivalents) and available dilution at discharge point. Two datasets have been collated as detailed in Box 3 (overleaf).

Data Set 1

Size of STP by PE (population equivalents)

By region, receiving water and discharge name

1561 records, regional breakdown as follows:

Anglian	295	Midlands	285
North East	240	North West	154
South West	192	Southern	61
Thames	159	Wales	175

Data Set 2

Dilution Available at discharge point as:

quotient of micro-low-flow mean and STP consented mean flow

424 data records available, regional breakdown as follows:

Anglian	62	Midlands	108
North East	82	North West	74
South West	0	Southern	18
Thames	68	Wales	23

Within the data: 277 records Dilution < 10
98 records Dilution < 1

Many dilutions quoted as value available in ditch or drain at immediate point of emission

Only 192 records explicitly named as discharges to rivers

Box 3 – Size and Dilution Available Datasets for STPs in England and Wales

The findings from the completed and further work on the risk assessment process of the European Notification System, and the prescribed method of calculating PEC values within the risk assessment method it details, can be applied in the wider context of all environmental risk assessment methods. The European model has been used due to the highly detailed and prescribed system of assessment, but these findings are equally valid in other risk assessment systems, in the estimation of environmental concentrations.

Three parts of this research work have been highlighted as possible material for journal papers. The three areas break down as follows:

i. NEXCES – the spreadsheet tool developed for the calculation of PEC values and the sensitivity analyses of measured and default values with that calculation.

ii. Compilation and analysis of Sewage Treatment Plant (STP) data for England and Wales, including restrictions and problems inherent in the dataset.

iii. Detailing the probabilistic risk assessments performed using the STP data (ii) and the NEXCES model (i), and conclusions drawn from these analyses.

2.3 EPSRC External Advisory Group:

The author was asked to attend an EPSRC meeting and join the EPSRC External Advisory Group, (EAG). The aim of the group was to discuss and agree a strategy for the strengthening and maintaining of links with current and graduated EPSRC students.

The three main areas for consideration were:

- a student web site and what content would be needed and required
- incentives to stay in touch and other link-building exercises
- how feedback would be gained at key stages in the development and implementation

Although this day of work was not directly related to research aims and goals, the chance to feed into the process of improving student support and possible intellectual forums for current and graduated students was a valuable one. The results seemed positive and many of the suggestions were taken on board.

2.4 Presentations and Conferences:

During this period a number of opportunities to present the progress of this research were taken. These are outlined below.

Cascade Brief

At the Environment Agency, Cascade Briefs are delivered monthly to keep everybody in touch with the overall aims and objectives of the organisation, and to update all employees with information on new initiatives and projects. These briefings include messages from the Chief Executive which are passed down eventually to the bulk of the workers.

At the National Centre, the Cascade Brief meetings also offer an opportunity members of the Centre to present their progress on various projects to their colleagues. Such an opportunity was taken early in this period to present the initial findings from the PEC calculation sensitivity analysis. Positive feedback was received as well as many constructive points on were further consideration needed to be made.

It is intended to present the final findings of this sensitivity work at a later date, at a similar meeting.

Brunel Graduate School

An internal Brunel University poster presentations day is run in the Faculty of Technology on an annual basis. It was decided that this would provide an excellent opportunity to present the poster that was being prepared for the SETAC conference. An early draft of the poster was completed and submitted.

Feedback on the poster was okay at this event although the subject of the majority of the other posters was of a more classical engineering bias. The limited interest in the current research, received at this event may have been due to the low number of attendees with similar backgrounds and research interests.

SETAC World Congress

The World Congress of SETAC (Society of Environmental Toxicology and Chemistry) was held at Brighton in May of this period. A poster of the current research was presented as part of the Student Forum at this meeting. The work was well received and developed some interesting discussion, various comments made where noted.

While at the meeting the Workshop on Probabilistic Risk Assessment was attended, which gave a detailed introduction to this approach to risk assessments and its use to date in assessing pesticides. The knowledge gained has helped and aided the work on the sensitivity analysis research.

Finally, the conference provided opportunities to meet and discuss the current research with many of the key people in this field some of whom had been contacted via email. In particular Dr. Jack de Bruijn who was a main contact for the SimpleTreat model was able to provide a Microsoft Excel spreadsheet of the model for use in this research.

Also of interest was a piece of research completed by Arnd Weyers on the analysis of almost 700 base set notifications to assess the sensitivities of the three acute aquatic toxicity test organisms used. Also an assessment of which test organism was the main driving force for classification and labelling was made.

EngD Annual Conference

This year a 20-minute oral presentation was given at the annual Engineering Doctorate conference, held this year at Brunel. A paper was also written on the current research work, this paper can be found in the Conference Proceedings for the Engineering Doctorate Conference 2000.

2.5 EuroLabCourse:

The EuroLabCourse was titled:

Environmental Risk Assessment: Advanced analytical techniques

It was felt that this course would provide a further opportunity to bridge the author's knowledge gaps in the sampling and analysis of ecotoxicological samples. The course was held in Ravenna, Italy, from 10-21 July 2000.

These EuroLabCourses are financed under the European 5th Framework and are intended to be interdisciplinary events in fully equipped laboratories and should include zoological, botanical, microbiological, geochemical, chemical and social aspects in the course.

The event brought together international experts and students from different professional backgrounds and different Member and Associate States, and combined practical work, lectures and fieldwork.

The emphasis was on laboratory analytical procedures and risk assessment, performed at Montecatini Environmental Research Centre and the University of Bologna site in Ravenna. The course programme included the following:

Field activities:

- Cruise in the coastal lagoon of Ravenna and sediment sampling.
- Trip to the reservoir of Ridracoli: presentation of the Operational Centre, visit to the water laboratory and treatment plant, sampling cruise in the reservoir.
- Trip to the protected oasis of Punte Alberete and the wetlands in North Ravenna.

Practical laboratory exercises:

- Analysis of organic and inorganic contaminants by GC/MS and ICP/AES in collected samples.
- Microbiology practise, Scanning Electron Microscopy (SEM) on environmental samples and pilot plants for bioremediation processes
- Vibrio fisheri luminescence inhibition test on sediment samples.

Lectures:

- Key background lecture - The State of the Environment and Contaminated Land.
- Environmental Impact Assessment on the port of Ravenna: characterisation of sediments in the view of their subsequent management.
- Research programs for soil remediation.
- Risk Assessment and Modelling.
- Reading the chronicle of 40 years of industrial pollution in the sediments of a coastal lagoon in Ravenna.
- The last two environmental accidents in Romania with cyanide and heavy metals.
- Environmental Risk of Chemicals: Assessment and reduction of the risk of contaminated sites.
- Occurrence of Polychlorinated biphenyl (PCBs) in soils: use of exogenous specialised biomass in their ex-situ aerobic bioremediation.
- European and Italian Law on Industrial Pollution.
- Criteria and Techniques for Monitoring and Sampling Coastal Areas.
- Biological metal mobilisation from metal-containing solids.
- Introductory lecture, In Vitro Transformation tests to assess the toxicological properties of environmental pollutants, and Scanning Electron Microscopy (SEM).
- Introductory lecture, Analysis of organic and inorganic contaminants in sediments by Gas Chromatography/Mass Spectrometry (GC-MS) and Inductively Coupled Plasma- Atomic Emission Spectrometry (ICP-AES).
- Introductory lecture, Ecotoxicological testing.
- Effectiveness of advanced instrumental techniques and sample preparation methods for the monitoring of traces of radioisotopes in the environmental and their risk assessment evaluation.
- Ecological Risk Assessment of sediments: Sediment Quality Triad (SQT) methodology.
- Sewage sludge disposal and utilisation possibilities.

2.6 Period of work at Head Office:

It was suggested that a short project at the Agency's Head Office would provide an opportunity to see how the current research fitted into the wider picture of the Agency's business. Steve Killeen, Head of Chemicals Policy, had been considering the possibility of combining health and environmental advice to SMEs (Small and Medium sized Enterprises) through a COSHH (Control Of Substances Hazardous to Health) type risk assessment approach. The Agency have an Intranet based system called NETREGS, and HSE (Health and Safety Executive) have a system for COSHH called COSHH Essentials, not yet available digitally. The proposed project involves an in-depth feasibility study of integrating these systems (see Box 4).

Objective

To respond to requests from SMEs for simple over-arching advice on chemicals control, encompassing both worker safety and environmental protection, by developing a unified chemical assessment system, accessible via the Internet.

Background

Current approaches by HSE to assist SMEs

HSE has recently published new guidance to help SMEs assess risks and control chemicals under the Control of Substances Hazardous to Health Regulations 1999 (COSHH). The guidance known as COSHH Essentials is a simple step by step guide through the risk assessment process leading to the selection of a control guidance sheet or sheets. These guidance sheets contain specific and targeted information on how to achieve adequate control for the particular chemical(s) and task(s) concerned. Public consultation gleaned that for the control of chemicals the distinction between worker and environmental protection is irrelevant to most firms, all they want is clear uniform guidance.

Current approaches by the environment Agency to assist SMEs

There are approximately 3.7 million businesses in UK 99.9% of which are SMEs's and 90% of which have less than 10 employees. To provide simple pollution control guidance to these businessses the Agency has been developing an Internet tool (NetRegs) which will become live in Autumn 2000. The approach differs from COSHH Essentials as it considers inputs and outputs from an SME site and provides management guidelines signposting regulatory requirements that would apply. This provides guidance on when an SME will come under different 'environmental' legislation and what they should do as a consequence.

Box 4 – Development of a Unified Chemical Assessment System for SMEs

Combining HSE and Agency approaches

The ultimate goal would be to integrate the two approaches to create an electronic, interactive, seamless system. This would enable users to extract sufficient information from one system to give them advice on how to control the risks from the substances they are using to worker's health and safety, and to the environment.

There would be clear benefits of such a system, should it prove feasible, in terms of reducing burdens on business by making compliance with health and safety and environmental legislation easier and more successful. The system would bring together the various aspects and requirements to one point of access, giving straightforward, practical and coherent guidance.

The availability of such a system should also meet wider objectives of waste minimisation and increased process efficiency and hence economic performance of the SME sector.

Feasibility

HSE and the Agency have conducted an initial assessment of the feasibility of developing a unified system.

Conclusions which can be drawn from this are:

- The starting points of the two systems are quite different. HSE focuses on chemicals while the Agency approach considers processes in a more holistic way.
- The strengths of the two systems are complimentary. HSE has developed a pragmatic hazard/risk assessment system, while the Agency has developed a comprehensive sign-posting system for legislative guidance and sector specific guidance.
- There is some degree of commonality in the underlying hazard information. COSHH Essentials is underpinned by information provided on safety datasheets under Chemicals (Hazard Information Packaging for Supply) regulations (CHIP).

Box 4 – Development of a Unified Chemical Assessment System for SMEs (continued)

After discussion with Supervisors it was decide not to pursue this project so late in the research programme. The PEC sensitivity analysis has produced many interesting areas for further work, which will be investigated in preference to the above project. Although it would have been nice to complete a period of work at the Agency's Head Office this project opportunity has come to late to fit into the remaining work schedule.

It is however still intended to review the research work completed in terms of the wider picture of the Agency's business and the goal of environmental protection, to conceptualise the work that has been completed as part of this Engineering Doctorate Programme.

2.7 Objectives Proposed for the Next Period:

Below in Box 5 the proposed objectives for the next period are outlined as well as an indication of timescales for the whole of the remaining period of registration.

- PEC Calculation Sensitivity Analysis

  Continue sensitivity analysis of Notification data,

  - Collate Regional Sewage Treatment Plant (STP) data
  - Analyse regional STP data and produce distribution curves for values – 30/10/2000
  - Write paper on analysis of Regional STP data 31/10– 10/11/2000
  - Probabilistic risk assessment using STP value distributions 13/11 – 22/12/2000
  - Write paper on probabilistic risk assessment using distribution data 3/1– 19/1/2001
  - Write paper on Excel spreadsheet model 22/1– 9/2/2001

  It is hoped that this work can be presented at an international conference some time in early 2001.

- Dissertation milestones
  - Outline of chapters and content 2/2/2001
  - Completed Introduction, background information... 1/6/2001
  - Complete first draft 27/7/2001

- 2020 Vision
  - Conceptualisation work 26/2 – 25/5/2000

Box 5 - Objectives proposed for then next 6 months

2.8 Aims and Objectives of the Engineering Doctorate Program:

Aims and Objectives of EngD Programme	How Attributes Have Been Demonstrated
REs should:	
(i) be equipped as engineering research-designers to plan and lead flexible and innovative R&D programmes that respond to customers' needs.	The work on the PEC sensitivity analysis has demonstrated both flexibility and innovation. A flexible approach has been required in obtaining and using the data obtained, which has not always been in the format required. Also the Excel spreadsheet model was developed to fulfil requirements not met by the existing PEC calculation models available.
(ii) be able to work effectively, and to form, work within and where necessary lead teams with a multi-disciplinary background to tight time schedules.	Much of the current work requires continual co-operation with contacts in Regional offices for data, as well as within the National Centre to ensure the right data is collated from the Regions, and that the analyses performed are appropriate.
(iii) possess comprehensive expert knowledge of the field of Environmental Technology, of techniques needed to balance social and economic benefit against resource utilisation and environmental impact, and of the processes of technology transfer needed to ensure the application of research into practice	The PEC calculation is and its underlying equations, as well as the default, measured and estimated values used to perform the calculation are understood in great detail. However, at each stage an effort is made to reflect on the wider picture and to put the relative sensitivity of values into the context of cost to the environment and industry. It is very important that in risk assessments that the methodologies are transparent and that any uncertainties are known along with an estimate of their magnitudes. This work aims to increase the transparency and knowledge of uncertainty of at least some of the values in the PEC calculation.
(iv) have demonstrated ability for originality and for innovation	Again the construction of the Excel spreadsheet, and STP data collation and analysis are both novel and innovative.
(v) possess a working knowledge of project management and business methods and their implications for research and development	When dealing with many data sources and trying to collate them all ready for analyses, timescales are very important, and the planning and project management has been very important in this part of the current research, to ensure realistic time constraints are given to those providing the data.
(vi) possess and have demonstrated a high level of communication and presentation skills	The progress on the current research has been presented in many different forums in this period, in a variety of media, including audio visual presentations, a written paper and poster presentations.

Table 7 – Progress to Date Towards Aims and Objectives of the Engineering Doctorate

The Joint Regulations (Section 4.4.1) also outline criteria that are necessary for eligibility to graduate as a Doctor of Engineering. Many of these are assessed as part of the taught modules, however two criteria of particular note are to be tested in the final *viva voce*, but are worth considering here and throughout the degree programme, these are to:

- Demonstrate evidence of innovation and a contribution to knowledge via research into either:
  - (i) novel understanding of the environmental consequences of systems for providing or using goods or services, or;
  - (ii) novel methods of improving the environmental performance of systems for providing or using goods or services thereby contributing to more sustainable development.
- Demonstrate an understanding of the context of the research: this must include the scientific context and, where appropriate should include the commercial and social context.

Further to these is the consideration that the work should meet the criterion of environmental technology, which is unique to the Brunel/Surrey Engineering Doctorate program. It is believed that this research will meet these criteria in the following ways:

The innovation and contribution to knowledge in this research shall primarily be in the area of risk assessment. The work on the Kennet & Avon Canal incident, although pollution management in a wider sense, did result in the production of some novel work including an analysis of the National Centre's contribution to the emergency response, and what expectations and requirements there were. It has not been decided however, whether this work will be presented in depth in the final dissertation.

From the initial study of existing risk assessment systems further areas of work were outlined and pursued. The PEC sensitivity analysis project is examining the sensitivities within the Notification System's calculation of predicted concentrations in the environment. However the findings from this work can and at least qualitatively will be applied more broadly to all environmental risk assessment systems, all of which must make some estimate of the concentration of a substance (or substances) in the environment.

An understanding of the context of the research will be necessary and demonstrated in the additional transparency this sensitivity works gives to the existing systems. The value of a sensitivity analysis on a calculation like this is that it can help to inform and direct further data requirements, research and model development.

This research is at the core of the activities of the NCEHS. As such environmental technology will be demonstrated through the development of improved risk assessment practices that while ensuring protection, don't over regulate, and where the main areas of variability and uncertainty are made more transparent. Such practices allow the regulators and environmental managers to make more informed decisions and help to promote sustainable development in the chemical field.

3 Project Planning Gantt Chart

The following insert is the updated version of the Gantt chart for this research work, showing all commitments and proposed periods of work until the end of registration for this course as well as proposed timescales for setting and sitting the assessment *viva voce*.

The milestones and periods of work outlined here are also detailed in Section 2.7.

ID	ⓘ	Task Name	Start
1	▦	Engineering Doctorate Program	Mon 15/09/97
2	▦	PEC sensitivity analysis	Mon 25/09/00
3	▦	36 Month Report - Deadline	Sun 01/10/00
4	▦	STW and Dilution data analysis	Mon 25/09/00
5	▦	Write paper on STW/dilution dat	Mon 30/10/00
6	▦	Supervisors Meeting (prov)	Fri 20/10/00
7	▦	Module - Talking to the media	Mon 23/10/00
8	▦	Probabilistic RA using STP/Dil.	Mon 13/11/00
9	▦	Write paper on probabilistic RA	Wed 03/01/01
10	▦	Module - (optional) Env. Man. Sy	Mon 04/12/00
11	▦	Supervisors Meeting (prov)	Fri 15/12/00
12	▦	Xmas 2000 HOLIDAY	Sat 23/12/00
13	▦	Write paper on Excel model/tool	Mon 22/01/01
14	▦	Module - (optional) Careers Advi	Thu 25/01/01
15	▦	Dissert. - Outline of chapters	Fri 02/02/01
16	▦	Write report on PEC project	Mon 12/02/01
17	▦	Supervisors Meeting (prov)	Fri 23/02/01
18	▦	Possible further work (2020 Visi	Mon 26/02/01
19	▦	42 Month Report	Mon 05/03/01
20	▦	42 Month Report - Deadline	Sun 01/04/01
21	▦	Supervisors Meeting (prov)	Fri 20/04/01
22	▦	Critical analysis and review - fina	Tue 29/05/01
23	▦	Dissert. - Intro., Bacground...	Fri 01/06/01
24	▦	Dissert. - First draft	Fri 27/07/01
25	▦	Submission of final dissertation	Mon 01/10/01
26	▦	Revision and viva prep.	Mon 01/10/01
27	▦	Viva Voce	Thu 01/11/01
28	▦	Corrections to dissertation	Mon 03/12/01
29	▦	Raleigh International	Mon 07/01/02

Project: EngD-99-2001
Date: Wed 26/09/01

Task	▬	Progress	▬	Summary	▬	Rolled Up Split	┈┈	Rolled Up Progress	▬	Project Summary	▬
Split	┈┈	Milestone	◆	Rolled Up Task	▬	Rolled Up Milestone	◇	External Tasks	▬		

ID		Task Name	Start
1		Engineering Doctorate Program	Mon 15/09/97
2		NEXCES Documentatio/paper	Wed 28/02/01
3		Submit NEXCES paper	Mon 02/04/01
4		42 Month Report - Deadline	Mon 02/04/01
5		Stats. analysis paper/pres.	Mon 02/04/01
6		Final draft of stas paper	Wed 18/04/01
7		Submit stats paper	Fri 04/05/01
8		SETAC conference Madrid	Sat 05/05/01
9		Stats. in NEXCES paper	Mon 14/05/01
10		Supervisors Meeting (prov)	Tue 22/05/01
11		Critical analysis and review - fin	Tue 29/05/01
12		Report Writing course	Tue 05/06/01
13		Materials Module	Mon 16/07/01
14		Dissert. - Intro., Bacground...	Fri 01/06/01
15		Dissert. - First draft	Fri 27/07/01
16		Dissert. - Final draft	Fri 31/08/01
17		Submission of final dissertation	Mon 01/10/01
18		Revision and viva prep.	Mon 01/10/01
19		Viva Voce	Thu 01/11/01
20		Corrections to dissertation	Mon 03/12/01
21		Raleigh International	Mon 07/01/02

Project: EngD-99-2001
Date: Wed 26/09/01

4 Glossary

The following is a glossary of terms that have been used and that have come up during this and other work at the Environment Agency.

AF	Assessment Factor
ALARA	As Low As Reasonably Achievable
ASL	Approved Supply List
BCF	Bio-concentration Factor
CA	Competent Authority
CAU	Chemical Assessment Unit
COSHH	Control Of Substances Hazardous to Health
CNU	Chemical Notification Unit
DETR	Department of the Environment, Transport and the Regions
DTA	Direct Toxicity Assessment
EA	Environment Agency
EASE	Estimation and Assessment of Substance Exposure
EC	European Community
EC_{50}	Effect Concentration for the median or 50th percentile
ECB	Environmental Chemical Bureau
EEC	European Economic Community
EFTA	European Free Trade Association
EINECS	European Inventory Existing Chemical Substances
ELINCS	European List of Notified Chemical Substances
EQS	Environmental Quality Standard
ERA	Environmental Risk Assessment
ESR	Existing Substances Regulation
ETS	Environmental Toxicology Section
EU	European Union
EURAM	European Ranking Method
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice
HEDSET	Harmonised Electronic Data SET
HRA	Human Risk Assessment
HSE	Health and Safety Executive

HTML	Hyper-Text Mark-up Language
IPS	Informal Priority Setting method
IUCLIDS	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
LC_{50}	Lethal Concentration for 50th percentile
LCA	Life Cycle Assessment
LEAPs	Local Environment Action Plans
LOAEL	Lowest Observable Adverse Effect Level
LOEC	Lowest Observable Effect Concentration
MATC	Maximum Acceptable Toxicant Concentration
NCEHS	National Centre for Ecotoxicology and Hazardous Substances
NEXCES	Nik's Excel Calculation for the Evaluation of Substances
NOAEL	No Observable Adverse Effect Level
NOEC	No Observable Effect Concentration
NONS	Notification Of New Substances
OECD	Organisation for Economic Co-operation and Development
PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
PPE	Personal Protective Equipment
(Q)SAR	(Quantitative) Structural Activity Relationship
RA	Risk Assessment
RCR	Risk Characterisation Ratio
RPE	Respiratory Protective Equipment
SETAC	Society of Environmental Toxicology and Chemistry
SME	Small to Medium Sized Enterprises
SNIF	Standard Notification Interchange Format
STP	Sewage Treatment Plant
TGD	Technical Guidance Document
UVCB	Substances of Unknown or Variable Composition, complex reaction products or Biological material
WAF	Water Accommodated Fraction
WWTP	Waste Water Treatment Plant

5 References

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42 Month Report

ENVIRONMENT
AGENCY

BRUNEL
UNIVERSITY

Engineering Doctorate in Environmental Technology

42 Months Report

1st April 2001

By
Nik Robinson

Executive Summary

This report is the seventh six-monthly and penultimate report tracking the progress of my research work throughout the duration of the Engineering Doctorate course. It contains an introduction to, and review of the work undertaken during this period as well as updated time-plans and a Gantt chart of the remaining period of registration on the Engineering Doctorate. For a more general introduction to the Environment Agency and the National Centre for Ecotoxicology and Hazardous Substances (NCEHS), I refer the reader to the first six-month report in this portfolio.

The work on the sensitivity analysis of the PEC (Predicted Environmental Concentration) calculation has continued. There has been some problems in compiling and analysing the Sewage Treatment Works data, and particularly in the statistical analysis needed of these data. Meanwhile the documenting of the spreadsheet model was completed and an example investigation carried out. This six-month period also included attendance at the European Member States' "Expert consultation on statistical extrapolation techniques for environmental effect assessment" in the capacity of an observer, and attendance at one of the Research Council's Graduate School Programmes.

The aims and objectives from the previous period have been reviewed and objectives for the final period are outlined. Finally, a revised Gantt chart is included, showing the proposed timescales for the remaining research, with modules and other overlapping commitments indicated. There is also a glossary of terms at the end of this report.

1 Introduction

This period has seen further progress with the research on the sensitivity analysis of the risk assessment procedure as part of the European Notification System. There has also been progress in the documentation of some of the aspects of this work that have been completed to date. Also the first of three papers for peer reviewed journals is about to be submitted to the journal of Environmental Toxicology and Chemistry, and acceptance has been received from SETAC (Society for Environmental Toxicology and Chemistry) for an oral presentation at the Madrid Conference in May.

One module was completed during this period; Talking to the media, which provided a great insight into communicating concepts succinctly and how to stick to key messages.

During this period the author was also invited to attend the European Member States' "Expert consultation on statistical extrapolation techniques for environmental effect assessment" as an observer. This proved to be a great insight into the development of European policy at the technical meeting level; it also provided an opportunity to meet key people in the research area.

A Research Council's Graduate School Programme was also attended, this being a weeklong team building and development programme. Much of the content only echoed topics that had previously been covered within the scope of the EngD modules, however the chance to work and inter-relate with PhDs and other EngD students of widely differing backgrounds and research areas was very useful and informative.

2 Review

2.1 Objectives from the Last Period:

The objectives outlined in the 36-month report at the beginning of this period can be seen repeated below (Box 1).

- PEC Calculation Sensitivity Analysis

  Continue sensitivity analysis of Notification data,
  - Collate Regional Sewage Treatment Plant (STP) data
  - Analyse regional STP data and produce distribution curves for values – 30/10/2000
  - Write paper on analysis of Regional STP data 31/10– 10/11/2000
  - Probabilistic risk assessment using STP value distributions 13/11 – 22/12/2000
  - Write paper on probabilistic risk assessment using distribution data 3/1– 19/1/2001
  - Write paper on Excel spreadsheet model 22/1– 9/2/2001

  It is hoped that this work can be presented at an international conference some time in early 2001.

- Dissertation milestones
  - Outline of chapters and content 2/2/2001
  - Completed Introduction, background information... 1/6/2001
  - Complete first draft 27/7/2001

Box 1 - Objectives set from previous 6-month period

2.2 The PEC Calculation Sensitivity Analysis

The original project proposal for this work is detailed in Box 2 in way of a summary of this work.

Through initial analyses of the data received from the National Centre for Environmental Data and Surveillance (NCEDS) it was found that the Dilution value was calculated in a different manner to the way the value is calculated in the EU risk assessment (see Box 3 for details).

Project Proposal 1

Sensitivity analysis of values in the environmental exposure section of the European Notification risk assessment system as performed in the EUSES computer program.

Project Area/Group: Chemical Assessment Unit

Background:

As part of the notification system a standard base set of information has to be supplied from which a risk assessment is made. The UK Competent Authority (the CAU and HSE) has approximately 1200 such notification records, and the New Chemical Database (NCD) has approximately 6500 records at the European Chemical Bureau (ECB). By conducting a detailed sensitivity analysis on the data variables that are used, it can be determined which values are of greatest importance and have the greatest effect on the calculation. This would mean in the case where an assessment highlights a cause for concern, the costs and benefits of refining the PEC or the PNEC values would be better understood.

Objectives:

Overall objective: To carry out a sensitivity analysis on the variables supplied in a notification in order to relate their effect on the calculated PEC value.

Specific objectives (i): To analyse and study the interrelation of various variables e.g. solubility, vapour pressure and partition coefficients in order to inform the multivariate sensitivity analysis.

Specific objectives (ii): To carry out single and multivariate sensitivity analysis on the PEC calculation of the EU notification process, in order to highlight critical and sensitive variables.

Specific objectives (iii): To report findings, including those variables with the most significant effect on the PEC value in order to allow these factors to be considered when planning further testing to refine assessments.

Methodology:

From the 1200 records held by the CAU, those with full base sets of data can be found and an initial trial sample selected and analysed.

A fuller analysis could then be made using all records that satisfy the base set and any other requirements.

Once the sensitive values have been highlighted, these findings could then be confirmed through the analysis of the full NCD data set at the ECB.

Risks and Constraints:

Initially methods for sensitivity analysis will need to be investigated, to see whether a standard spreadsheet can be used or whether some form of MATLAB or C++ program is required. Also the CAU's New Chemicals data set needs to be checked to highlight those suitable for study.

In-depth sensitivity analysis of available and suitable UK data set records, with a view to highlighting the key variables in the PEC calculation, those having the greatest effect on the resulting PEC value. Reporting and publishing of sensitivity findings.

The larger EU data set could then be analysed in light of findings from UK sensitivity analysis to confirm these finding in the larger, EU database. Reporting and publishing of results will ensue.

Some form of blind labelling system may be required to protect the 'commercial in confidence' nature of some of the data. The further analysis of the EU database would help to strengthen previous findings but would not be essential.

Box 2 – PEC Sensitivity Analysis Project Proposal from 24-Month Dissertation

When further information was requested from the NCEDS it was found that the data used to calculate the Dilution value were not available, for this reason the Regions were approached for the data individually.

European Union calculation for deriving Dilution Factor:

$$Dillution = \frac{Effluent\ discharge\ rate + River\ flow}{Effluent\ discharge\ rate}$$

Environment Agency calculation for deriving Dilution value:

$$Dillution = \frac{River\ flow}{Effluent\ discharge\ rate}$$

Where *River flow* is assumed to be equal to dry weather flow (DWF) or micro low flow mean, both of which are standard hydrometry measures

Effluent discharge rate is assumed to be equal to consented mean flow, which approximates to a reasonable worst case value

Box 2 - Equations for the calculation of Dilution for comparison

From the Regions it was possible to get the data split into consented mean flow and a measure for river flow, and then from these values the required Dilution value could be derived.

Another issue that arose from approaching the Regional offices for the data, was that to make the data request feasible a lower limit on the size of STPs that were of interest had to be specified. This meant that the data received would not be a true random sample of the distribution, being skewed by the lack of data below the lower cut-off point.

While collating these new data from the regions, an attempt was made to investigate the kinds of statistical methods that would be needed to interpret the data, and a start was made on the documenting of the spreadsheet model for the risk assessment of substances.

In documenting the spreadsheet model, the model itself was modified a number of times to make some of the functions and operations more transparent. Through running examples on the model it was found that in the Columns orientation that it was in, the limit to the number of runs per individual sheet was just over 250, whereas in Row orientation it was possible to have more than 5000 runs. The new layout for the spreadsheet is detailed in Table 1(a, b, c), Appendix 5.1 and a schematic of the risk assessment system and the equations used is also included in this Appendix (Figure 2).

2.3 Peer Reviewed Papers:

Three parts of the research had been highlighted as possible areas for journal papers. The three were:

i. NEXCES – the spreadsheet tool developed for the calculation of PEC values and the sensitivity analyses of measured and default values with that calculation.

ii. Compilation and analysis of Sewage Treatment Plant (STP) data for England and Wales, including restrictions and problems inherent in the dataset.

iii. Detailing the probabilistic risk assessments performed using the STP data (ii) and the NEXCES model (i), and conclusions drawn from these analyses.

The first paper has been completed and is due for submission to the Journal of Environmental Toxicology and Chemistry (Journal Impact Factor = 2.46). Feedback on early drafts of the paper suggested that a worked example demonstrating the power of the spreadsheet model to calculate many risk assessments simultaneously would aid understanding. This worked example took the form of an investigation of the effects of measurement error on the resulting RCR (Risk Characterisation Ratio) values.

The variability in the measurement of the octanol-water partition coefficient (*Kow*) and the vapour pressure (*VP*) of a test substance were investigated. The test guidelines as produced by the Organisation for Economic Co-operation and Develoment (OECD) for the two methods were used as standard error values.

It was assumed that variability would be normally distributed around the mean (Base Set) value and the error given in the test guidelines would be equal to 3 standard deviations (99.7 %) about this mean.

Then a number of runs of the calculation were performed with the *VP* or *Kow* set at a random value from the normally distribution of probable measured values. To determine the number of runs that were required to achieve a good statistical fit, normally distributed numbers with mean 0 and standard deviation 1 were generated at sample sizes of 100, 500, 1000, 2000, 5000 and 10000 (see Appendix 5.4). From the plot of these distributions it was found that visually the plots approached a normal distribution at 5000 samples and above. For this reason 5000 samples were run for each of the investigations (*VP*, *Kow*).

Two graphs were produced of the resulting RCR values from normally distributed *VP* values and from normally distributed log *Kow* values (see Appendix 5.1, Figures 3 & 4 respectively).

It is easily observed that the error from measurement can cause a far greater effect for the *Kow* value than for vapour pressure. The resulting range for the RCR within ±2 SD (this encompasses 95% of the data) of the mean, is 1.5 - 2.3 for variation in *Kow* and only 1.908 – 1.923 for variation in *VP*.

An attempt has been made to determine through which algorithm the random numbers are generated in Excel, however to date the only information that has been found is for the formula command RAND():

> The first random number:
> random_number=fractional part of (9821 * r + 0.211327),
> `where r = .5`
>
> Successive random numbers:
> random_number=fractional part of (9821 * r + 0.211327),
> `where r = the previous random number`
>
> This formula will provide up to 1 million different numbers.

(http://www.microsoft.com/support/, March 2001)

Work on the statistical analysis will be completed by early mid April and the resulting paper should be available for submission by the end of April, or just after return from the SETAC conference.

2.4 Presentations and Conferences:

No specific opportunities for presenting the research have been available during this period, however an Abstract was submitted to SETAC, and a poster has been prepared for the Brunel Graduate School poster day.

SETAC Conference, Madrid

An abstract was submitted and was accepted for a platform presentation at the Madrid conference in May. The title of the abstract was, "Standard and default values in the exposure assessment of chemicals in Europe" and the full submission can be found in Appendix 5.2. This presentation will include the preliminary and any further results and conclusions drawn from the analysis of the STP data that has been collated.

Brunel Graduate School

An internal Brunel University poster presentation day is run in the Faculty of Technology on an annual basis. A poster has been prepared demonstrating the work on the spreadsheet model and outlining an example investigation that has been carried out on the model. A copy of the poster is included in Appendix 5.3

2.5 Objectives Proposed for the Next Period:

Below in Box 5 the proposed objectives for the next period are outlined as well as an indication of timescales for the whole of the remaining period of registration.

- PEC Calculation Sensitivity Analysis
  - Analyse regional STP data and produce distribution curves for values – 18/4/2001
  - Completed paper on analysis of Regional STP data 04/5/2001
  - Probabilistic risk assessment using STP value distributions 14/5 – 30/5/2001
  - Completed paper on probabilistic risk assessment using STP data 30/5/2001
  - Present STP statistical work at SETAC, Madrid 5/5– 13/5/2001
- Thesis milestones
  - Completed Introduction, background information... 1/6/2001
  - Complete first draft 27/7/2001
  - Submit final draft 31/8/2001

Box 5 - Objectives proposed for then next 6 months

2.6 Aims and Objectives of the Engineering Doctorate Program:

Aims and Objectives of EngD Programme	How Attributes Have Been Demonstrated
REs should:	
(i) be equipped as engineering research-designers to plan and lead flexible and innovative R&D programmes that respond to customers' needs.	The work on the PEC sensitivity analysis has demonstrated both flexibility and innovation. A flexible approach has been required in obtaining and using the data obtained, which has not always been in the format required. Also the Excel spreadsheet model was developed to fulfil requirements not met by the existing PEC calculation models available.
(ii) be able to work effectively, and to form, work within and where necessary lead teams with a multi-disciplinary background to tight time schedules.	Much of the current work requires continual co-operation with contacts in Regional offices for data, as well as within the National Centre to ensure the right data is collated from the Regions, and that the analyses performed are appropriate.
(iii) possess comprehensive expert knowledge of the field of Environmental Technology, of techniques needed to balance social and economic benefit against resource utilisation and environmental impact, and of the processes of technology transfer needed to ensure the application of research into practice	The PEC calculation is and its underlying equations, as well as the default, measured and estimated values used to perform the calculation are understood in great detail. However, at each stage an effort is made to reflect on the wider picture and to put the relative sensitivity of values into the context of cost to the environment and industry. It is very important that in risk assessments that the methodologies are transparent and that any uncertainties are known along with an estimate of their magnitudes. This work aims to increase the transparency and knowledge of uncertainty of at least some of the values in the PEC calculation.
(iv) have demonstrated ability for originality and for innovation	Again the construction of the Excel spreadsheet, and STP data collation and analysis are both novel and innovative.
(v) possess a working knowledge of project management and business methods and their implications for research and development	When dealing with many data sources and trying to collate them all ready for analyses, timescales are very important, and the planning and project management has been very important in this part of the current research, to ensure realistic time constraints are given to those providing the data.
(vi) possess and have demonstrated a high level of communication and presentation skills	The progress on the current research has been presented in many different forums in this period, in a variety of media, including audio visual presentations, a written paper and poster presentations.

Table 1 – Progress to Date Towards Aims and Objectives of the Engineering Doctorate

The Joint Regulations (Section 4.4.1) also outline criteria that are necessary for eligibility to graduate as a Doctor of Engineering. Many of these are assessed as part of the taught modules, however two criteria of particular note are to be tested in the final *viva voce,* but are worth considering here and throughout the degree programme. These are to:

- Demonstrate evidence of innovation and a contribution to knowledge via research into either:
  (i) novel understanding of the environmental consequences of systems for providing or using goods or services, or;
  (ii) novel methods of improving the environmental performance of systems for providing or using goods or services thereby contributing to more sustainable development.
- Demonstrate an understanding of the context of the research: this must include the scientific context and, where appropriate should include the commercial and social context.

Further to these is the consideration that the work should meet the criterion of environmental technology, which is unique to the Brunel/Surrey Engineering Doctorate program. It is believed that this research will meet these criteria in the following ways:

The innovation and contribution to knowledge in this research shall primarily be in the area of risk assessment. The work on the Kennet & Avon Canal incident, although pollution management in a wider sense, did result in the production of some novel work including an analysis of the National Centre's contribution to the emergency response, and what expectations and requirements there were. This work will be presented briefly in the final thesis. The majority of the thesis however, will concentrate on the development of the NEXCES spreadsheet model, the underlying assumptions and background concepts, and the use of this with the STP data to demonstrate the level of protection afforded to particular situations in the UK by the European risk assessment system.

An understanding of the context of the research will be necessary and demonstrated in the additional transparency this sensitivity works gives to the existing systems. The value of a sensitivity analysis on a calculation like this is that it can help to inform and direct further data requirements, research and model development. The investigation of real STP values also demonstrates the level of protection afforded by the generic system to the country and regions within it.

This research is at the core of the activities of the NCEHS. As such environmental technology will be demonstrated through the development of improved risk assessment practices and greater knowledge of the sensitivities within them. Such practices allow the regulators and environmental managers to make more informed decisions and help to promote sustainable development in the chemical field.

3 Project Planning Gantt Chart

The following insert is the updated version of the Gantt chart for this research work, showing all commitments and proposed periods of work until the end of registration for this course as well as proposed timescales for setting and sitting the assessment *viva voce*.

The milestones and periods of work outlined here are also detailed in Section 2.5.

4 Glossary

The following is a glossary of terms that have been used and that have come up during this and other work at the Environment Agency.

AF	Assessment Factor
ALARA	As Low As Reasonably Achievable
ASL	Approved Supply List
BCF	Bio-concentration Factor
CA	Competent Authority
CAU	Chemical Assessment Unit
COSHH	Control Of Substances Hazardous to Health
CNU	Chemical Notification Unit
DETR	Department of the Environment, Transport and the Regions
DTA	Direct Toxicity Assessment
EA	Environment Agency
EASE	Estimation and Assessment of Substance Exposure
EC	European Community
EC_{50}	Effect Concentration for the median or 50th percentile
ECB	Environmental Chemical Bureau
EEC	European Economic Community
EFTA	European Free Trade Association
EINECS	European Inventory Existing Chemical Substances
ELINCS	European List of Notified Chemical Substances
EQS	Environmental Quality Standard
ERA	Environmental Risk Assessment
ESR	Existing Substances Regulation
ETS	Environmental Toxicology Section
EU	European Union
EURAM	European Ranking Method
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice
HEDSET	Harmonised Electronic Data SET
HRA	Human Risk Assessment
HSE	Health and Safety Executive

HTML	Hyper-Text Mark-up Language
IPS	Informal Priority Setting method
IUCLIDS	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
LC_{50}	Lethal Concentration for 50th percentile
LCA	Life Cycle Assessment
LEAPs	Local Environment Action Plans
LOAEL	Lowest Observable Adverse Effect Level
LOEC	Lowest Observable Effect Concentration
MATC	Maximum Acceptable Toxicant Concentration
NCEHS	National Centre for Ecotoxicology and Hazardous Substances
NEXCES	Nik's Excel Calculation for the Evaluation of Substances
NOAEL	No Observable Adverse Effect Level
NOEC	No Observable Effect Concentration
NONS	Notification Of New Substances
OECD	Organisation for Economic Co-operation and Development
PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
PPE	Personal Protective Equipment
(Q)SAR	(Quantitative) Structural Activity Relationship
RA	Risk Assessment
RCR	Risk Characterisation Ratio
RPE	Respiratory Protective Equipment
SETAC	Society of Environmental Toxicology and Chemistry
SME	Small to Medium Sized Enterprises
SNIF	Standard Notification Interchange Format
STP	Sewage Treatment Plant
TGD	Technical Guidance Document
UVCB	Substances of Unknown or Variable Composition, complex reaction products or Biological material
WAF	Water Accommodated Fraction
WWTP	Waste Water Treatment Plant

5 Appendices

Section	Title
5.1	Figures and Tables from new spreadsheet model
5.2	Abstract for SETAC Conference, Madrid
5.3	Poster for Brunel Graduate School
5.4	Distributions of Randomly Generated Normally Distributed Numbers

5.1 Figures and Tables from new spreadsheet model

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	P	Q
1	Name	MOLW	Kow	VP	SOL		Chemical Class	Biodeg	Prod Vol	Import	Export	L(E)C50 Fish	L(E)C50 Daphnia	L(E)C50 Algae	PECregional$_{water}$	
2	Comment	Base Set	Base Set	Base Set	Base Set		From pick list AX4:AX22	From pick list BB4:BB8	Base Set	Base Set	Base Set	Base Set	Base Set	Base Set	Assumed to be negligible	
3	Eqn. No.	~	~	~	~		~	~	~	~	~	~	~	~	~	
4	Value															
5	d/c/e	e	e	e	e		e	e	e	e	e	e	e	e	e (c)	
6	Units	g/mol	~	Pa	mg/l		~	~	Tonnes/Yr	Tonnes/Yr	Tonnes/Yr	mg/l	mg/l	mg/l	mg/l	
7	Calculation	197.3	10000	0.043	7.5		Predom. Hydro.	No Biodeg.	10	0	0	0.6	2.3	0.86	0	

Table 1 (a) - Complete spreadsheet for risk assessment of water compartment at local scale

	A	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
1	Name	Capacity$_{stp}$	Waste$_{inhab}$	Effluent$_{stp}$		Elocal$_{water}$	Kbio$_{stp}$	Log Koc	Koc	HENRY	Fstp$_{water}$	Clocal$_{inf}$	
2	Comment	Default	Default	= Capacity$_{stp}$ * WASTE$_{inhab}$		= Manually entered	Rate from descriptive value	Log Koc = x log Kow + y (from QSAR and chemical class)		= MW * VP / SOL	= Value from SimpleTreat model	= E.local$_{water}$ * 10000000 / Effluent$_{stp}$	
3	Eqn. No.	~	~	1 (19)		(2)	2, DEG1	4, QSAR1	5	6 (7)	ST3	7 (17)	
4	Value	10000	200			0.05							
5	d/c/e	d	d	c		e (c)	c	c	c	c	c	c	
6	Units	eq	l/d/eq	l/d		kg/d	h^{-1}	~	l/kg	Pa.m3/mol	~	mg/l	
7	Calculation	10000	200	=R7*S7		0.05	=VLOOKUP(H7, $BB$4:$BC$8, 2)	=(VLOOKUP (G7, $AX$4:$AZ$22 ,2) * LOG10 (C7)) + VLOOKUP (G7, $AX$4:$AZ$22 ,3)	= 10^(X7)	= D7 * B7 / E7	From SimpleTreat 3.0 debugged using macro	=V7 * (10 ^ 6) / T7	

Table 1 (b) - Complete spreadsheet for risk assessment of water compartment at local scale (continued)

	A	AD	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP
1	Name	SUSP$_{water}$	DILUTION	Foc$_{susp}$		Kp$_{susp}$	Clocal$_{eff}$	Clocal$_{water}$ (prov)	Clocal$_{water}$	PEClocal$_{water}$	Min L(E)C50	AF	PNEC$_{water}$	RCR$_{water}$
2	Comment	Default	Default	Default		= Foc$_{susp}$ * Koc	=Clocal$_{inf}$* Fstp$_{water}$	= Clocal$_{eff}$ / ((1 + (Kp$_{susp}$ * SUSP$_{water}$ * 10E-6))* DILUTION)	Check if value > water solubility	=Clocal$_{water}$ + PECregional$_{water}$	= min[L(E)C50 (fish, daphnia, algae)]	= 1000 (at Base Set)	= min. L(E)C50 / AF	= PEClocal$_{water}$ / PNEC$_{water}$
3	Eqn. No.	~	~	~		9 (9)	10 (18)	11 (30)	12	13 (33)	14	~	15	16
4	Value	15	10	0.1								1000		
5	d/c/e	d	d	d		c	c	c	c	c	c	c	c	c
6	Units	mg/l	~	kg/kg		l/kg	mg/l	mg/l	mg/l	mg/l	mg/l	~	mg/l	~
7	Calculation	15	10	0.1		=AF7 * Y7	=AB7 * (AA7 / 100)	= AI7/((1+(AH7 * AD7 * (10 ^ -6))) * AE7)	= IF (AJ7>E7, E7, AJ7)	= AK7 + P7	= MIN(L7:N7)	1000	= AM7 / AN7	= AL7 / AO7

Table 1 (c) - Complete spreadsheet for risk assessment of water compartment at local scale (continued)

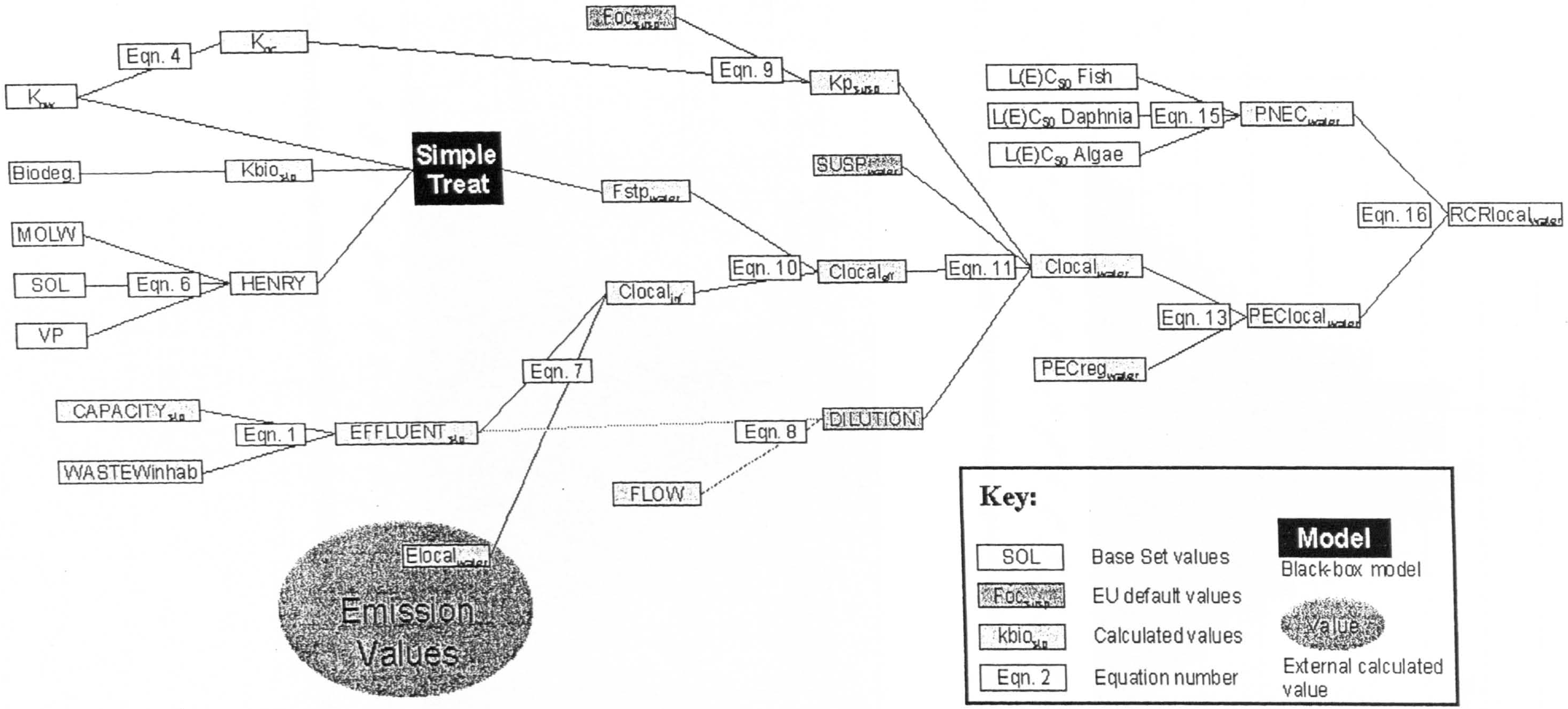

Figure 2 - Schematic diagram of the parameters involved in calculating the local PEC for water, amended and modified [4]

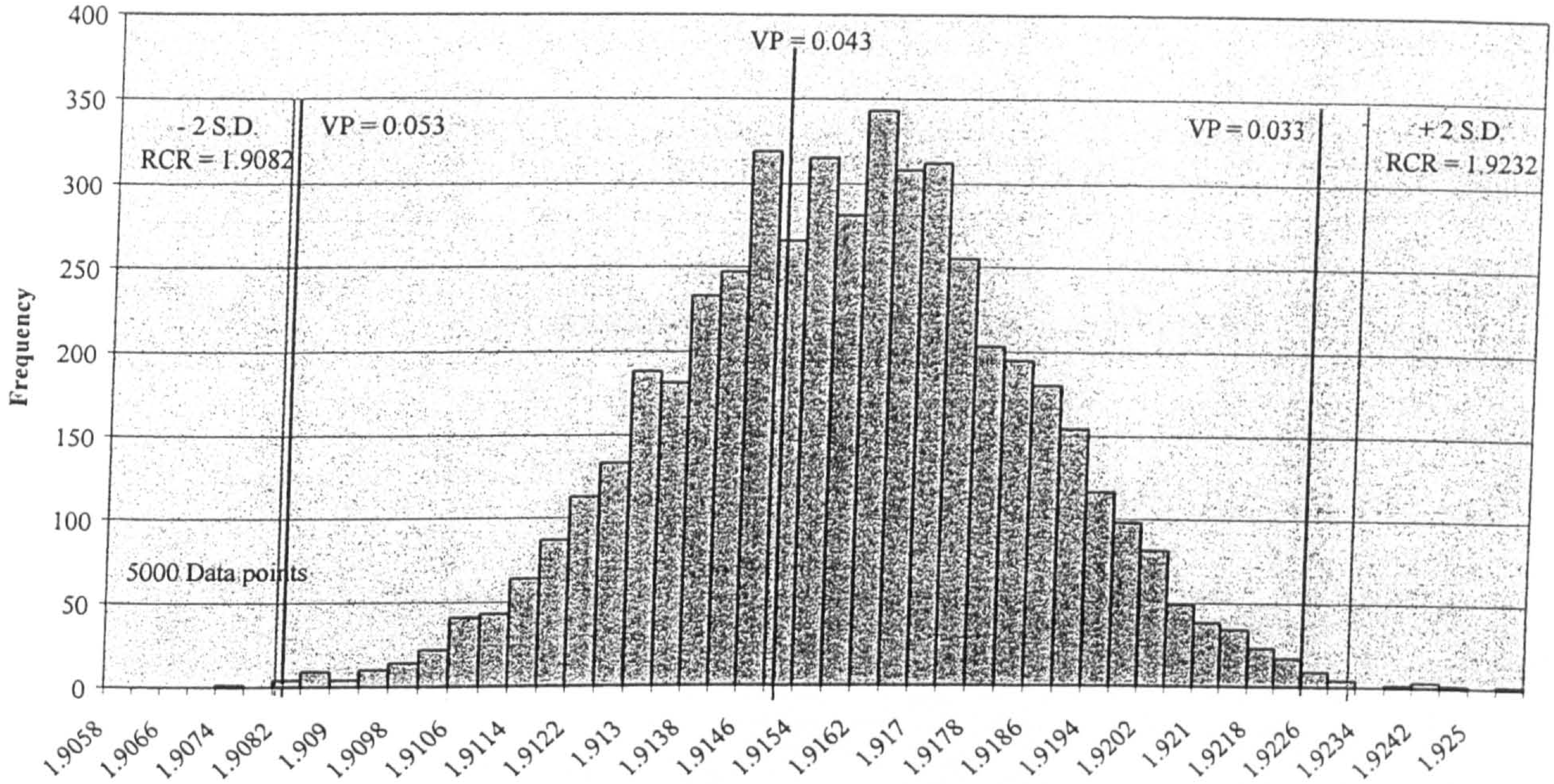

Figure 3 - RCR distribution from normally distributed vapour pressure (VP) values

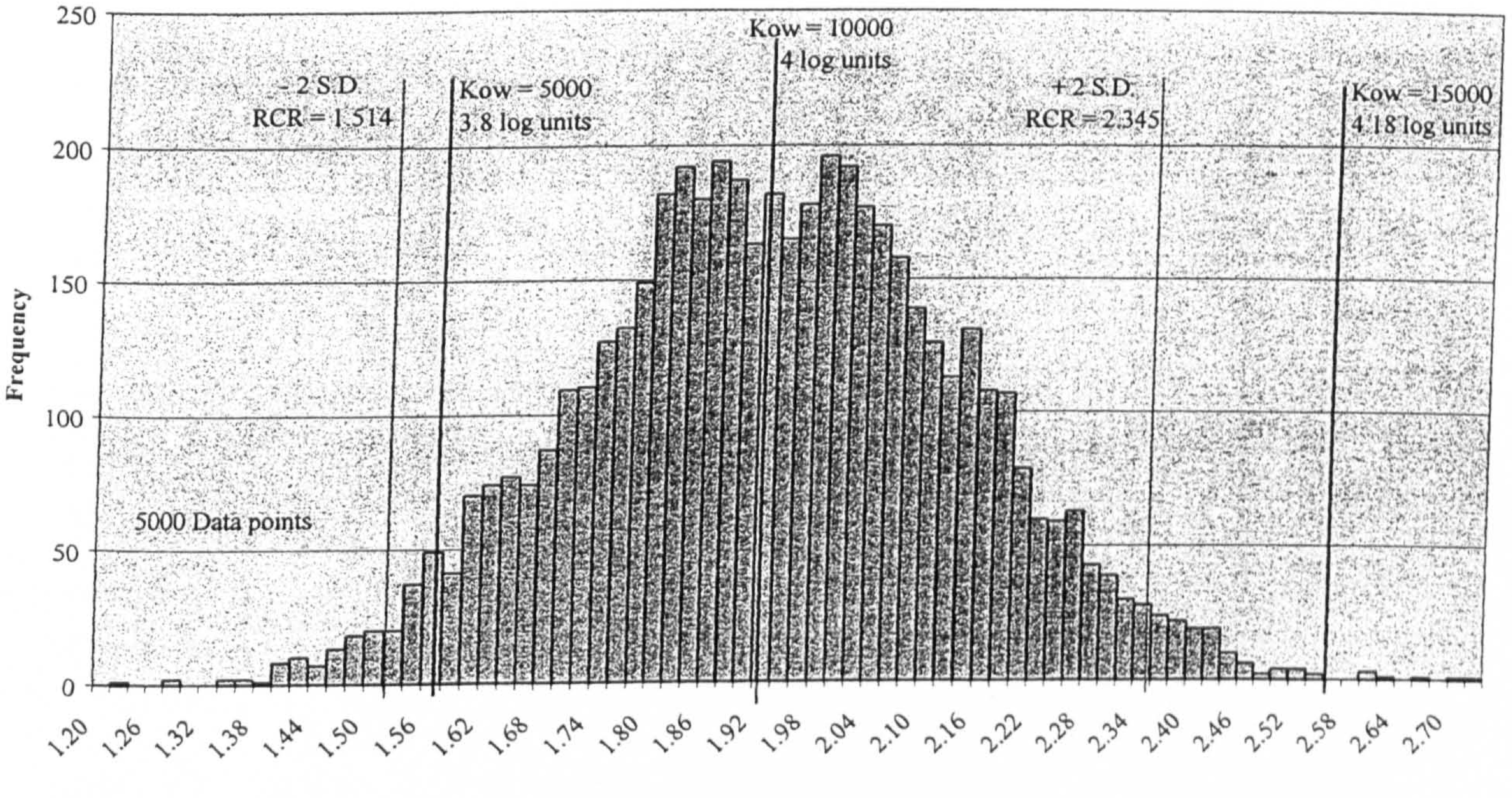

Figure 4 - RCR distribution from normally distributed Log partition coefficient (Kow) values

5.2 Abstract for SETAC Conference, Madrid

Robinson N.L.
Grimes S.M
Wharfe J.R.

Key words: Environmental risk assessment, Statistical analysis, European notification system

Presenter: N.L. Robinson, Brunel University

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Preference: platform, but will accept poster
1st Choice: 4A - Addressing the uncertainty of ERA
2nd Choice: 4C – Site-specific ecological risk assessment

I want to be considered for the Young Scientist Award and will be below 30 years of age at the time of the meeting: No

Standard and default values used in the exposure assessment of chemicals in Europe. Robinson N.L.[1,2], S.M. Grimes[1] and J.R. Wharfe[2]. [1]Brunel University, Uxbridge, UK; [2]National Centre for Ecotoxicology and Hazardous Substances, Environment Agency, Wallingford, UK.

In Europe the EC Directives 67/548/EEC, 93/67/EEC and Regulations Nos. EEC 793/93 and EC 1488/94 require that environmental risk assessments be performed on all notified new chemicals and priority existing substances respectively. The EC has produced a technical guidance document (TGD, EC 1996) that outlines the procedure for this assessment. This procedure is also automated in the computer programme EUSES (European Union System for the Evaluation of Substances). The TGD and EUSES outline a generic system for the assessment of chemicals in a non-existing model environment, using average and reasonable worst case values as default values in the calculations. The strength of such a generic assessment approach is the general applicability of the results, and general acceptance across European Member States. This work examines the actual values found in England and Wales for two such default values used in the model and presents a statistical analysis of those values. The size of the Sewage Treatment Plant (STP) in Population Equivalents (PE) is examined, along with the Dilution Factor at the point of effluent discharge from the STP. The aim of this work is to examine the general applicability of the generic environmental risk assessment performed, as defined in the TGD and EUSES, with particular reference to the conditions in England and Wales.

5.3 Poster for Brunel Graduate School

Robinson N.L.[1,2], S.M. Grimes[1] and J.R. Wharfe[2]

[1]Centre for Environmental Research, Brunel University, Uxbridge, UK
[2]National Centre for Ecotoxicology and Hazardous Substances, Environment Agency, Wallingford, UK.

INTRODUCTION

The Dangerous Substances Directive (67/548/EEC) and its amendments require an environmental risk assessments on all "New Substances". A technical guidance document (TGD) outlines the procedure for this assessment. The procedure is also automated in the computer program EUSES (European Union System for the Evaluation of Substances). This generic system for assessing chemicals uses average, reasonable worst case and default values in the calculations.

There are however, discrepancies between EUSES and the TGD. Also problems have been highlighted concerning EUSES, including the lack of transparency, poor user interface and the inability to run multiple assessments side by side for comparison. The European environmental risk assessment model is detailed in Figure 1.

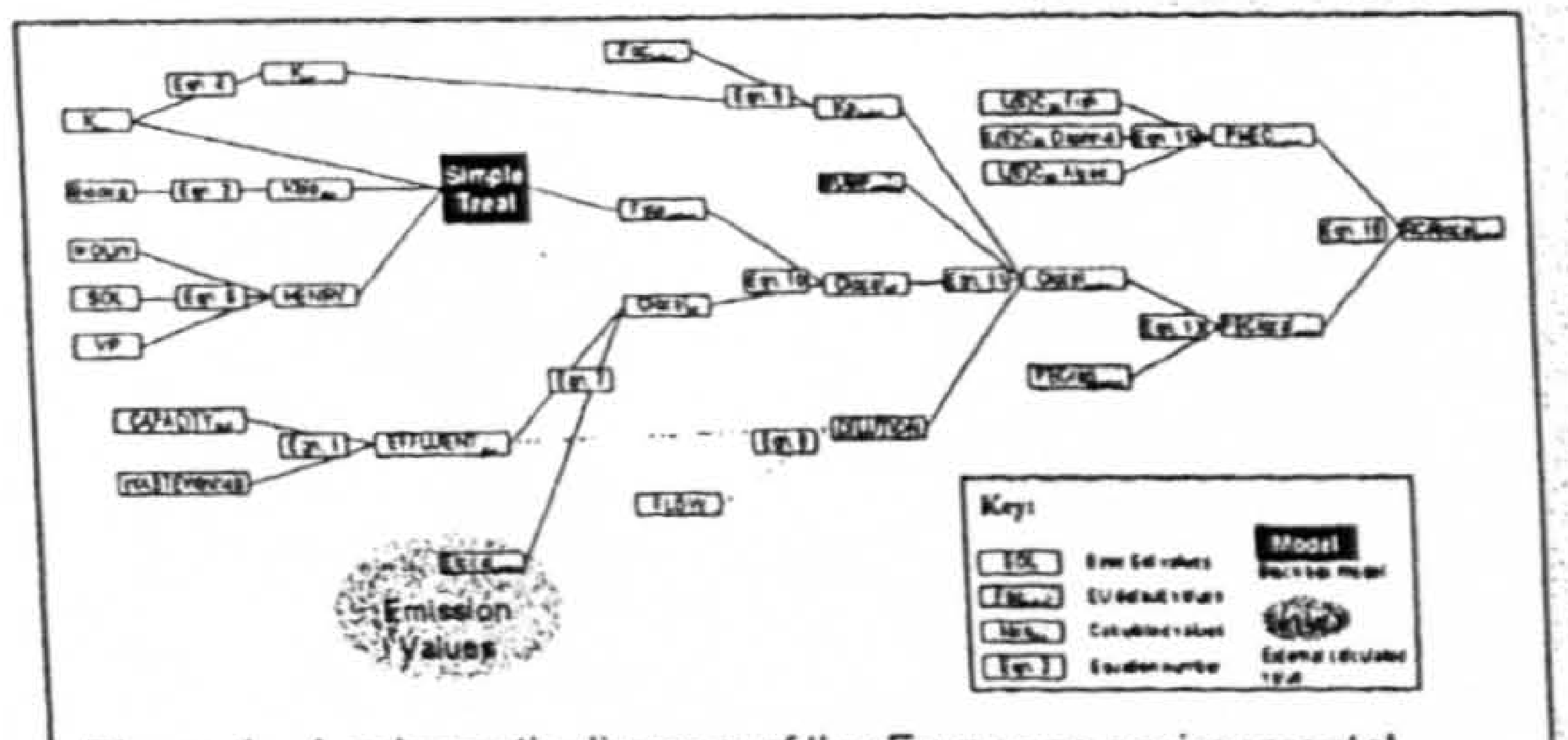


Figure 1 - A schematic diagram of the European environmental risk assessment process

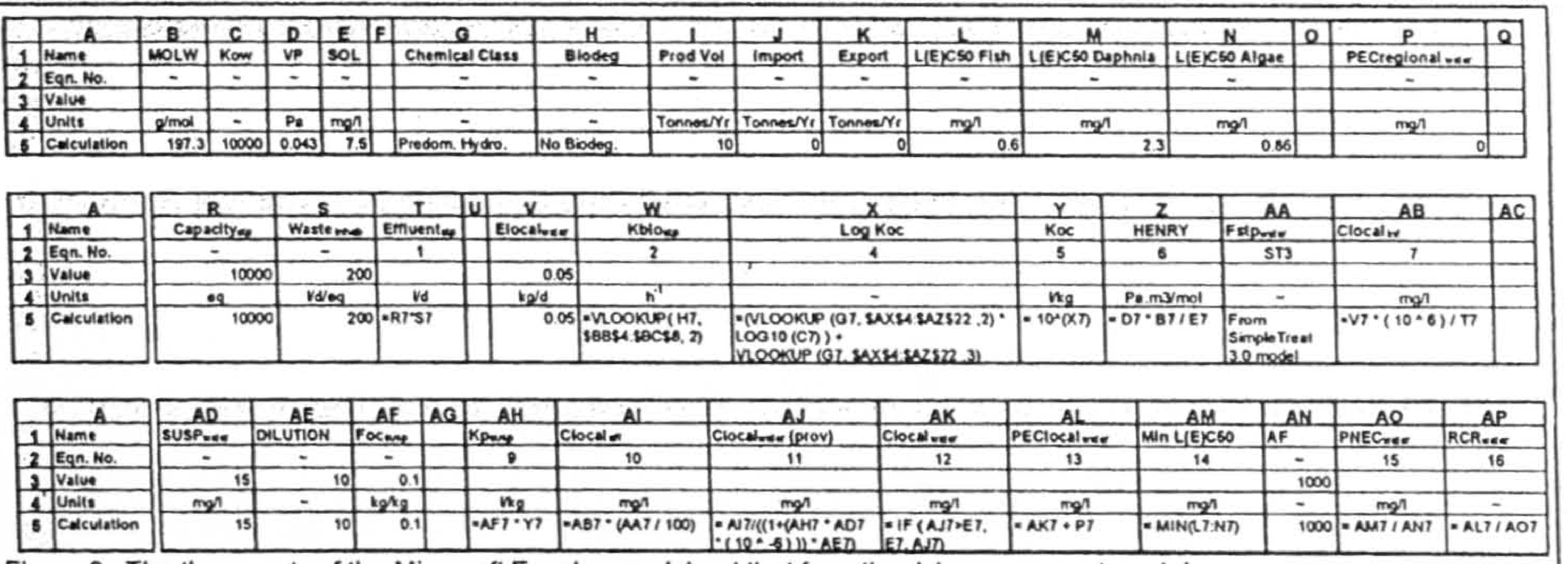
This risk assessment framework was constructed in a Microsoft Excel spreadsheet in a transparent way (as detailed in Figure 2), with the opportunity to run many instances of the same assessment numerous times to compare and highlight sensitive values. Many of the problems with EUSES were fixed in this model.

EXAMPLE

The effect on the resulting Risk Characterisation Ratio (RCR) of variability in measuring the octanol-water partition coefficient (*Kow*, Column C) and the vapour pressure (*VP*, Column D) of a test substance were investigated, based on standard published precision measurements.

For this example it was assumed that variability would be normally distributed around the mean value and the error given in the test guidelines would be equal to 3 standard deviations (99.7 %) about this mean.

A sample size of 5000 data points from separate runs of the calculation was used, based on the good approximation to a normal distribution afforded by such a sample.



a

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Name	MOLW	Kow	VP	SOL		Chemical Class	Biodeg	Prod Vol	Import	Export	L(E)C50 Fish	L(E)C50 Daphnia	L(E)C50 Algae		PECregional$_{water}$	
2	Eqn. No.	-	-	-	-		-	-	-	-	-	-	-	-		-	
3	Value																
4	Units	g/mol	-	Pa	mg/l		-	-	Tonnes/Yr	Tonnes/Yr	Tonnes/Yr	mg/l	mg/l	mg/l		mg/l	
5	Calculation	197.3	10000	0.043	7.5		Predom. Hydro.	No Biodeg.	10	0	0	0.6	2.3	0.86		0	

b

	A	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
1	Name	Capacity$_{stp}$	Waste$_{inhab}$	Effluent$_{stp}$		Elocal$_{water}$	Kbio$_{stp}$	Log Koc	Koc	HENRY	Fstp$_{water}$	Clocal$_{eff}$	
2	Eqn. No.	-	-	1			2	4	5	6	ST3	7	
3	Value	10000	200			0.05							
4	Units	eq	l/d/eq	l/d		kg/d	h^{-1}	-	l/kg	Pa.m3/mol	-	mg/l	
5	Calculation	10000	200	=R7*S7		0.05	=VLOOKUP(H7, $BB$4:$BC$8, 2)	=(VLOOKUP (G7, $AX$4:$AZ$22 ,2) * LOG10 (C7)) + VLOOKUP (G7, $AX$4:$AZ$22 ,3)	= 10^(X7)	= D7 * B7 / E7	From SimpleTreat 3.0 model	=V7 * (10 ^ 6) / T7	

c

	A	AD	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP
1	Name	SUSP$_{water}$	DILUTION	Foc$_{susp}$		Kp$_{susp}$	Clocal$_{eff}$	Clocal$_{water}$ (prov)	Clocal$_{water}$	PEClocal$_{water}$	Min L(E)C50	AF	PNEC$_{water}$	RCR$_{water}$
2	Eqn. No.	-	-	-		9	10	11	12	13	14	-	15	16
3	Value	15	10	0.1								1000		
4	Units	mg/l	-	kg/kg		l/kg	mg/l	mg/l	mg/l	mg/l	mg/l	-	mg/l	-
5	Calculation	15	10	0.1		=AF7 * Y7	=AB7 * (AA7 / 100)	= AI7/(((1+(AH7 * AD7 * (10 ^ -6))) * AE7)	= IF (AJ7>E7, E7, AJ7)	= AK7 + P7	= MIN(L7:N7)	1000	= AM7 / AN7	= AL7 / AO7

Figure 2 - The three parts of the Microsoft Excel spreadsheet that form the risk assessment model

The resulting RCR values (Column AP) were examined. Two graphs were produced of the resulting RCR values from normally distributed *VP* values and from normally distributed log *Kow* values (Figure 3 & 4 respectively).

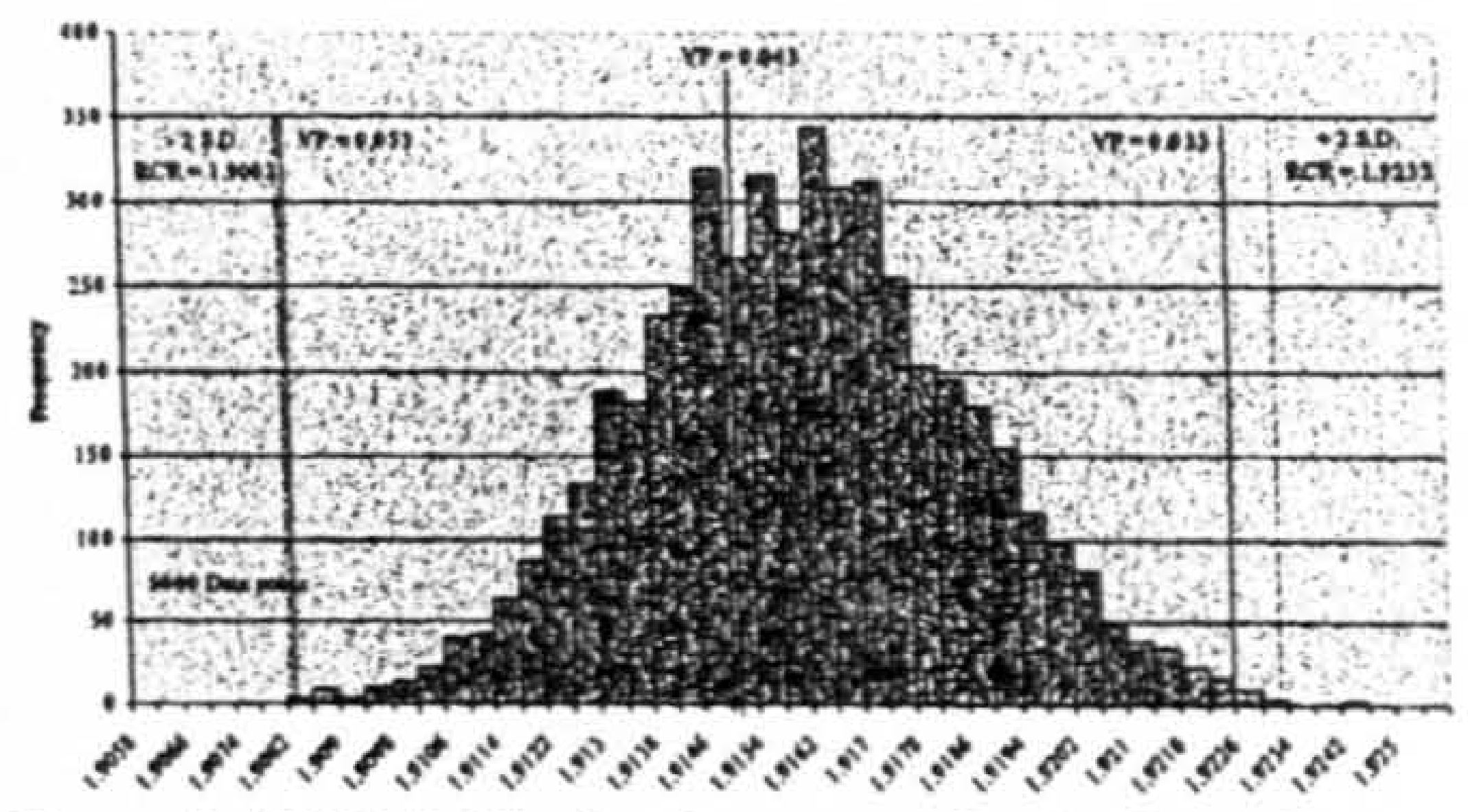


Figure 3 - RCR distribution from normally distributed vapour pressure (VP) values

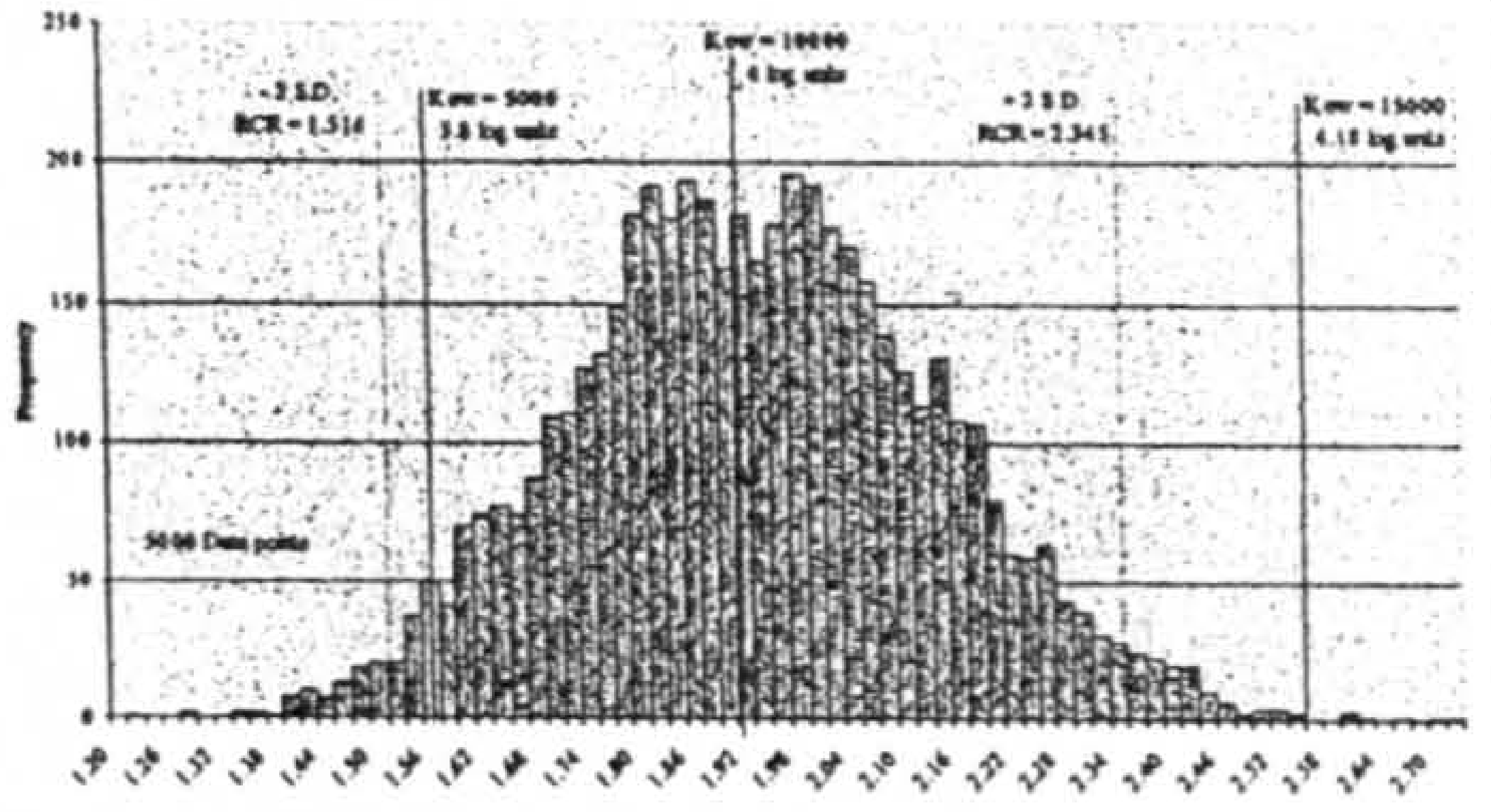


Figure 4 - RCR distribution from normally distributed octanol-water partition coefficient (Kow) values

It is easily observed that variability in measurement causes far greater effect for the *Kow* value than for vapour pressure. The resulting range for the RCR within ±2 SD (this encompasses 95% of the data) of the mean, is 1.5 - 2.3 for variation in *Kow* and only 1.908 - 1.923 for variation in *VP*.

CONCLUSIONS

The spreadsheet model provides a usable and powerful tool for the investigation of risk assessments, allowing thousands of iterations of an assessment to be performed simultaneously. The model allows uncertainty and sensitivity analyses to be performed quickly and accurately, informing risk assessors of where data refinements are required.

FURTHER WORK

Work is currently being carried out to model actual characteristics of sewage treatment plants in the UK to compare the result with European default values used in the generic assessments. By examining these values, the level of protection afforded in the UK by the generic system can be demonstrated.

ACKNOWLEDGEMENTS - The authors would like to thank the EPSRC (Engineering and Physical Science Research Council) and the Environment Agency for their financial support of this Engineering Doctorate project. Gratitude is also extended to members of the National Centre for Ecotoxicology and Hazardous Substances within the Environment Agency whose help has been invaluable.

5.4 Distributions of Randomly Generated Normally Distributed Numbers

Distributions from Various Sized Samples of Randomly Generated Normally Distributed Numbers