Draft Final Report R&D Project 332

A UNIFIED INFORMATION SYSTEM TO SATISFY THE NRA'S REQUIREMENT FOR ECOTOXICOLOGY INFORMATION: THE SPECIFICATION STUDY

WRc plc

February 1992
R&D 332/3/W

A UNIFIED INFORMATION SYSTEM TO SATISFY THE NRA'S REQUIREMENT FOR ECOTOXICOLOGY INFORMATION: The Specification Study

M G C Baker, S D Atkins, G Coles, S Hedgecott, R Fleming, D Cox and S Goodwin

Research Contractor:
WRc plc
Henley Road Medmenham
PO Box 16 Marlow
Buckinghamshire SL7 2HD

National Rivers Authority
Rivers House Waterside Drive
Almondsbury Bristol
Avon BS12 2UD

NRA Draft Final Report 332/3/W

National Rivers Authority
Rivers House Waterside Drive
Almondsbury Bristol
Avon BS12 2UD

Tel: 0454 624400
Fax: 0454 624409

Dissemination status
Internal: Restricted
External: Restricted

Research contractor
This document was produced under R&D Contract 332 by:

WRc plc
Henley Road Medmenham
PO Box 16 Marlow
Buckinghamshire SL7 2HD

Tel: 0491 571531
Fax: 0491 579094

WRc Report № NR 3008/Project № 4272

NRA Project Leader
The NRA's Project Leader for R&D Contract 332:

R Milne - Welsh Region

Additional copies
Further copies of this document may be obtained from Regional R&D Co-ordinators or the R&D Section of NRA Head Office.

CONTENTS

Page

APPENDICES

LIST OF TABLES

LIST OF FIGURES

CONTENTS

Page

APPENDICES

LIST OF TABLES

LIST OF FIGURES

EXECUTIVE SUMMARY

The objective of this study has been to specify an information system which, if effectively managed, would satisfy the requirements for ecotoxicology information within the NRA. Establishing such a system is a multistage process that entails:

(i) an assessment of the need for information;

(ii) proposals for specific solutions to satisfy this need;

(iii) an investigation into the feasibility of these solutions;

(iv) a detailed specification of the information system; and

(v) an implementation plan.

The objective of this study was to consider stages (i) to (iii). The remaining stages will require the involvement of information technologists within NRA, since more detailed discussions and studies are required before a system can be selected, specified and implemented.

In addition to the specification of an information system, a number of pieces of supporting work have been produced with direct relevance to the type of system (e.g. internal or external), its information sources, and data requirements for the derivation of water quality objectives (e.g. EQSs, Likely Safe Environmental Concentrations).

KEY WORDS

Information storage and retrieval, Information technology, Toxicology, Environmental Quality, Databases.

1. INTRODUCTION

At present the NRA has no central in-house source of information on the ecotoxicology of substances. Consequently it uses external services such as WRc's Information Service on Toxicity and Biodegradability (INSTAB) to satisfy its requirements for toxicity information. However, the introduction of legislation, changes in NRA policy, and the NRA's continued research into improved application of ecotoxicology have led to an increased requirement for information.

In 1991 the NRA asked WRc to carry out a feasibility study for an information system capable of providing ecotoxicology data on a national basis. In carrying out this project consideration has been given to relevant work on information systems recently completed in NRA Anglian Region (Contact: A Ferguson). This project examined the sources of information, and the benefits and problems associated with obtaining data on the fate and behaviour of chemical contaminants (Baker *et al* 1991). In addition work is in progress within Severn Trent Region (Contact: G Dolby) on developing a Pollution Incident Management System for Lap-Top PCs.

The primary aim of this project is to objectively specify an information system that, if effectively managed, will be able to provide the NRA with ecotoxicology data. This objective has been achieved by assessing the information needs of the NRA on a national basis (Section 2), identifying potential solutions (Section 3) and examining their feasibility (Section 4). The NRA will need to consider all these potential solutions and select the most appropriate after discussion with its information technology specialists.

In addition a number of pieces of supporting work have been produced as part of this project. These include a consideration of the benefits and disadvantages of databases and information systems (Appendix D) and the second concerns the derivation of Environmental Quality Standards (EQSs) and Likely Safe Environmental Concentrations (LSECs) (Appendix E and F respectively).

2. THE RESULTS OF THE INTERVIEW AND QUESTIONNAIRE SURVEYS

2.1 Introduction

According to the Central Computing and Telecommunications Agency (CCTA) Guidelines on appraising investment in information systems (CCTA 1989) a clear understanding of "needs" must be obtained before an information system is proposed. The NRA's information requirements were assessed by two surveys during July and August 1991. NRA personnel with an involvement in ecotoxicology were selected by key contacts for their participation in these surveys from every region and head office. In total 34 staff were involved in the interview survey and 21 (out of 32) replied to the questionnaire survey.

The results obtained from these surveys are presented in Appendix A and are summarised below in Sections 2.2 to 2.6.

2.2 Toxicology experience and training of survey participants

In both the interview and questionnaire surveys most participants (65% and 82% respectively) were relatively new in their position (<1 - 5 years) (Appendix A2.1).

A large percentage (77%) of the NRA personnel in the interview survey reported that their experience in ecotoxicology was gained from "on-the-job experience". Only a small percentage (12%) of these people, however, had worked in ecotoxicologically orientated positions or had relevant academic experience. This is similarly reflected in the responses received from the questionnaire survey (Appendix A2.3).

The majority of the participants had no toxicology training. Results from the interview survey indicated that 18% had attended external courses and only 3% had attended internal courses. A lower percentage is reflected in the questionnaire survey (Appendix A2.2).

There appear to be few NRA internal courses concerning ecotoxicology. Most participants who had received in-house training indicated that it had taken place before the privatisation of the water industry. However, Severn Trent region has reported that staff are trained in basic ecotoxicology.

2.3 Present use of toxicity data within the NRA

The toxicity data requirements within the NRA have been suggested in NRA report 254/1/A (Baker *et al* 1991), and in excess of 90% of the responses from both surveys agreed with the division into the 3 broad areas (Appendix A3):

(i) Incident management;

(ii) Consent setting (including planned discharges);

(iii) Strategic policies (R&D, long term planning, monitoring, legal requirement, catchment management, EQS derivation, legislation).

Participants in both surveys were primarily involved in incident management and to a slightly smaller extent in consent setting and strategic policies. Participants were not necessarily restricted to one area.

2.3.1 Frequency of use and speed of information retrieval

Frequency of use

Both surveys indicated a variable requirement for toxicity data within NRA. Information is typically required once a month (or less), but a significant number of participants indicated that they require it more frequently (Appendix A3.3).

Time requirement for information

Both surveys indicated that the speed requirement for information can be divided into short- (<1 day), medium- (<1 month) and long-term (>1 month). Incident management has the most immediate need for information (<1 day). Consent setting appears to have a medium term need, and strategic policies a variable response time according to the policy area (e.g. R&D has a long term requirement and catchment management a medium term requirement) (Appendix A3.3).

2.3.2 Quality, amount and detail of data required

Data quality

Both surveys revealed that there is no time during a pollution incident for data quality assessment to be carried out. A large percentage (55% interview survey; 94% questionnaire survey) of participants felt that data quality was important or very important, and consequently there is a need for assessed data to be available in such situations. However, a significant percentage (45%) of the interview survey results indicate that the quality of data used during such situations is considered unimportant compared to the urgency for such data (Appendix A3.5).

The quality of data for both consent setting and strategic policies was considered to be very important in both surveys (>88% interview survey; >92% questionnaire survey).

Amount and detail of toxicity information

The amount and detail of information gathered during pollution incidents was considered not to be a major consideration in the interview survey (71%), with only a few types of information needed. However, a number of participants in both surveys felt that the amount and detail of information was important (19% interview; 50% questionnaire), or very important (10% interview; 44% questionnaire), in spite of the problems of assessing large quantities of data in the limited time available (Appendix A3.6).

The amount and detail of data gathered for consent setting and strategic policies are considered to be very important, as a consequence of the long term decisions that are based on these data and thus the scrutiny that it comes under.

2.3.3 Presentation of Data

All participants involved in the surveys indicated that the presentation of toxicity data is important when applying it to a problem. The formats preferred by participants depended on their operational/strategic area(s) of involvement.

Presentation of data for use in pollution incidents was considered to be best achieved through a substance profile in the interview survey (96%). This would have the advantage of quickly conveying the relevant assessed information required in a pollution incident without the need for searching a number of toxicity information sources. However, participants of the questionnaire survey (41%) perceived that a short advisory/report would be of most use during an incident. This may be due to some misinterpretation of the question, since it would take more time to extract information from a short advisory or report than from a substance profile (see Appendix A3.7 and Glossary).

Presentation of data for consent setting and strategic policies as perceived to be best achieved through a short advisory and a detailed report, respectively. However, both surveys demonstrated that a combination of formats would be helpful (Appendix A3.7).

2.3.4 Storage of Toxicity Data

Most storage of data within NRA is not central and is restricted to personal and/or departmental filing. In addition it appears that a number of these systems were not designed to provide toxicity data and consequently are not particularly user friendly (i.e. data is not indexed by substance).

Computer databases used for toxicity information storage comprise a very small proportion of the methods of storage within NRA (21% questionnaire survey; 4.0% interview survey). Time for setting up and maintaining databases appears to be a problem in a number of the regions. Additionally their availability appear to be limited to the departments that created them, as other departments are unaware of their existence (Appendix A3.8).

Approximately 28% of participants of the interview survey reported that they did not store toxicity data for future reference. Consequently, when required again a request for toxicity data needs to be repeated (Appendix A3.8).

2.3.5 Obtaining toxicity data

Set procedure for obtaining and using data

The interview survey indicate that there is largely no set procedure for obtaining toxicity information (82%). The participants who used a set procedure (18%) were exclusively involved in incident management. Additionally there appear to be no procedures or guidance available for using toxicity data to solve operational or strategic policy problems (Appendix A3.2).

Individuals responsible for obtaining data

The interview survey revealed that approximately 74% of the interviewees obtain data themselves, whilst approximately 26% delegate this task to other staff. No figures are available from the questionnaire survey (Appendix A3.10).

Use of data by staff in the group/department

The majority of the participants in both surveys reported that other staff in their group/department used toxicity data. Approximately 87% of participants reported that between 1 and 10 staff used toxicity data, and 10% reported 11 or more using such data (Appendix A3.12).

Use of external organisations to obtain data

The majority of those interviewed reported that they use external organisations to supply them with toxicity data (91%), in contrast to the questionnaire survey that reported only 50% usage of external organisations. The interview survey demonstrated that the range of organisations consulted is large and appears to be a result of personal contacts rather than use of existing services. WRc (37%) is the most frequently used organisation (and only service), followed by MAFF (15%) and manufacturers (13%) (Appendix A3.11).

2.4 Specific requirements for toxicity data

2.4.1 Type of toxicity data used

In general participants of both surveys involved with incident management primarily use acute data (77% interview survey, 42% questionnaire survey). LC50s are most commonly utilised (Appendix A4.1).

The determination of discharge consents appears to be established principally by using chronic (32% questionnaire survey; 46% interview survey) and acute toxicity data (32% questionnaire survey; 40% interview survey), as well as quality standards and guidelines (15% questionnaire survey; 10% interview survey).

The interview survey indicated that strategic policies principally require chronic toxicity data (48%). However, other information such as acute toxicity data, quality standards and bioaccumulation data are also used.

A small number of NRA personnel reported that they require mammalian toxicity data for incident management, consent setting and strategic policies. A general indication of such toxicity is principally needed, although a few participants (2 out of 34) of the interview survey indicated that they require more specific data (e.g. chronic, teratogenicity, carcinogenicity, mutagenicity).

2.4.2 Other data used

The majority of the participants combine the use of toxicity data with other data, principally guidelines and quality standards (not necessarily with a toxicological basis). However, data on the fate and behaviour, occurrence/use, health and safety, and physical and chemical properties of substances are also used (Appendix A4.2).

2.4.3 Access to additional data to satisfy information requirement

The majority of participants indicated that they would like to have access to additional data to satisfy their need for information. In particular water quality data, biological monitoring data, field study data, incident reports, discharge consents (brief details only), and a greater range of toxicity data were highlighted by the surveys (Appendix A4.3).

2.4.4 Interpretation of data

The majority of participants of the surveys reported that they interpret data (76% interview survey, 89% questionnaire survey). Both surveys, (particularly in the questionnaire survey, 82%), indicated that participants experienced problems with interpretation. This problem could primarily be attributed to the limited time available for the task (58% interview survey; 81% questionnaire survey). Some participants, however, indicated that problems with interpretation stemmed from their limited knowledge of ecotoxicology (Appendix A4.4).

A large number of participants (89%) use both internal and external contacts for guidance during data interpretation.

2.4.5 Understanding of basic acute toxicity data (LC50) and its application to a real situation

Approximately 56% and 55% participants of the interview and questionnaire surveys respectively had a correct understanding of an LC50. However, a significant proportion of participants have only an adequate or poor understanding of this result.

The majority of the participants from both surveys understood that the application of an LC50 to the environment is not a straightforward transition. A small percentage (9% interview survey, 5% questionnaire survey), however, were not aware of this (Appendix A4.5).

2.5 <u>Sources of information</u>

2.5.1 Present sources of information

The participants of both surveys revealed that they rely heavily on printed texts, external organisations and contacts within the NRA as sources of information. Few (19% interview survey, 8% questionnaire survey), use computer (both PC and on-line) and hardcopy databases.(Appendix A5).

On-line databases

A small number of participants (4 out of 34 interview survey; 4 out of 20 questionnaire survey) reported that on-line databases are used as a source of information. Only a very small number of databases are used (between 2 and 3) and access appears to be fairly frequent. Over 50% of staff using such databases access them between 1 and 5 times per month. Few of the participants (1 from each survey) had received training for on-line searching and only one (questionnaire survey) had such training maintained.

Most of the NRA personnel that use on-line databases report that they are not useful, mainly because they do not contain relevant or useful information, data quality cannot be judged and that they are not cost effective.

Obtaining data from separate NRA regions

Participants of both the questionnaire and interview survey reported that they obtained data from other regions (35% and 75% respectively). Also some participants were used by NRA personnel in other NRA regions as a source of information (15% and 56%) (Appendix A5.1).

2.5.2 Concept of an information unit

The majority of participants (in excess of 80%) were in favour of an "information gathering unit" providing relevant data to them, and possibly helping with interpretation (Appendix A5.4).

2.5.3 Concept of a computer database

The majority of participants (65% questionnaire survey; 94% interview survey) were in favour of a computerised pollution database containing relevant detail and subject coverage on toxic substances (e.g. substance profiles for incident management) (Appendix A5.4).

2.5.4 Are information sources satisfactory?

The majority of participants (70%) felt that the information sources available to them at present did not satisfy their requirement for information (Appendix A5.5). Perceived improvements that were suggested included:

(i) Improve the sources of information and make access easier;

(ii) Supplement published literature data with secondary data (e.g. toxicity test data, incidents or details of consents);

(iii) Produce a common dataset on a list of substances;

(iv) Reduce the number of sources that need to be consulted.

2.6 Future information requirements for toxicity information

The majority of participants (70% questionnaire survey; 83% interview survey) felt that their requirement for information would increase. For those able to specify how, the areas of change reported were numerous (Appendix A6).

3. PROPOSAL FOR A UNIFIED INFORMATION SYSTEM

3.1 Introduction

The toxicity requirements of the NRA have been established by interview and questionnaire surveys (Section 2) and an important finding concerning the participants (potential users of the system) was that most appeared to have gained their ecotoxicology experience from work rather than from formal training. Additionally there was often a lack of understanding of the basic principles underlying the application of such information.

Section 2 summarises the results of the survey and divides NRA's information need into:

(i) Incident management;

(ii) Consent setting (including planned discharges);

(iii) Strategic policies, a "catch-all" category which encompasses areas such as catchment management, R&D, monitoring, policies, legislation, EQS derivation and others.

Using these areas of requirement and the data gathered from the surveys, it has been possible to establish user specifications for an information system, the types and presentation of data that are required, and also other aspects of ecotoxicological information that the NRA may wish to consider in the future.

Sections 3.2 and 3.3 contain brief details of the toxicity needs of NRA personnel and outline possible strategies for information systems and their management that would satisfy the short- and long-term information requirements.

3.2 The toxicity information requirement of the NRA

Both surveys demonstrated that NRA staff strongly favour the existence of a unit providing toxicity information and support, but would also benefit from a computerised database that was available for personal use (Sections 2.5.2 -2.5.3).

Additionally the results suggest that the NRA requires a system capable of satisfying a variable demand for toxicity information, in terms of the frequency and extent of access, and the speed and detail of reply. At present it appears that there is a low usage of toxicity data by NRA staff (typically once a month), which could be a reflection of the limited time available for obtaining and evaluating data (Section 2.3.1). However, it is anticipated that this will increase with the introduction of new legislation (e.g. Groundwater Directive) and changes in NRA policy (e.g. introduction of toxicity-based consents) (Section 2.6).

The speed of response and detail of data required by NRA staff varies according to the operational task or strategic policy for which they require information (Section 2.3.1). In general pollution incidents require basic toxicity data immediately, discharge consents require detailed data within a few weeks and certain strategic policies (e.g. EQS derivation, R&D) require extensive data within a few months. However, there is considerable overlap, in terms of detail of data and speed of response, with some of the strategic policies. For example NRA staff involved with monitoring or catchment management have indicated that they require basic or detailed data, respectively, within a few days.

NRA staff indicated during the surveys that they require assistance with the interpretation and evaluation of data (Section 2.4.4), since time constraints typically prevent proper assessment of the information being used.

The introduction of a consistent approach for obtaining and using toxicity data during pollution incidents, when setting discharge consents and for certain strategic policies (e.g. catchment management, monitoring, EQS derivations) would benefit the NRA, by ensuring that:

(i) the minimum dataset needed to resolve a particular problem has been gathered;

(ii) its interpretation is objective; and

(iii) the consequences of this exercise are justifiable (Section 2.3.5).

The types of toxicity data most commonly used within the NRA (Section 2.4.1) are acute (LC50s) and chronic (sublethal, lethal) values, principally for fish and invertebrates. The introduction or increased usage of additional data, such as bioaccumulation, behavioural-, physiological- or community-responses, and environmental fate and behaviour of contaminants, would benefit the NRA by improving the quality of the dataset used when assessing the environmental impact of a substance or process.

At present the NRA uses only a small amount of mammalian toxicity data. However, recent legislation (e.g. Groundwater Directive), problems experienced with surface water contamination (e.g. algal blooms), and the uses to which some rivers are put (e.g. potable water abstraction) suggest that the NRA will need to take more account of mammalian toxicity, in particular for humans and livestock.

The surveys indicated a need for data produced within the NRA (such as monitoring data, lists of consents and incidents) to be made more widely available to NRA staff, in order to support data from other sources (Section 2.4.3).

3.3 Proposal for a Unified Information System for the NRA

3.3.1 System specification

The unified information system required by the NRA needs to satisfy a number of requirements:

(i) Availability as a national resource;

(ii) Compatibility with the NRA's existing systems and IT strategy;

(iii) A short-term solution that is compatible with any long-term solution, better able to satisfy the NRA's requirements, but more difficult to implement;

(iv) Capability for responding appropriately to users needs, in terms of frequency of access, speed of reply and detail of reply;

(v) Inclusion of assessed and interpreted data;

(vi) Effective presentation of data to users according to operational/strategic areas for which they require the data.

3.3.2 Short term solution

A short term solution that is capable of satisfying all the requirements identified above in Section 3.3.1 is summarised in Figures 3.1 and 3.2. It is recommended that this is based on mainframe or PC. The incorporation of ORACLE relational databases into NRA's information technology strategy and the availability of IBM-compatible PCs throughout the NRA make either option viable.

The database system is intended to provide:

(i) Ecotoxicological data (e.g. acute and chronic (lethal and sublethal) data for aquatic organisms);

(ii) Mammalian toxicological data, in particular for humans and livestock;

(iii) Bioconcentration data;

(iv) Environmental fate and behaviour data (e.g. persistence, routes of removal from the environment);

(v) Water quality standards, both for drinking water and for the protection of aquatic life (e.g. suggested no adverse response levels (SNARLs), likely safe environmental concentrations (LSECs), environmental quality standards (EQSs)).

Although biological monitoring data, water quality data, details of field studies, incidents and consents are presently available on systems within the NRA, the package could incorporate brief details of such data and thus provide a useful source of centralised supporting information.

The presentation of data, in terms of the detail required for each operational or strategic task, is important to NRA staff (Section 2.3.3). Therefore it is proposed that data should be presented as:

(i) Profiles of substances, incorporating an environmental impact summary and brief details on topics of interest to NRA; and

(ii) Short advisories/reports containing detailed data on the environmental impact of substances.

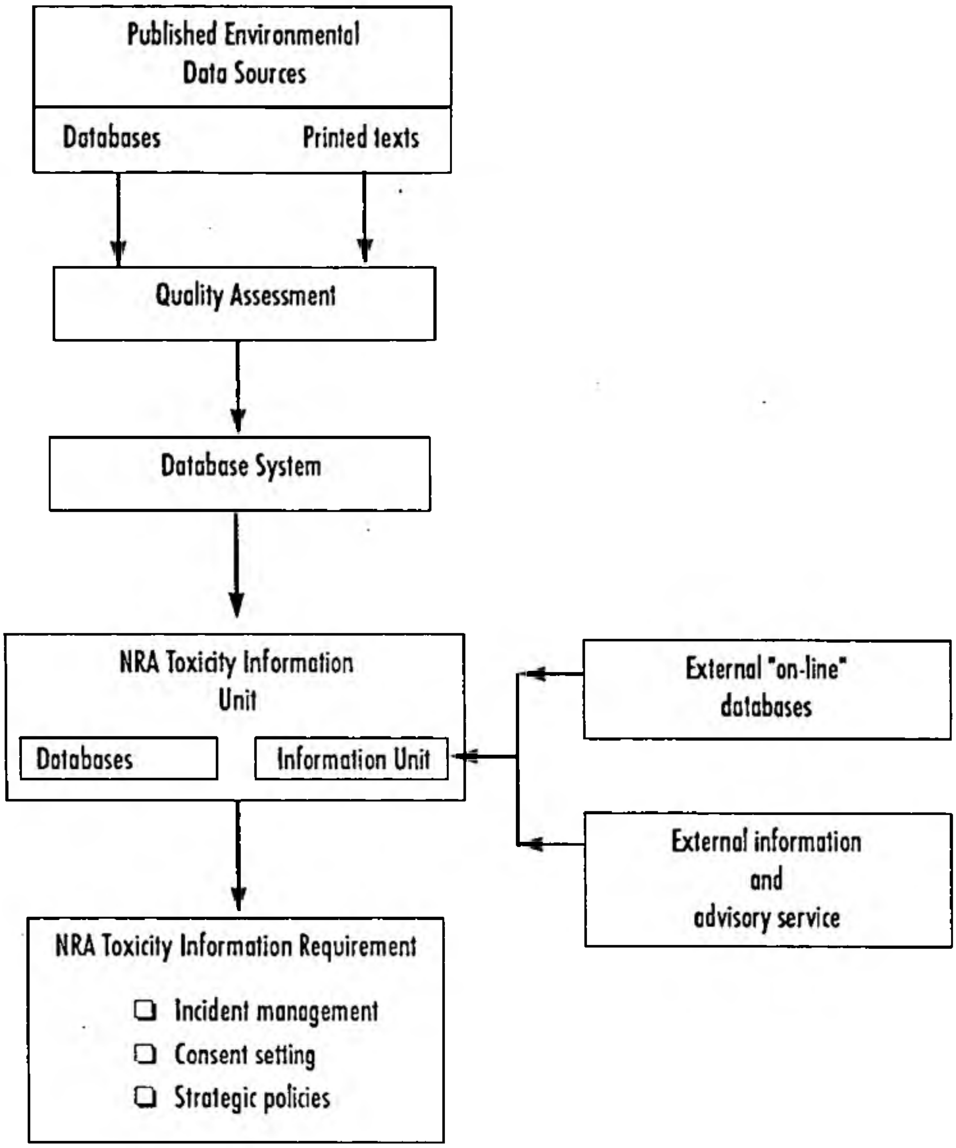
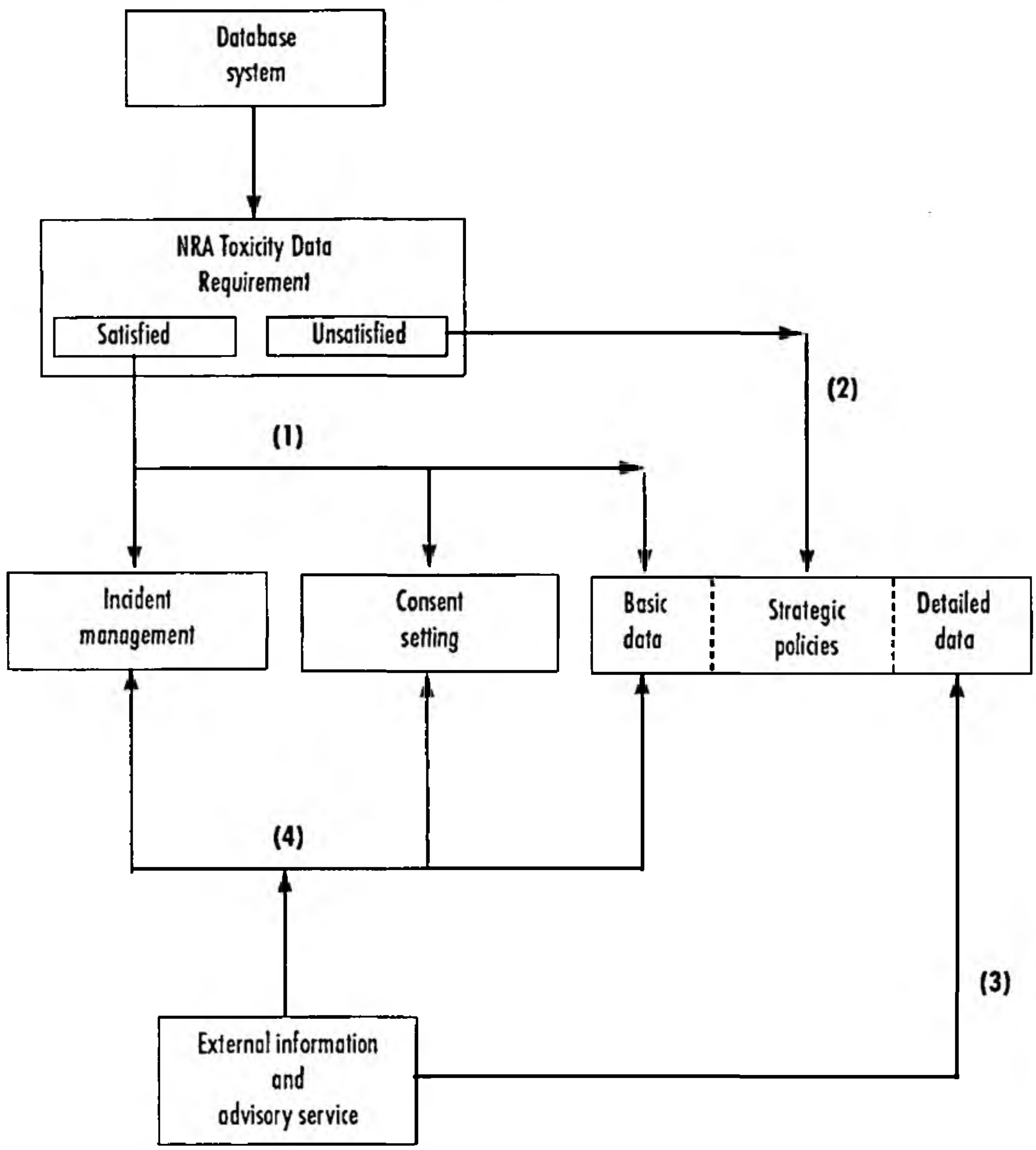


Figure 3.1 Sources of Information and Outputs of the Information System



Notes:

- The database system and the toxicity information available within it would satisfy the incident management, consent setting and certain strategic policy (eg. catchment management) requirements of the NRA (1).
- However the package would **not** satisfy the detailed data requirement of some strategic policies eg. EQS derivation (2). Consequently an information unit would be needed to provide such support (3) and also back up to database users (4), due to the initial low substance coverage of the database (6).

Figure 3.2 Features of the Short Term Solution

Presentation of data in this way will effectively satisfy the majority of the NRA's requirements for toxicological and related information. The profiles are intended for use in incident management (and certain strategic policies such as catchment management), and will contain brief details on identification, toxicity and environmental fate of water contaminants. The short advisories/reports are intended to satisfy the requirements of staff involved in consent setting and strategic policies and will contain detailed toxicology and related information, sufficient to allow the user to calculate a likely safe environmental concentration (LSEC).

The detailed information requirements of some of the NRA's strategic policies (e.g. EQS derivation, assessment of the impact of widespread contamination) are unlikely to be satisfied by this short term solution. Consequently the NRA would benefit from establishing a central information unit, either internally or externally, to provide assessed and interpreted data to all the regions. This central unit should have access to a mainframe computer containing both toxicological information and supporting data generated by the NRA, that is capable of downloading information to the PCs. In addition it would require facilities to access other data sources, such as on-line databases and external services.

3.3.3 Long term solution

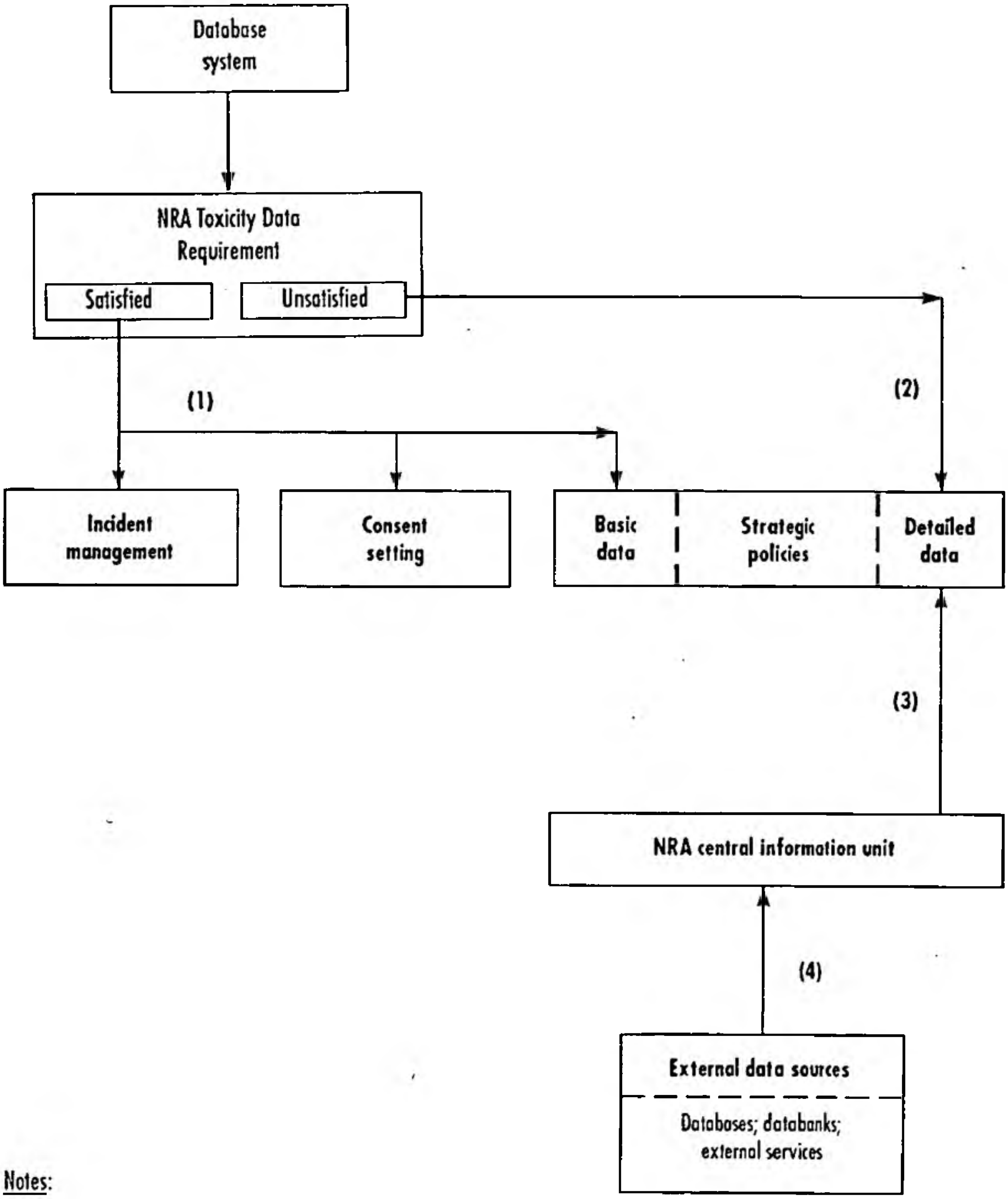
One possible development of the short-term solution is the production of a Knowledge Based System (KBS) as an intelligent front end to the database (Figures 3.1 and 3.3). KBSs are computer programs that simulate in part the knowledge and reasoning of experts giving advice, often (but not exclusively) used for when diagnosing a fault in a complicated process. They do this mainly by encoding expertise in a large number of rules concerning areas of expert knowledge. When an KBS is run, it prompts a user or reads a file for the information it needs. Using this information, with the rules it has been given, enables it to infer the solution to a problem.

In this application, an KBS could allow users to obtain advice on the likely impact of substances on the environment, whether or not they are experienced or inexperienced in ecotoxicology.

The long-term solution would thus contain all the features of the short-term solution, as well as encapsulating the knowledge of experts on how to interpret the information contained therein. This has the advantage that key expertise is preserved and made widely available to less experienced staff.

The proposed KBS is likely to prove useful in decision making for incident management, consent setting and certain strategic policies (e.g. catchment management) and would additionally satisfy the NRA's requirement for general information, through the availability of profiles and advisories outlined in Section 3.3.2.

However, the system is unlikely to satisfy the detailed information requirements of some of the NRA's strategic policies (e.g. EQS derivation). Consequently, as proposed in Section 3.3.2, the NRA would from benefit in establishing a central information unit, either internally or externally, for the provision of such data and its interpretation.



Notes:

- The database system would be an advance over the short term solution, since it would feature an expert system to enable environmental hazard assessments to be carried out. The toxicity information available through this system would satisfy the incident management, consent setting and certain strategic policy (eg. catchment management) requirements of the NRA (1).

- However the package would **not** satisfy the detailed data requirement of some strategic policies eg. EQS derivation (2). Consequently an NRA central information unit would be needed to provide such support (3). Such a facility would require access to extensive external data sources (4).

Figure 3.3 Features of the Long Term Solution

3.3.4 Unified Information System

A scheme for the effective management of both the short- and long-term solutions for a unified information system is proposed in Figure 3.4 and the outputs of the system are presented in Figure 3.1. Because of the length of time and cost implications of fully establishing and maintaining such an information system, the NRA should consider the benefits of linking with an existing advisory or information service, to ensure that all requirements for toxicological and related information are satisfied.

It is anticipated that the NRA regions would be provided with updates of the database package, either directly by the external "PC database" supplier or via a central data handling facility within the NRA.

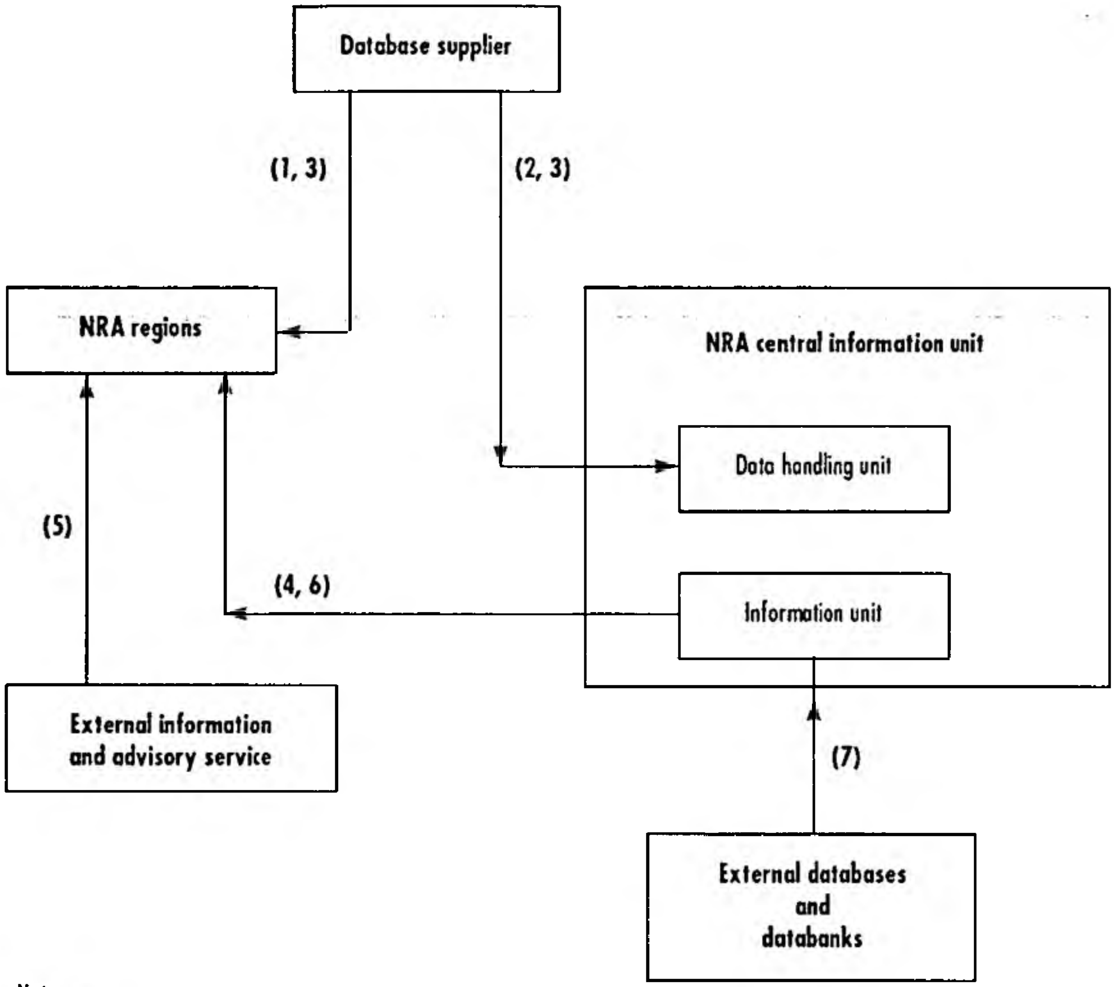
NRA regions could also be provided with a toxicity database (derived from the PC package) for incorporation onto "lap-top" PCs presently used by pollution control staff in the field. Additionally it is recommended that the provision of 24 hour support for toxicity information during pollution incidents is available, either centrally within NRA or externally.

The solutions proposed in Sections 3.3.2 and 3.3.3 are unlikely to satisfy the detailed data requirements of certain NRA strategic policies (e.g. EQS derivation). Provision of such data could be resolved by:

(i) The NRA setting up a central information unit able to obtain, evaluate and provide detailed data to regions. This unit would require facilities to link with a number of external databases or information services;

(ii) NRA regions consulting an external enquiry and advice service;

(iii) Alternatively a combination of these two solutions could be adopted.



Notes:

- NRA regions could be provided directly with updates of the database system (1) from the database supplier or via a central data handling unit at NRA (2) for dissemination to the regions.
- In addition Pollution Control staff could be provided with a toxicity database (derived from the information contained in the PC package) for incorporation onto "lap-top" PCs presently used in the field (3). Toxicological support (24 hour) for such staff should be provided and could be set up centrally within NRA (4) or come from an external information and advisory service (5).
- The proposed database system is unlikely to satisfy the detailed data requirement of some of the NRA's strategic policies. Provision of such data could be resolved in two ways:

  (a) NRA establishes an information unit that can provide assessed toxicological information to regions (6). Such a unit will require facilities to link with external databases or databanks (7).

  (b) However if an information unit is not set up, NRA could consult directly with an external information and advisory service (5).

Figure 3.4 Proposed Unified Information System

4. PROPOSED STRATEGY FOR THE UNIFIED INFORMATION SYSTEM

4.1 Introduction

This section explores the feasibility of the proposed solutions for a unified information system outlined in Section 3. It focuses on how far each system will achieve the objectives of the project, at what cost, and with what benefits for the NRA.

Section 4.2 and Table 4.1 summarise the options for an information system and recommend general short- and long-term solutions. They do not, however, recommend the database system for use by the NRA since more detailed discussions and studies are required before such a system is selected. However, they do highlight the major advantages of each option.

Sections 4.3 to 4.6 assess of the constituents the information system (i.e. database package, database package with Knowledge Based System (KBS) and information unit) and examine the information content, users, data volume, frequency of use, maintenance, ownership, interfaces and costs, as recommended by Central Computing and Telecommunications Agency (CCTA) Guidelines (CCTA 1989). Additionally the important benefits and disadvantages of specific solutions or systems have been highlighted.

Table 4.1 Summary of the available solutions for a unified information system

Feature	Database system	Knowledge based system associated with a database	Information unit
Information	Ecotoxicology and supporting data.	Ecotoxicology and supporting data and a KBS to assist in decision making for incident management, consent setting and catchment management.	Ecotoxicology and supporting data and additionally experienced scientists to offer advice to assist in decision making for incident management, consent setting and strategic policies.
Presentation	Substance profiles and short advisory/report.	Substance profiles and short advisory/report and numerical or qualitative advice from KBS.	Data presented according to individual users needs.
Systems	DG-Oracle-system; PC "Fixed Field" system; PC "Text Retrieval" system.	KBS to run on DG, PC or a combination of the two.	The system would be the same for an internal unit, but an external unit should have its own database.

...../continued

Table 4.1 (continued)

Feature	Database system	Knowledge based system associated with a database	Information unit
Users	All Systems can accommodate users.	All Systems can accommodate users.	Either type of unit can accommodate users.
Data volume	All systems can incorporate information on 60 000 substances.	A KBS can be developed to work on a database of this size.	Not relevant.
Frequency	All systems are unlikely to be overloaded.	The KBS is unlikely to be overloaded.	The information unit is unlikely to be overloaded
Maintenance	ORACLE system limits who can maintain system, whereas users of PC databases have to update the database themselves.	Same applies as for database system.	Not relevant.
Ownership	Data belong to NRA, whereas the system is the copyright of its producer.	Data belong to NRA, whereas the system is the copyright of its producer.	Data would be owned by an internal unit, but purchased from an external unit.
Interfaces	All systems can interface with external databases and internal systems.	The KBS can interface with systems containing the data that it requires.	External unit could not interface with NRA systems. Internal unit could interface with both internal and external systems.
Approximate costs for system[2]	£60K DG-ORACLE system; £37K PC fixed field; £35K PC text retrieval (exclusive of data).	£20 - £100K (×2) or £50 - £100K for incident management; £100 - £150K for each KBS for consent setting and catchment management.	£149K to establish an internal unit (£100K to maintain); £75K to obtain information from an external service[1].
Benefits and disadvantages	Listed Section 4.3.10.	Listed Section 4.4.7.	Listed Section 4.5.5.

NOTES [1] Based on present demand for information
[2] Cost for information unit includes toxicity data

4.2 Unified Information System

There appear to be three broad solutions for an information system:

(i) a database system and information unit (Section 3.3.2);

(ii) a database system with a KBS and an information unit (Section 3.3.3);

(iii) use of a 24 hour information and advisory service to provide ecotoxicology and related data.

It is not the aim of this project to recommend one of these solutions as the information system for the NRA, since all could satisfy its requirements for ecotoxicology information. Selection of a system will require much discussion with NRA's information technology specialists and should involve development of a detailed specification of the system, ready for implementation. Whichever solution is chosen, it is important to ensure that it is implemented in full rather than being built up of features from different solutions added on over time.

4.2.1 Structure of the system

Section 3 outlines possible short- and long-term solutions for an internal information system. These solutions include a database package, providing assessed and interpreted toxicity data, in conjunction with a central information unit. The database package is designed to satisfy the requirements of users involved in both incident management and consent setting, whilst the information unit is primarily designed to provide information to satisfy those personnel requiring more detailed data. Additionally the KBS is intended to provide specific support (e.g. impact assessment) for pollution control, consent setting and catchment management (Section 4.4). Table 4.1 presents a summary of the constituents of the information system, their likely usage and predicted costs.

Establishing an information system is a multistage process which requires careful monitoring of each stage. Therefore immediate implementation of the whole system would be impractical and it is recommended that initially only the database package should be established. Additional support (internally or externally) from a central facility would be required for users of this database to satisfy any enquiries concerning:

(i) the use of the package;

(ii) detailed toxicity information; and

(iii) basic toxicity information for substances not included on the database.

Initially support for enquiries on the database system would be best provided by the organisation responsible for producing and supplying it, and any requests for toxicity information should be directed to an established information and advisory service.

4.2.2 Cost implications

The cost of the database and information unit (excluding toxicity information) is likely to fall approximately between £110 and £135K using an external advisory service for support, and between £184 and £209K using an internal information system (see Sections 4.3, 4.5 and Figure 3.2).

The cost of establishing the database, information unit and KBS is high and could be in the range £204 to £359K using an internal unit and £130 to £285K using an external system, depending on how many applications the KBS is used for (see Sections 4.3, 4.4, 4.5 and Figure 3.3).

4.2.3 Benefits and disadvantages

Despite the large investment required to develop an internal information system there are significant advantages compared to an external system (see Appendix D4):

(i) The NRA would become more independent in satisfying its need for information;

(ii) Information could be tailored specifically to meet the NRA's needs;

(iii) Information would be both assessed and interpreted;

(iv) The availability of such a system could increase the application of ecotoxicity data within the NRA.

However, the major disadvantages of establishing an internal system are:

(i) The substantial effort and time needed to accumulate information on a large number of substances. The NRA would therefore, need to also establish reliable links with external data sources to allow them to obtain information on a 24 hour basis; and

(ii) The cost involved in fully implementing the information system is high and needs to be carefully considered against the demand for information.

In contrast the benefits of using an external information and advisory service to provide data are:

(i) Information would be available 24 hours a day, every day;

(ii) Information would be both assessed and interpreted, and tailored to individual users needs;

(iii) Information would be available on a large number of substances; and

(iv) This option would be cheaper than an internal system.

However, the disadvantages of an external system are:

(i) It would not interface with NRA systems;

(ii) It may not encourage use of ecotoxicology data throughout the NRA (since people might not know of the service or may be dissuaded from using it for general enquiries); and

(iii) In some circumstances information may not be available to users within the desired time (e.g. assessment of available information for a consent needed within 1 day).

4.3 Database system

4.3.1 Type of information available

The database package is designed to provide toxicity data to NRA users. However, when assessing the potential impact of a substance, a considerable amount of supporting data are also needed. Inclusion of such data on the database would widen its potential use within NRA. Consequently it is recommended that the database package should contain data on:

(i) identification;

(ii) occurrence and use;

(iii) aquatic toxicity (both freshwater and saltwater);

(iv) bioaccumulation (both freshwater and saltwater);

(v) potential hazard to human health;

(vi) fate and behaviour;

(vii) analysis; and

(viii) physical and chemical properties.

The database is not designed to supply details on the toxicity of complex effluents (e.g. paper and pulp mill), but would supply information on the major constituents of these effluents. In addition, for specific operational areas (e.g. pollution incidents or catchment management) there would be no advice or actions provided on how to deal with spillages of substances, or indeed with how to identify the likely cause of a pollution event. This type of application could be best satisfied by an "KBS" or an information unit (Sections 4.3 - 4.4).

Substance-Profile

The proposed substance profile (see Glossary) is designed to rapidly provide basic assessed information on the aquatic toxicity, fate and behaviour of substances. In particular the information presented in the proposed profile would be of use to NRA staff involved in incident management and certain strategic policies (e.g. catchment management) and would also provide useful background information to those involved in establishing discharge consents.

The substance profile will cover the areas outlined in Section 4.3.1 (i) to (viii) (see Table 4.2). In addition summaries of the profiles will be available and are designed to provide both qualitative and quantitative information on the toxicity, fate and behaviour of substances in the environment (see Table 4.3).

Table 4.2 Type of information present in the proposed substance profile

Type of Information	Data Provided
Identification	Chemical abstracts number; IUPAC name; Chemical group; HAZCHEM code; Synonyms.
Occurrence	Levels in media (NRA data could be added here) and whether it is found naturally or through anthropogenic activities.
Use	Its uses and the types of industry that use it. Potential sources of contamination (point and diffuse).
Aquatic toxicity	The most sensitive species or life stage will be identified where possible. In addition information on indigenous species will be provided when available and a "quality of data" assessment will be given.
	Where possible toxicity data for a representative of each of the following taxa will be provided: algae, plants, annelids, echinoderms, molluscs, crustaceans, insects and fish.
- Acute	Freshwater and saltwater fish, invertebrates and plants acute toxicity data (LC50 or EC50).
- Chronic	Both lethal and sublethal (e.g. growth, reproduction, avoidance) toxicity to freshwater and saltwater fish, invertebrates and plants.
- Toxic mode of action	Where possible will attempt to identify site(s) of action.
- Symptoms of poisoning	Where possible will attempt to detail the symptoms of poisoning. (NRA data could be added here).
Bioaccumulation	Bioconcentration factors (log); Log Kow; Body burdens (species, exposure, levels); fish tainting levels; food chain biomagnification.
Mammalian Toxicity	Summary of hazard posed to humans and livestock.
Fate and behaviour	The profile will attempt to identify how the substance will partition in the aquatic environment (e.g. sediments, water); its biodegradability (e.g. in water, sediments, soil, sewage sludge); its fate in water (e.g. principal route of removal); and persistence (e.g. half lives in water, sediment and soil).
Standards and Guidelines	EQS; Water quality criteria; LSEC.
Analysis	Appropriate analytical method and limit of detection.
Physical/Chemical Properties	Chemical structure; chemical mass; Physical appearance; Melting point; Boiling point; Flash point; Solubility; Henry's Law constant; Vapour pressure; Dissociation constant; Octanol water partition coefficient; Soil adsorption constant.

Table 4.3 Type of information present in the summary of the proposed substance profile

Type of Information	Data Provided
Identification	Chemical abstracts number; IUPAC name; Chemical group; HAZCHEM code; Synonyms.
Fish Toxicity	LC50 and high, medium or low toxicity statement.
Invertebrate Toxicity	LC50 or EC50 and high, medium or low toxicity statement.
Plant and algal toxicity	LC50 or EC50 and high, medium or low toxicity statement.
Bioaccumulation	Bioconcentration factor and high, medium or low bioaccumulation potential statement.
Environmental Partitioning	Sediments, water.
Persistence	Half-life and high, medium or low persistence statement.
Standards	EQS, LSEC, WQC.

Short advisory/report

The proposed short advisory/report (see Glossary) is designed to provide critically assessed information on the aquatic toxicity of chemical contaminants. It is likely to be of particular use to NRA personnel involved in establishing discharge consents and would also provide a suitable source of background information for certain strategic policies (e.g. R&D).

Table 4.4 summarises the information that these advisories/reports would contain. It is intended that an assessment of the toxicity to both fish and invertebrates will be available for both short- and long-term exposure and for lethal and sublethal effects. Additionally as a consequence of both the number of taxa covered by each advisory/report and the detailed data that each provides, it is likely that sufficient data will be available for the derivation of a likely safe environmental concentration (LSEC) (Appendix F). Finally it is intended that each advisory/report will have a summary highlighting the major points concerning the substance's toxicity.

Table 4.4 Type of information present in the proposed substance advisory/report

Type of Information	Data Provided
Identification	Chemical abstracts number; IUPAC name; Chemical group; HAZCHEM code; Synonyms.
Toxicity to fish	An assessment of the acute and chronic (lethal and sublethal) toxicity.
Toxicity to invertebrates	An assessment of the acute and chronic (lethal and sublethal) toxicity to a selection of invertebrate taxa. Sensitive groups will be identified.
Toxicity to algae and plants	An assessment of the acute and chronic (lethal and sublethal) toxicity.
Bioaccumulation	An assessment of the bioaccumulation potential.
Standards	Information on EQS or LSEC.

4.3.2 System strategies

There are a number of database system strategies that the NRA could adopt. Each system has been selected according to NRA's information technology strategy and either one could be selected for the information system, or alternatively a combination of (i) to (iii) could be used. The characteristics of the proposed systems are outlined below:

(i) Data General UNIX-based ORACLE system, with customised "front-end" to enquire for substance name and give an index of substances to pick from, and data interface procedures for information transfer to and from local and remote systems. Access would be local or by dial-up modem from remote sites;

(ii) PC-based "fixed field" database (see Glossary), using a commercially available database package (e.g. Dbase IV), again with customised front-end;

(iii) PC-based text retrieval database (see Glossary), similar to WRc's "AQUASEARCH" product.

On the basis of the results of the surveys (Section 2), it is currently envisaged that data would need to be accessed by substance name (including synonyms, identification codes or numbers). However, it is important for the NRA to consider whether at a later date, it may wish to search by other criteria, e.g. LC50, as this has a direct bearing on the type of system selected.

4.3.3 Usage of database system

The results, obtained from the questionnaire and interview surveys (Section 2), on departmental organisation and use of toxicity information within NRA, suggest that the potential number of users of the unified information system are approximately 40 - 130 per NRA region (except HQ), thus 400 - 1300 nationally. However, it is likely that the highest number of users (130/region) is an overestimate at the present time, since organisation and function of departments varies between NRA regions. For instance operational responsibilities (e.g. pollution control and establishing discharge consents), satisfied in some regions by two departments, are satisfied by one in others; effectively reducing the number of potential users.

Nevertheless the number of present users is likely to increase with the introduction of new legislation, new NRA policies, or an increased awareness of ecotoxicology, particularly in regions where such information is poorly used.

Assuming that the frequency of use statistics (Section 2.3.1) can be applied to a population of 400 - 1300 users nationally, there will be between 100 - 300 accesses to the database daily. The systems outlined in Section 4.3.2 (i) - (iii) therefore, would be able to cope with the existing numbers of users within NRA and also could cope with an increase in usage.

However, for DG-ORACLE, NRA's computer systems managers and administrators need to assess the impact of increased usage of their systems, although the usage figures above are unlikely to be of concern to them. Nevertheless they will be concerned about the volume of data, and their data communications' capacity.

With a PC based "fixed field" or "text retrieval" databases each user would require access to a PC with sufficient storage and processing capacity to run the system. Additionally each user would have to be provided with a user software license, together with a customised "front-end" to enable them to use the system, and additionally an arrangement could be made with the software licenser for a multiple user license for use within the NRA.

4.3.4 Data volumes

Expected number of compounds

NRA are likely have a priority list of the most problematic substances and these will obviously require attention first for the system. Based on information available through the Information Service for Toxicity and Biodegradability (INSTAB), WRc estimate that approximately 200 - 300 chemicals would be on this list. However, in the long term it is likely that a large number of substances will be required on the database (e.g. 5000 or more, especially if trade chemicals and mixtures are included (maximum 60 000)). But despite this large number of compounds, only limited published information will be available on most, although NRA in-house toxicity testing could add to this limited dataset.

Amount of information per compound

The amount of assessed and interpreted information produced for intensively researched substances (approximately 200) is likely to be equivalent to 3 pages (maximum) of A4 text for the substance profiles and 5 pages (maximum) for the short advisory/reports. Information on the poorly studied substances are likely to be limited. Consequently approximately 1 - 1.5 A4 pages text (maximum) for the substance profile and 2 - 2.5 pages (maximum) for the short report/advisory are likely.

One page of A4 size text consists of about 3000 characters (ca. 3 kilobytes (K)) as a practical maximum, and about half that on average. For the first 200 substances therefore, 3 pages of profile and 5 pages of report would result in a maximum of 24K (9 + 15 = 24K) per substance, or about 5 Megabytes (maximum). For 5000 substances taking a maximum of 12.5K each (5 + 7.5 = 12.5K), the number of Megabytes would be about 60. For 60 000 substances taking the number of kilobytes would be 750 Megabytes. The capacity required by the database systems therefore, is large, but it would take a considerable amount of time to accumulate information on 5000 substances and also the number of Megabytes required should be considered as a maximum.

Capacity of the database systems

All the systems (with the appropriate hardware) are capable of running the database package.

The amount of indexing required by the DG-ORACLE system is minimal, since only one entry point (i.e. the substance name) is required. The total storage overhead is likely to be 100%, implying storage requirements of 10 Mb/125 Mb/1, 500 Mb for 200, 5000 and 60 000 substances respectively and would be confirmed by NRA's technical specialists.

The typical PC hard disk sizes are of the order of 30 Megabytes, although older machines could only have 10 Megabytes. Assuming storage overhead of 100%, the storage of only 200 intensively studied substances, which would require 10 Megabytes, would be feasible on a PC "fixed field" database. However, optical storage technology (especially for read-only usage) is advancing, allowing volumes of storage of the order of a Gigabyte (1000 Megabytes), in which case all substances can be stored in this way. Additionally capacity may be improved through data compression routines (which some PC packages offer), but this may compromise the speed of retrieval.

The storage requirement for an inverted file index retrieval system (e.g. PC "free text" searching database AQUASEARCH) is greater than for other databases (approximately 150% - 200%) and again information on only 200 substances could be run on this, but a 5000 or 60 000 substance database would not. As with the PC "fixed field" option outlined earlier, optical storage technology may make this system a feasible option.

4.3.5 Frequency of use

It is unlikely that systems outlined in Section 4.3.2 (i) - (iii) would ever be overloaded with users accessing information.

A number of points concerning usage have already been highlighted in Section 4.3.3. Nevertheless the remote use of the DG-ORACLE system would primarily be limited by the availability of modems on the DG machine. Consequently all users could not possibly be using the system at the same time. The number of possible concurrent users is likely to be small, e.g. approximately 4 - 8. Consequently the system itself could never be overloaded.

Similarly the PC based systems (Section 4.3.2 (ii) - (iii)) are unlikely ever to be overloaded, since these systems are single-user orientated.

4.3.6 Maintenance

Control of the maintenance of the database must be held by a centralised function.

Since the data are all held in one place for the DG-ORACLE system, there is no problem with data consistency. ORACLE allows full control over who is allowed to add, update and delete data from the database, and procedures and security features are needed to ensure that the database is correct and up-to-date. The maintenance facilities are not required to be unusually easy to use, since a relatively small number of staff would have the ability to change data. Backup of the data would presumably be provided by NRA's computing support, but separate procedures could be implemented if necessary.

The distributed PC "fixed field" and "text retrieval" systems would have to ensure that the users cannot change the data in the system, even if they are given the facility to add their own local material to it. The updates to the system would have to be distributed either on "floppy disk" or by electronic means. The local PC update procedure would have to be easy to use, since it would be implemented by a variety of users. Backup would have to be provided both centrally and by the users themselves and qualified support would have to be available both on the software and the data.

Adding, updating and deleting data is intrinsically more complex in a PC text retrieval system (Section 4.3.2 (iii)). Fixed-field databases (Section 4.3.2 (iii)) and their indexes are simple to update interactively. Text retrieval systems, or "inverted file" systems have to regenerate their entire index every time the data are changed.

4.3.7 Ownership

A DG-ORACLE system would be written by ORACLE programmers employed directly or sub-contracted by the NRA, and therefore the software would legally be copyright to them, and usable freely under their ORACLE licence.

The database licences for the "fixed field" PC database system would be held presumably, by the NRA (either locally or nationally). The copyright to any program or procedures written as a user interface would be held by NRA.

The distributed PC software package for the "text retrieval" database package would be less well defined in terms of ownership. The database licenses would be held, presumably, by the NRA (either at local or national level). The copyright to any program or procedures written as a user interface would either be held by the NRA or the software licenser for the database (e.g. in the case of the WRc database package AQUASEARCH, the changes are made to the software package by the manufacturers).

In either case, the ownership of the information within the system would have to rest with the NRA and consideration of the copyright of any information supplied to the system by interfaces to commercial databases would be needed. Additionally information acquired from a commercial database and then distributed must be covered in an agreement with the commercial database provider.

4.3.8 Database Interfaces

Assuming that NRA has a full implementation of ORACLE, interfaces to other local databases can be made by either 'batch' interfaces (e.g. production of an exported data file for use by that system and vice versa), or more interactively by using the 3GL interfaces (Third generation languages, like 'C' calling ORACLE commands). This would require bespoke programming for each interface and the system design would have to take these into account, to avoid data inconsistencies between the systems.

Interfaces to remote systems (e.g. external on-line databases) would be of the 'batch' kind only, and would depend on proper license agreements to the use of the data obtained. The data obtained would have to be processed into the correct format for the information system.

Only the 'batch' interfaces would be available for fixed field PC based systems, due to the standalone nature of the solution. The data obtained would have to be processed into the correct format for the information system and copyright would again have to be taken into account.

Additionally only 'batch' interfaces would be available for text retrieval PC based systems, but minimal processing of the data obtained would be needed, due to the free-text searching capability of a text retrieval system and again copyright would require consideration.

4.3.9 Costs

It is difficult to be precise on the costs of each database system without having specified the desired system more fully, but certain costs would be similar for any system, with regard to the data and functional specification. Each system, however, would have its own "unique" costs (see Table 4.5).

Exploitation of NRA's staff skills for the writing and maintenance of the DG-ORACLE system would reduce its costs. No additional software licences should be needed unless NRA's ORACLE license has a limit on the number of users.

The areas of increasing cost for the PC systems are on the ongoing supply of update media and any supply of optical or other disk controllers and disks if the amount of storage space exceeds that which seems reasonable. Individual or group licenses from the software publishers will have to be purchased, but these would be reasonable (typically from £100 for every PC). Administration costs would be increased as a number of update floppy disks would have to be produced and sent out of a regular basis. It is inevitable that an element of PC support would also be needed from the central information unit.

However, WRc already has a text retrieval system (e.g. AQUASEARCH), and a good relationship with the software producers (who may be eager to get their product more widely known within the NRA), the costs of the software production may be considerably less than for a "fixed field" PC database.

Table 4.5 Comparison of the costs likely to be incurred with a ORACLE or PC system

Features	Database system costs (£K)		
	ORACLE	PC fixed field	PC text retrieval
Data requirements	2	2	2
Data structure specification	1	1	1
Functional system specification	3	3	3
System process specification	5	5	5
System testing	7	7	7
Data licensing costs	*	*	*
Support costs (e.g. qualified technical support and database administration)	*	*	*
Data table design	2	2	-
System and interface specification and coding	5	5	5
Hardware costs** (e.g.. additional modems, disk storage)	25	5	5
Running costs (e.g. telephone and processing time, "rental" and license maintenance)	5	-	-
Data preparation	5	6	6
Update media (e.g. floppy disks)	-	1	1
Total	60	37	35

NOTES * Not enough information to specify

** £10K per annum for DG-ORACLE system. Costs are inclusive of running costs for PC fixed field and text retrieval databases

4.3.10 Benefits and disadvantages

Each system has a number of features that are beneficial or are a disadvantage for the NRA. The features are listed according to the database system in Table 4.6.

Table 4.6 The benefits and disadvantages of the proposed database systems

Database system	Benefits	Disadvantages
DG-ORACLE/UNIX	The system would be understood and controlled by the NRA, their own people would be more confident in its reliability, because they, essentially, would have produced it in-house. The Database is one that is known to them, and they have expertise in the efficient management of ORACLE.	The system is remote from the user, and liable to communications problems "noise"; a misprint is more dangerous with critical numerical data than with text.
	Interfaces would be more easily produced and understood, since ORACLE uses the industry-standard SQL query language for database administration and 3GL program production.	With the system potentially dependent on a single processor, any down time of that processor is more critical than if data were distributed.
	The NRA Information Unit have total control over the data content and system maintenance at one location only.	The concept of a single access point (e.g. substance name) is limiting. Free-text searching will not be available as an option later without considerable cost in processing time. There is also no allowance for imprecision in substance specification.
	The system has definite advantages for Management both in financial and access control.	
	As a relational database, (e.g. add, update and delete data).	
	The single access point (e.g. substance name) makes it simpler for the user.	
PC-based fixed field	Local control of data and processing.	There is a possibility of a lack of consistency between machines (e.g. a floppy disk update lost in the post).
	PC licenses, maintenance and peripherals tend to be cheaper than those for mini-mainframes.	The larger versions of the system may require individual hardware upgrades (e.g. an optical or other disk).
	Portability (e.g. no dependency on communication lines, nor, theoretically, on power supply).	

...../continued

Table 4.6 (continued)

Database system	Benefits	Disadvantages
	As a fixed-field database, it would be simple to maintain (i.e. add, update and delete data). The single access point (substance name) makes it simple for the user.	The concept of a single access point (e.g. substance name) is limiting. Free text searching will not be available as an option later without considerable cost in processing time. There is also no allowance for imprecision in substance specification. Having to adapt a PC database package, with the possibility of functional limitation. Inflexibility of the interface capability.
PC-based "free text" searching	WRc have had experience of this; one version of the system already exists. Local control of data and processing. PC licenses, maintenance and peripherals tend to be cheaper than those for mini-mainframe. Portability (e.g. no dependency on communication lines, nor, theoretically, on power supply). As a free-text database, it is flexible in its searching capability. All text could be indexed, and so any document could be retrieved from imprecise information.	There is a possibility of a lack of consistency between machines (e.g. floppy disk lost in the post). The larger versions of the system may require individual hardware upgrades (e.g. an optical or other disk). The use of a free-text database is inappropriate for essentially numerical data, with an obvious key field for retrieval. Maintenance of the database is slightly more complex for the user, unless extra resources are devoted to writing the system. There is a larger storage overhead. Inflexibility of the interface capability.

4.4 Database system and associated knowledge based systems (KBSs)

KBSs have the ability to encapsulate knowledge or expertise and make it more widely available. As such they complement databases, which encapsulate information, by providing an interpretation of or advice on the meaning of the data or advise an action to be taken. (A description of the key features of KBS was given in Section 3.)

4.4.1 Application of Knowledge-Based Systems

In order to review the feasibility of an integrated information system incorporating a KBS, it is necessary to identify how such a system may be used, by whom and for what purpose.

The following five KBS applications have been identified which are extensions to the ecotoxicological database and enable greater use to be made of the data within it:

(i) Incident management - to advise on the constituent substances complex effluents or formulations prior to accessing the database by substance name;

(ii) Incident management - to identify the likely pollutant from details of symptoms and upstream discharges prior to the results of chemical analysis;

(iii) Incident management - to advise on the action to be taken depending upon the volume and toxicity of the pollutant and the details of the site;

(iv) Consent setting - to assist the user to undertake an impact assessment to determine the likely safe environmental concentrations of substances within the proposed discharge;

(v) Catchment management - to advise on the safe volumes, concentrations and storage requirements of toxic chemicals within the catchment.

Clearly the scale and information requirements of each of these applications varies significantly. Applications (i) and (ii) are relatively small KBS, whereas (iii), (iv) and (v) are medium to large developments, depending upon the number of substances they would cover. The following sections assume that a medium sized application would be required initially.

4.4.2 System strategies

Using a KBS with a database means that there are three main options envisaged:

(i) Mainframe processing using remote PC terminals

This would utilise a mainframe computer (NRA have a Data-General UNIX based system with ORACLE database) where the database and interrogation software would reside. Access would be local or via modem-linked remote PCs at other sites. Data would be transferred down this link with the KBS residing on the mainframe.

(ii) PC based processing

This would utilise PCs with the database and its interrogation software (including the KBS) residing on its hard disk. The data would be held on a central PC and updates of that data periodically transferred to remote sites by floppy disk or electronic means.

(iii) PC and mainframe processing combination

This would utilise a combination of options (i) and (ii). The relevant parts of this database and its data would reside on the mainframe. This would then be transferred to the PC when required. The KBS would reside on the PC.

4.4.3 Usage of the system

Although the number of users of the database identified in Section 4.3.3 is relatively large it is assumed that only a proportion of these would require access to a specific KBS application. Some of the KBS applications will require data transfer between the mainframe and the KBS. Some will be able to work alone from user input only. Therefore, the performance will depend on each application (Section 4.4.1) and the option chosen (Section 4.4.2).

It is envisaged that for the option outlined in Section 4.4.2 (i), the number of concurrent users envisaged would not pose a problem for system performance.

For the second option (Section 4.4.2 (ii)) each user would require their own PC with sufficient storage and processing capacity. If this was assessed properly then performance would be sufficient. In addition, each KBS used on each PC would require a software licence. In certain circumstances it may be possible to acquire a site licence.

Usage of the third option (Section 4.4.2 (iii)) would depend on the speed of transfer of data down the line to the PC. However, bearing in mind the low number of users at any one time, this is not likely to cause a problem. Again, KBS used on each PC would require a software licence. In certain circumstances it may be possible to acquire a site licence.

4.4.4 Maintenance of the knowledge base

The maintenance and updating of the knowledge contained in the KBS would, again, depend on the option chosen. However, all updates should be under the control of a Knowledge Base Administrator (KBA) who would authorise changes and be responsible for updates.

Due to the evolving nature of KBS development the knowledge contained would need to be refined after delivery. This is due to the complex nature of verifying that knowledge, and further requirements that inevitably arise after delivery. One method of achieving this (outside of final system testing) is for the system to keep a log of each interaction with it. This log could then be used to check that the system advice/conclusions are correct. Perhaps once or twice a year the log would be inspected. This would suggest changes and/or further knowledge to be incorporated in the knowledge base. It is important to realise that the system must be tested after each change to ensure that it performs to expectations.

Using the option detailed in Section 4.4.2 (i) it would be possible to update the knowledge base centrally and, hence, this would be a relatively easy task for a trained knowledge engineer.

Using the PC options (Section 4.4.2 (ii) - (iii)) would mean that new versions of the knowledge base would need to be distributed to each PC and user. This would require more administration than above and require a trained knowledge engineer to perform the changes. Once distributed, the user would load the new version onto the PC.

4.4.5 Ownership

A licence for the use of the software would have to be paid for each deliverable copy used. This would depend on the number of installations and on the KBS option chosen. If the KBS software resided on each PC then discounts for many copies are available. It may be possible to obtain a site licence which would reduce the costs.

As far as ownership of the knowledge contained was concerned this would depend on whether its source was the NRA itself or an external organisation. Incorporation of the knowledge of another organisation could cost more than simply the development costs of such a system. Final ownership would be a matter of negotiation between the NRA and the organisation providing the knowledge.

4.4.6 Costs

The following are very broad estimates based on the assumed requirements stated previously. It is impossible to estimate the costs of delivery licences because this depends on the type and number of computer terminals or PCs required.

For the options in Section 4.4.2 (ii) - (iii) where the KBS can be developed using a PC based toolkit, cost estimates are as follows:

(i) Incident management - to advise on the constituent substances within complex effluents or formulations prior to accessing the database by substance name.

Cost: £20K to £40K

(ii) Incident management - to identify the likely pollutant from details of symptoms and upstream discharges prior to the results of chemical analysis.

Cost: £20K to £40K

(iii) Incident management - to advise on the action to be taken depending upon the volume and toxicity of the pollutant and the details of the site.

Cost: £50K to £100K

(iv) Consent setting - to assist the user to undertake an impact assessment to determine the likely safe concentration of substances within the proposed discharge.

Cost: £100K to £150K

(v) Catchment management - to advise on the safe volumes, concentrations and storage requirements of toxic chemicals within the catchment.

Cost: £100K to £150K

For the option outlined in Section 4.4.2 (i) where the KBS would need to be developed in a suitable language on the mainframe, the costs are likely to be 50 to 100% higher.

4.4.7 Benefits and disadvantages of using a KBS

There are a number of benefits of using a KBS (listed below) and the benefits and disadvantages of each option in Section 4.4.2 are detailed in Table 4.7:

(i) It would enable the NRA to utilise rare or often unavailable expertise and make it available to other, less skilled staff. This will lead to more efficient solutions than would be achieved otherwise;

(ii) It would ensure a more efficient storage and use of ecotoxicological data and knowledge;

(iii) Constantly consulted experts would be free to perform more productive tasks;

(iv) The NRA would to be more independent in this area;

(v) Advice from such a system would be available to those who require it on a 24-hour basis. This may not be possible using an external service or just a database retrieval system;

(vi) It would carry out tasks in a consistent and complete manner and derive solutions that can be explained or justified;

(vii) A complete audit trail of a consultation with the system would be produced, greatly aiding Quality assured operation;

(viii) Task would be completed in a shorter time than was previously possible;

(ix) All the above would reduce costs.

Table 4.7 The benefits and disadvantages of the proposed knowledge based systems

Database system	Benefits	Disadvantages
Mainframe processing processing using remote terminals	Maintenance of the knowledge base would be relatively straightforward.	WRc know of no KBS development toolkit available for the mainframe option. This would severely limit the KBS development options to the use of a programming language which will increase cost of development.
	Interfacing to ORACLE would be possible subject to its disadvantages.	If any development environments are available at all then they would cost considerably more than a PC based system.
		Cost of development on a mainframe would be higher than a PC based system.
PC based processing	Cheapest method of development. Plentiful choice of suitable development software. A more user-friendly interface can be built. There would be no variable demand for information due to PC being a single user.	Maintenance of the KBS would be more difficult due to the necessity of issuing new versions when changes take place. However, proper administration and control would overcome this. Requests for knowledge maintenance would need to be coordinated, most probably by the original developers. Licensing costs for all of the software installed on the required PCs will be higher than the mainframe.
PC and mainframe	The data could be stored centrally. Plentiful choice of suitable development software. A more user-friendly interface can be built. Single-user and no speed of access problem. No variable demand for information.	Maintenance of the KBS would be more difficult due to the necessity of issuing new versions when changes take place. However, proper administration and control would overcome this. Requests for knowledge maintenance would need to be coordinated, most probably by the original developers. Licensing costs for all of the software installed on the required PCs will be higher than the mainframe. Data may be downloaded from the mainframe as required by the KBS. This may be subject to delay because the KBS will be selective about the data it chooses to download. This means that several transfers may be needed to perform a single consultation. However, this would only apply to some of the applications and may not be a limiting factor.

4.5 Information Unit

This unit would provide or direct toxicology support throughout the NRA and could also be the unit responsible for coordinating updates for the database package. To function effectively it would require toxicologists to select and process information and would need a number of reliable links to external data sources.

If located centrally within the NRA, the unit will have access to the database package and would need to establish links with external data sources (e.g. "on-line" database hosts and an information and advisory service). Similarly if the unit is located externally (e.g. at an information and advisory service), NRA staff will have access via the service to similar sources. Regardless of where the unit would be located its principal functions would be to provide detailed or basic (in the short term) data on the toxicity of substances, and to provide support to NRA personnel for general enquiries on ecotoxicology (e.g. interpretation).

4.5.1 Frequency of use

The frequency of use and variable demand for information (e.g. complexity of enquiry) by NRA personnel will determine how efficiently both an internal or external unit can function. At present there is typically a low usage of toxicity data within the NRA (Section 2.3.1), although this is likely to increase in the near future.

If the NRA establish an internal unit it is advisable to maintain a small one (e.g. 2 - 3 people) at first, with access to a number of data sources (e.g. on-line hosts), which can be expanded with the demand for toxicity information. Additionally it is advisable to establish or maintain links with an existing information and advisory service for use as an alternative information source, or for occasions when there is a great demand for information.

An external unit is unlikely to suffer from the variable demands that an internal unit (in the short term) could be prone to. Frequency and variable demand for information are therefore, unlikely to effect the response time.

The NRA would benefit from 24 hour toxicological support for pollution incidents. The frequency of such requests is likely to be low and therefore, it may be more cost effective for such a service to be handled externally.

4.5.2 Maintenance

Maintenance of the information unit will relate mainly to the staff and available sources of information. However, it is important that the unit's development is periodically monitored to ensure that the NRA's need for detailed ecotoxicological information is satisfied.

Personnel employed in an internal information unit will require a considerable amount of training in order to effectively locate and interpret data. Training courses on the retrieval of information for particular on-line databases are available from a number of hosts (e.g. DIALOG). Maintaining this training is essential, since hosts continually modify searching strategies to improve data retrieval and staff will be unaware of these changes unless courses are attended regularly. Additionally personnel not experienced in specific areas of the water industry (e.g. sewage treatment, water treatment) or toxicology (e.g. environmental relevance of ecotoxicology tests) would benefit from training in such areas, since this would help them in the interpretation of data.

The data sources used by the unit to retrieve information will require maintenance. The unit would benefit from a continual awareness of new developments (e.g. recent publications, or new on-line, CD-ROM or PC databases) and would need to be able to gain access to select any suitable sources.

Maintenance (e.g. personnel, training and sources) would not be of concern to NRA if an external information and advisory service were selected, since these would be financed by the organisation that offers the service.

4.5.3 Information unit interfaces

The internal information unit will need to interface with both NRA databases and external data sources either via the database package or by other means.

Although it is not the aim of this project to identify specific internal databases with which the information system should interface, it is desirable that any proposed system is capable of interfacing with the NRA's mainframe and PC databases (e.g. WIS (water information system and CHEMSAFE)).

Recommended external interfaces include the 24 hour toxicity information and advisory service provided at WRc and links with institutes such as Plymouth Marine Laboratory (PML) and Institute of Freshwater Ecology (IFE) may also prove useful. Additionally interfaces with on-line databases and databanks available on the hosts STN, DIALOG, CIS and TDS Numerica would be beneficial.

External information and advisory services could not interface with the NRA's internal databases, but could offer similar (or more extensive) links with external data sources.

4.5.4 Costs

The cost of establishing an information unit is likely to be high and it is important that this cost is justifiable against the demand for information.

Staff costs and costs associated with sources of information are likely to be the main areas of expenditure. Table 4.8 details the expected cost of setting up an internal information unit. The initial outlay for the unit would be for 3 experienced staff and necessary training, provision of 24 hour call-out, and acquiring specific sources of information or establishing links with data sources. In total therefore, it is estimated that to set up a unit for the provision of toxicity data only, the cost could be approximately £149K, excluding the cost of the database base system and information. Maintenance of the unit would be less at £100K (excluding database).

The cost of using an external information and advisory service (e.g. WRc) would be approximately £75K (including database and information) at present demand (Table 4.8). This is cheaper, but does not have the advantages of an internal information unit (Section 4.2.3, Appendix D4).

Table 4.8 The approximate cost of establishing an internal and external information unit

	System cost (£K)	
Feature	Internal	External
Staff and overheads (e.g. 3 toxicologists)	100	
Staff costs for 24 hour standby for emergency call out	3	
Training (e.g. on-line database searching, areas of the water industry)	11	
Database package (see Section 4.3.9)	-	
Texts (extensive)	3	
External data sources (e.g. on-line, WRc 24 hour callout)	**24	75
Maintenance of current awareness (e.g. Journals, Conferences)	8	
Total	149	*75

NOTES * Including toxicity information. Based on 1992/1993 figures

** This figure is based on WRc's expenditure for on-line databases and 24 hour call out. An information unit at NRA, without a similar internal database used by WRc, could spend considerably more on on-line searching than has been estimated.

4.5.5 Benefits and disadvantages

The benefits of an information unit (either internal or external) are that:

(i) It would be a central facility for users to obtain information or guidance on problems, thus ensuring, through discussion that the users' needs would be satisfied;

(ii) Data sources not available through the database package could be accessed by this unit.

(iii) It would facilitate centralised updating of any database and KBS, thus ensuring consistency between NRA regions.

The disadvantage of an information unit relates to its use within the NRA and its cost. The unit may not be used to its full potential, as some personnel may prefer to use personal contacts (internally or externally) to obtain information, and thus, consequently, in such instances a consistent approach to obtaining and using toxicology information within NRA might not be achieved. Additionally the costs of establishing an internal information unit are high in comparison to the use of an external information and advisory service.

5. PROJECT DISCUSSION AND RECOMMENDATIONS

5.1 Survey results

An understanding of the information requirements of the NRA was obtained from the results of two surveys carried in July and August 1991, targeting personnel who use ecotoxicology to solve operational problems (Section 2). The most notable findings of these surveys are as follows:

1. Most participants (potential users of the system) appeared to have gained their ecotoxicology experience from work rather than from formal training. Additionally many lack an understanding of the basic principles underlying the application of ecotoxicology information.

2. The findings of the surveys suggest that the NRA's information requirements can be divided into 3 broad areas:

   (i) Incident management;

   (ii) Consent setting (including planned discharges);

   (iii) Strategic policies (a "catch-all" category which encompasses areas such as catchment management, R&D, monitoring, policies, legislation, EQS derivation and others).

   Each of these three areas has different information requirements, in terms of the type of data, speed of response, detail of reply and frequency of need. However, all areas are similar in that they require data to be both assessed and interpreted.

3. The results of both surveys indicate that NRA personnel strongly favour the existence of a unit providing toxicity information and support, but would also benefit from a computerised toxicology database available for personal use.

5.2 Proposed solutions

Based on the identified requirements of the NRA, possible strategies have been proposed for a unified information system that will provide both ecotoxicological and supporting data (Section 3). This unified information system will comprise a combination of:

(i) A database package (run under mainframe ORACLE or on PCs);

(ii) A knowledge based system (KBS) (run on ORACLE, PC or both);

(iii) An information unit (either internal to the NRA or an external advisory service).

The types of information that ought to be made available on the database system have been identified. The proposed database system will be accessible by substance name or identification codes only, and it is important that the NRA considers whether it may wish, at a later date, to search by other criteria (e.g. LC50), as this has a direct bearing on the type of system selected.

It is proposed that different levels of interrogation of the database will be possible, with the output varying accordingly. Substance profiles and short advisories/reports would be most useful for staff involved in incident management, consent setting and certain strategic policies (e.g. catchment management, monitoring). However, the requirements of staff involved with certain strategic policies such as R&D, long term planning, and assessment of widespread contamination would not be satisfied by such reports, and consequently an information unit providing both data and ecotoxicological support is proposed to satisfy their needs.

An initial feasibility study of the proposed solutions has been carried out (Section 4). This includes consideration of the level of usage, volume of data, frequency of access, maintenance requirements, ownership, interfaces and costs of each of the proposed options for the database system (including the KBS) and information unit (summarised in Table 4.2). The benefits and disadvantages of an internal and an external system are also considered and a general strategy proposed. The cost of the solutions are between £110 and £209K for a database and information unit, and between £130 and £359K for a database in association with a KBS. The actual cost depends on the database option selected, whether the information unit is internal or external to the NRA, and the type and number of KBSs selected. The cost of using just an external information and advisory service is approximately £75K (based on the current demand for data) (Section 4).

5.3 Applications of ecotoxicology data

As well as proposing a specification for an information system, this project has attempted to identify the ecotoxicological (and related) information requirements for the derivation of environmental quality standards (EQSs) and likely safe environmental concentrations (LSECs) for chemicals (Appendix E and F, respectively). These appendices include a consideration of the application of these "standards" to different situations, and will be of use to NRA staff who need to apply ecotoxicology data to estimate "safe" concentrations for chemicals.

5.4 Recommendations

The NRA need to examine the results of the surveys and consider the level of future demand for ecotoxicological information and support against the cost implications of establishing an internal unified information system, as opposed to alternative solutions (e.g. PC database for hazardous chemicals, use of external data sources).

If it is considered that the demand justifies establishing an information system, the various strategies proposed in this report need to be considered in order to determine which is most appropriate to the NRA's requirements. This will need to be followed by the development of a detailed strategy specification before full implementation in both the short- and long-term.

Whichever strategy is chosen, the following recommendations are made:

(i) Ecotoxicological and supporting data should be available as both substance profiles and short advisories/reports;

(ii) In the short-term, information should be presented on a database system (run on mainframe ORACLE or PCs), with additional support from an external information and advisory service;

(iii) If a KBS is desired, this should be introduced in the long-term. However, the database system (i.e. the short-term solution) must have been previously designed with this in mind;

(iv) The NRA should consider including in-house data (e.g. monitoring data, incident reports, consent details, and so on) on the database system;

(v) The database (and in the long-term the KBS, if required) should be made available on "lap top" PCs for use during pollution incidents;

(vi) If an internal information unit is established, this should comprise experienced toxicologists providing data and advice, and should have links with a number of external data sources.

It is important at all stages of the strategy specification and subsequent implementation that the NRA monitors for any change in requirements for ecotoxicological information. The developmental progress and efficiency of the system should also be monitored before, during and after implementation.

REFERENCES

Agg, A.R. and Zabel, T.F. (1989) Environmental quality objectives and effluent control, *Chemistry and Industry,* 1989, 443-447.

Baker, M.G.C, Rogers, H.R., Johnson, C., Fawell, J.K. and Wright, K. (1991) Fate and behaviour of chemical contaminants in the aquatic environment: A review of the sources of information. WRc report NR 2726. National Rivers Authority 254/1/A.

Cairns, J.C. (1986) The myth of the most sensitive species; multispecies testing can provide valuable evidence for protecting the environment, *BioScience*, **36,** No. 10, 670-672.

Cartwright, N. and Painter, H. (1991) An assessment of the environmental quality standards for inorganic nutrients necessary to prevent eutrophication (nuisance growth of algae). WRc Report No. NR 2397.

CCTA (1989) Appraising investment in information systems. Systems development set B4, The information systems guides, Central Computing and Telecommunications Agency, John Wiley and Sons Publisher.

CEC (Council of the European Communities) (1975) Directive concerning the quality required of surface water intended for the abstraction of drinking water in the Member States (75/440/EEC), *Official Journal,* **L194,** 25 July 1975.

CEC (Council of the European Communities) (1976a) Directive on pollution caused by certain dangerous substances discharged into the aquatic environment of the community (76/464/EEC), *Official Journal,* **L129,** 18 May 1976.

CEC (Council of the European Communities) (1976b) Directive concerning the quality of bathing water (76/160/EEC), *Official Journal*, **L31,** 5 February 1976.

CEC (Council of the European Communities) (1978) Directive on the quality of fresh waters needing protection or improvement in order to support fish life (78/659/EEC), *Official Journal,* **L222,** 14 August 1978.

CEC (Council of the European Communities) (1979) Directive on the quality required of shellfish waters (79/923/EEC), *Official Journal,* **L281,** 10 November 1979.

CEC (Council of the European Communities) (1980) Directive relating to the quality of water intended for human consumption (80/778/EEC), *Official Journal,* **L229,** 30 August 1980.

Crane, M. (1990) A review of the use of aquatic multispecies systems for testing the effects of contaminants. WRc DoE 2587-M.

Crane, M., Johnson, I. and Adams, N. (1991) Ecotoxicology - new approaches. WRc report No. NR 2676.

Crane, R.I., Zabel, T.F. and Fawell, J.K. (1988) Proposed environmental quality standards for trichlorobenzenes in water, WRc report no. DoE 1646-M/2.

Crossland, N.O. (1986) Predicting the hazards of chemicals to aquatic environments, *Chemistry and Industry*, 1986, 740-744.

Gardiner, J. and Mance, G. (1984) Proposed environmental quality standards for list II substances in water. Introduction. WRc Technical Report TR 206.

Hunt, D.T.E. (1989) Discharge control by direct toxicity assessment (DTA) - interim protocol. WRc PRS 2160-M/1.

Kimerle, R.A., Werner, A.F. and Adams, W.J. (1985) Aquatic hazard evaluation principles applied to the development of water quality criteria. In: *Aquatic Toxicology and Hazard Assessment: seventh symposium ASTM STP 854,* Edited by R.D. Cardwell, R. Purdy and R.C. Bahner. ASTM Philadelphia.

Könemann, W.H. (1984) Ecotoxicology and environmental quality. Chapter 6 In: *Environmental Protection: Standards, Compliance and Costs,* Edited by T.J. Lack, WRc/Ellis Horwood.

MAFF/ADAS (1980) Water quality for crop irrigation: guidelines on chemical criteria. MAFF/ADAS Information Leaflet 776.

OECD (1991) Draft report of the OECD workshop on the extrapolation of laboratory aquatic toxicity data to the real environment. Environment Directorate, OECD.

Otter, R.J. (1979) Environmental quality objectives, *Chemistry and Industry*, 1979, 302-305.

Price, D.R.H. and Pearson, M.J. (1979) The derivation of quality conditions for effluents discharged to freshwaters, *Water Pollution Control,* **78,** 118-138.

Stephan, C.E., Mount, D.I., Hansen, D.J., Gentile, J.H., Chapman, G.A. and Brungs, W.A. (1985) Guidelines for deriving numerical national water quality criteria for the protection of aquatic organisms and their uses. US EPA, Washington DC. National technical information service PB85-227049.

US EPA (1984) Estimating "concern levels" for concentrations of chemical substances in the environment. Environmental Effects Branch, Health and Environmental Review Division, February 1984.

US EPA (1985) Technical support document for water quality based toxics control. US EPA, Washington DC.

US EPA (1987) Guidelines for deriving ambient aquatic life advisory concentrations. Office of Water Quality Regulations and Standards, Criteria and Standards Division, Washington DC.

WRc (1976) Emission standards in relation to water quality objectives. WRc Technical Report TR 17.

GLOSSARY

CENTRAL INFORMATION UNIT

A facility located centrally within NRA, ideally comprising:

(i) A data handling unit. This would handle all updates of the database, ensure coordinated dissemination to regions and provide computing support for users.

(ii) An information unit. This would provide assessed and interpreted data to users, particularly those with involvement in certain strategic policies (e.g. EQS derivation).

FIXED-FIELD DATABASE

A database using structured data records to organise information in "fields". Enquiries can be made about individual data items and their values, typically using indices related to one or more fields. Fields must be of a specific length, and of a specific data-type (e.g. text, integer). Validation rules may be specified to limit the permissible values of a field.

An advantage of fixed-field databases is that individual fields can be updated or modified in isolation.

Table 1:

	Field1	Field2	Field3
Record 1	Datum	Datum	Datum
Record 2	Datum	Datum	Datum
Record 3	Datum	Datum	Datum

Example:

LC50	Concentration	Organism	Data quality
1	10 mg/l	Fish	Good
2	1 mg/l	Insect	Moderate
3	5 mg/l	Mollusc	Poor

The sort of query best answered by a "fixed-field" database would be of the form: FIND ALL LC50's WITH

(a) CONCENTRATIONS BETWEEN 1 AND 10 mg/l which relate to

(b) INSECTS OR FISH and the data also are from

(c) GOOD QUALITY studies.

Specific fields are specified together with acceptable ranges of values. In the example above, only LC50 1 satisfies all criteria.

Databases that may be described (loosely) as "fixed-field" include relational databases (e.g. ORACLE) and many other PC-based packages (e.g. Dbase IV).

FREE-TEXT DATABASE

A database designed to facilitate retrieval of textual information. A free-format document is fed into the database, and specified sections of it are indexed, word-by-word (an "inverted-file" index) to produce a list of all the words and pointers to those sections of the documents they occur in. It may also be possible to index the word position within the document. Boolean logic (AND, OR and NOT operators) is used to specify which combination of terms should occur in the retrieved document set. Since the retrieval process consists of comparing sets of document numbers to find those document numbers that satisfy the conditions, the speed of retrieval does not depend on the amount of text in the database.

The sort of query best answered by a "free-text" database would be of the form: FIND ALL LC50's WHERE

(a) "FISH" occurs within 3 words of "INDIGENOUS" or

(b) "COASTAL" occurs in the same sentence as "SALTWATER" or "ESTUARINE" BUT ONLY IF

(c) the document doesn't contain "TROPICAL".

An example of free text satisfying this query is: The salmon, an **indigenous fish** species, of Scottish **coastal** and **estuarine** waters has been reported to have a 96 hour **LC50** value of 1 mg/l following exposure to dichlorvos (at 10°C, under **saltwater** conditions).

INFORMATION SYSTEM

A flexible package capable of providing toxicology and related information to satisfy the needs of all its users. In contrast to the information available on databases and databanks, it is designed to provide information to help solve operational problems. This is achieved not only by access to a wide number of data sources, but also through the involvement of relevant experts that channel interpreted information or advice to the users.

SUBSTANCE PROFILE

Presents basic toxicology and supporting data to allow rapid use or interpretation. It is intended to satisfy the requirement of staff involved in incident management and certain strategic policy areas (e.g. catchment management). It will also provide staff involved in consent setting with useful background information.

SHORT ADVISORY OR REPORT

Presents a critical assessment of substance toxicity, and also includes relevant supporting data. It is intended to satisfy the requirement of staff involved in setting consents and will also provide staff involved in certain strategic policies (e.g. R&D planning) with useful background information.

APPENDIX A

THE RESULTS OF THE QUESTIONNAIRE AND INTERVIEW SURVEYS

CONTENTS

A1. INTRODUCTION

The NRA's requirement for toxicity information was established by two surveys carried out in July and August 1991. NRA personnel involved in ecotoxicology were selected by a key contact in Head Office and each region, and were asked to participate in either the interview or questionnaire survey.

In total, 34 NRA personnel were interviewed and 20 (out of 32) personnel responded to the questionnaire survey. The interview survey was, by far, the most successful method of obtaining data and is strongly recommended for any further NRA R&D with a similar requirement for information.

The data obtained from both surveys was sufficient to propose a unified information system (Section 3.4) and also contains valuable information on the methods of storing of data, sources of information, extent of communication within NRA and maintenance of current awareness. Additionally possible problem areas (e.g. current awareness, training) and areas of improvement (e.g. national lists of consents/incidents) are highlighted by the data.

A2. THE PARTICIPANTS INVOLVED IN THE SURVEYS

A2.1 Length of time working in present position

The majority of participants had only been in their position for a short time (see Table A2.1).

A2.2 Toxicology Training

The majority of participants have had no toxicology training, only a few had attended external courses and fewer still had received any in-house training (see Table A2.2).

Table A2.1 Number of years in present position

	Survey	
Years in position	Interview (%)	Questionnaire (%)
<1	20	15
1 - 5	62	50
6 - 10	3	5
11 - 15	3	15
>15	12	15

Table A2.2 Extent of formal toxicology training received by participants

	Survey	
Toxicology Training	Interview (%)	Questionnaire (%)
External	*18	5
Internal and external	**3	0
None	79	95

NOTES * External courses include: BIBRA mammalian toxicology course; conferences and seminars; Ecotoxicology course at the Robens Institute; Workshops at WRc.

** Internal courses included Seminars and workshops within NRA; training dates back to pre-privatisation.

A2.3 Toxicology Experience

The majority of participants had obtained their knowledge on ecotoxicology from work experience. Few had any academic background relating to ecotoxicology (see Table A2.3).

Table A2.3 The toxicology experience of the participants

	Survey	
Toxicology Experience	Interview (%)	Questionnaire (%)**
Work experience	*76	NA
Academic training	15	NA
Both academic and work experience	9	NA

NOTES * Only 11.5% of participants had worked in ecotoxicology orientated positions
** Three participants had relevant work or academic toxicology experience
NA Not asked

A3. PRESENT USE OF TOXICOLOGY DATA

Incident management, consent setting (including planned discharges) and strategic policies appear to be the three main areas of toxicity information requirement within the NRA.

The majority of participants from the interview and questionnaire surveys (91% and 95% respectively) agreed with this broad division of information requirement. However, a few participants of the interview survey thought that additional categories, such as "widespread contamination", "legal requirements" and "herbicide/pesticide applications", should be included.

A3.1 Present areas of involvement of survey participants

The areas of involvement of the participants are shown in Table A3.1. The three areas of requirement (Section A3) are well represented between both surveys, with participants involved in incident management being particularly prominent.

Table A3.1 Present areas of involvement of participants

	Survey	
Areas of involvement	Interview (%)	Questionnaire (%)
Incident management (I)	29	10
Consent setting (C)	9	0
Strategic policies (SP)	9	5
I and C	15	20
I and SP	6	10
C and SP	9	10
I, C and SP	23	45

A3.2 Set procedure for obtaining and using toxicology data

In general it appears that there are few examples of a set procedure for using and obtaining data. Only 18% and 35% of participants of the interview and questionnaire survey respectively claimed they followed a set procedure. Participants of the interview survey were referring to pollution incidents and the procedure was for obtaining information only. Limited supporting information was provided in the returned questionnaires.

A3.3 Frequency of toxicology data requirement

There is a varied use of toxicology information. In general, however, there appears to be a low demand (see Table A3.2).

A3.4 Speed requirement for data

The speed of data required for each area of information need (Section A3) is variable, but appears to be short term for incident management (I) and certain strategic policies (SP), and medium to long term for discharge consent setting and certain strategic policies.

Table A3.2 Demand for toxicity information

		Survey
Frequency	Interview (%)	Questionnaire (%)
Every day	12	6
Once a week	17	0
Twice a week	9	12
Once a fortnight	12	6
Once a month	29	19
Less than once a month	12	51
Never	9	6

Table A3.3 Speed requirement for data

	Survey					
	Interview (%)			Questionnaire (%)		
Speed	I	C	SP	I	C	SP
Immediately	88 *(17)	0	0	59	0	8
<1 day	8 *(50)	0	0	24	14	0
2 - 6 days	4 *(25)	6	14	12	43	23
1 - 4 weeks	0 *(8)	88	57	5	29	46
5 - 8 weeks	0 *(0)	6	0	0	14	23
>8 weeks	0 *(0)	0	29	0	0	0

NOTES * For post pollution investigations

A3.5 Data Quality

In general, quality of data is perceived to be very important for all areas listed in Section A3, although certain participants felt that, for pollution incidents, the quality of data is not a major consideration when considered with the speed that it is needed.

Table A3.4 Importance of data quality for incident management (I), discharge consent setting (C) and strategic policies (SP)

	Survey					
	Interview (%)			Questionnaire (%)		
Importance	I	C	SP	I	C	SP
Very Important	32	88	100	69	43	54
Important	23	12	0	25	57	38
Not a major consideration	45	0	0	6	0	8

A3.6 Amount and detail of toxicology data required

Results from the interview survey indicate that in general limited information is required for pollution incidents and more detailed information is required for both consent setting and strategic policies. However, the participants of the questionnaire survey perceived that the amount and detail of information was important for all areas of requirement (Table A3.5).

Table A3.5 Amount and detail of toxicity information

	Survey					
	Interview (%)			Questionnaire (%)		
Importance	I	C	SP	I	C	SP
Very Important	10	53	85	44	29	46
Important	19	47	15	50	64	38
Not a major consideration	71	0	0	6	7	16

A3.7 Presentation of data

The majority of both surveys (100% interview, 95% questionnaire) agreed that presentation of data is important for each area of requirement. Three formats were proposed: Substance profile (A), short advisory or report (B) and detailed report (C). Participants felt presentation of data in substance profiles or short advisory/reports or a combination of formats would be most useful (Table A3.6).

Table A3.6 Presentation of data

	Survey					
	Interview (%)			Questionnaire (%)		
Format	I	C	SP	I	C	SP
Substance profile (A)	96	12	7	29	14	29
Short advisory/report (B)	0	29	14	41	33	21
Detailed report (C)	0	0	72	0	33	21
A and B	0	18	0	24	0	8
A and C	4	18	0	6	0	0
B and C	0	24	0	0	20	21
A, B and C	0	0	7	0	0	0

A3.8 Storage of toxicity data

The results of the interview and questionnaire surveys show that 72% and 85% respectively of participants store toxicity data. Methods of storage are identified in Table A3.7.

Table A3.7 Storage of toxicity data

Storage	Survey: Interview (%)	Survey: Questionnaire (%)**
Hardcopy filing	*92	74
Computer database	4	21
Microfiche	4	5

NOTES * 17% of these participants filed data by substance
** 50% indexed by substance and the remainder filed data under subject areas, e.g. incidents

A3.9 Dissemination of toxicology data

Participants of the interview survey (82%) report that they disseminate toxicity information within or between regions and the frequency of dissemination is low (see Table A3.8).

Approximately half (59%) disseminated it within their region only and 41% disseminated information both within and between regions. Participants of the questionnaire survey report that of data disseminated either within or between regions, 60% occurs within the region and 32% between regions. Only a few (13%) participants reported that this dissemination was based on a formal directory of expertise.

A3.10 Obtaining data

The results confirm that a wider number of personnel are involved in obtaining information than just the participants of the survey (see Table A3.9).

Table A3.8 Frequency of dissemination of toxicity data

	Survey			
	Interview (%)		Questionnaire (%)	
Frequency	Within region	Between regions	Within region	Between regions
Once a week	12	0	0	0
Once a month	42	10	25	0
Less than once a month	46	90	75	100

Table A3.9 Obtaining information

Obtaining information	Survey: Interview (%)	Questionnaire (%)
Participant only	29	NA
Participant and other staff	45	NA
Other staff only	26	NA

NOTES NA Not asked

A3.11 Use of external organisations to obtain data

Both surveys indicate that external organisations are used to obtain data (91% interview, 53% questionnaire). The number of organisations are extensive (see Table A3.10).

Table A3.10 Use of external organisations

Organisations consulted	Survey: Interview (%)	Questionnaire (%)
WRc	37	33
MAFF	15	0
Manufacturers' data	13	28
Harwell	6	11
IFE	6	0
University departments	6	0
Water Utilities	4	0
ICI (Brixham)	4	0
RSC	1	0
Consultants contracted for R&D	1	11
BIBRA	1	0
PML	1	0
Institute of weed control	1	0
CONCAWE	1	0
HMIP	1	0
Fire service	0	11
Acer Environmental	0	6

A3.12 Use of toxicology data by group or department

Participants of both surveys (88% interview, 80% questionnaire) reported that their department or group uses toxicology data. In addition Table A3.11 gives an indication of the numbers of personnel within that use toxicology information.

Table A3.11 Numbers of personnel that use toxicology information

Number of personnel	Survey Interview (%)	Questionnaire (%)
1	21	17
2 - 5	21	59
6 - 10	43	8
11 - 15	7	8
16 - 20	4	8
>20	4	0

A4. SPECIFIC REQUIREMENTS FOR TOXICOLOGY DATA

A4.1 Types of toxicology data used

Table A4.1 outlines the broad areas of toxicology data that are used for incident management (I), consent setting (C) and strategic policies (SP).

Data used for incident management is primarily acute LC50 data. EC50 data and "No observed effect concentrations" (NOECs) are also used, but to a smaller extent. Additionally lethal and sublethal chronic data are also used.

Data used for consent setting comprise both lethal and sublethal chronic data. A few participants reported that they particularly search for data from "early life stage" (ELS) tests. The use of acute data are primarily limited to LC50s. EC50 data and Microtox data are used by fewer participants.

Data used for strategic policies varies and are extensive. Both lethal and sublethal chronic data are used and acute LC50 data are frequently used. In addition, a number of participants from the interview survey felt that the data used were too extensive to list and preferred to describe it as that required to complete an aquatic toxicity assessment.

Additionally, a number of participants involved in all three areas of requirement reported that they use mammalian toxicology data. Most only use summaries of toxicity, but others use specific information, for example on acute toxicity or carcinogenicity.

Table A4.1 Types of toxicology data used for incident management (I), consent setting (C) and strategic policies (SP)

	Survey					
	Interview (%)			Questionnaire (%)		
Toxicity data used	I	C	SP	I	C	SP
Acute	77	40	29	42	32	31
Chronic	9	46	48	36	32	33
Standards and guidelines	7	10	10	9	15	16
Other (Body burdens; symptoms of poisoning)	7	4	14	13	21	20

A4.2 Use of additional types of data

A large proportion of participants (90%) use additional data to that reported in Section A4.1. Table A4.2 lists the types of data used.

A4.3 Type of data that participants would like to access

The majority of participants of both surveys (approximately 85%) would like access to more data than they have access to at the moment. The data obtained during the surveys is outlined in Table A4.3.

Table A4.2 Use of additional types of data

	Survey	
Type of data	Interview (%)	Questionnaire (%)
Guidelines and standards	*20	0
Fate and behaviour	19	24
Health and safety	13	19
Identification	12	23
Physical	12	3
Chemical	12	-
Regulations on handling and use	2	0
Safe water drinking levels	2	3
Biological monitoring data	1	3
Other (e.g. Toxicity to sewage treatment; incident reports; occurrence and use; fish tainting levels; manufacturers' data; analysis)	8	25

NOTES * Not necessarily derived from toxicity data

A4.4 Interpretation of data

Participants of both surveys (76% interview, 89% questionnaire) reported that they interpret their own data. A large percentage found it to be a problem (82% questionnaire), in particular with regard to the amount of time it took (58% interview, 81% questionnaire). In addition, participants indicated that it was also due to a lack of understanding of how to apply toxicology data (56% questionnaire). To overcome the problems of interpretation, participants (89%) reported that they use internal or external contacts for guidance (see Table A4.4).

Table A4.3 Type of data that participants would like access to

Type of data	Survey: Interview (%)	Survey: Questionnaire (%)
Wider range of toxicity data	29	0
Field data (i.e. biological monitoring)	18	46
Incident reports	17	27
Field studies	10	0
Fate and behaviour data	5	3
National list of consents	4	18
Water quality data and legislation	4	0
Identification	6	0
Health and safety	2	3
Areas of expertise/contacts in NRA	2	0
Other (Fish tainting data; manufacturers'/industrial telephone numbers; trade name database)	4	3

Table A4.4 Interpretation of data

Contacts	Survey: Interview (%)	Survey: Questionnaire (%)
Internal	30	NA
External	13	NA
External and internal	57	NA

NOTES NA Not Asked

A4.5 Definition of an LC50

Approximately half the participants of both surveys (56% interview, 55% questionnaire) had a correct understanding of an LC50 and a small number had a poor understanding (9% interview, 5% questionnaire). The remainder or participants had an adequate understanding.

The majority of participants understood that the application of an LC50 to an environmental problem was not straight forward, but 42% (questionnaire survey) were unsure how to or would apply it with reservations. The remainder of participants indicated that they would use an LC50 as a guideline of toxicity only.

A4.6 Problems with toxicology data

The major problem with the toxicology data available appeared to be with interpretation and sources of information (see Table A4.5).

Table A4.5 Problems with toxicology data

Problem	Interview survey (%)
Quality assessment/interpretation	60
More toxicity data needed	*34
No priority list of substances available with data	4
Limited fate and behaviour data available	2

NOTES * This can also be atrributed to interpretation to an extent

A5. SOURCES OF INFORMATION USED BY THE NRA

A5.1 Sources of information

The sources of information used by the NRA to obtain toxicology information are listed in Table A5.1. Additionally, participants of both surveys (75% interview, 35% questionnaire) reported that they obtain information from contacts in other NRA regions and a smaller percentage (56% interview, 15% questionnaire) report that NRA personnel contact them for information.

Table A5.1 Sources of information used by NRA for toxicology data

	Survey	
Sources	Interview (%)	Questionnaire (%)
Printed text	30	28
External organisations	28	28
Internal contacts	23	36
Computer database - PC	9	*8
Computer database - on-line	7	-
Hardcopy database	3	0

NOTES * all types of computer databases

A5.2 Current awareness

Participants report (62% interview, 42% questionnaire) that current awareness on toxicology is maintained in their group or department. The methods of current awareness are listed in

Table A5.2. However, participants felt that such awareness requires improvement (82% interview, 56% questionnaire).

Table A5.2 Current awareness of toxicology

	Survey	
Types of current awareness	Interview (%)	Questionnaire (%)
Abstracts	33	25
Journals/reports	30	25
Verbal communication	*15	5
Current contents	13	25
Bulletins	4	20
Press cuttings	2	0
Manufacturers' data	2	0
Seminars	2	0

NOTES * Including external/internal contacts

A5.3 Use of on-line databases

A small percentage of participants reported that they use on-line databases (12% interview, 22% questionnaire). In general 2 - 3 databases were used and accessed approximately 1 - 5 times a month. The participants of the interview survey felt that there were problems using these databases and that they were not useful (e.g. do not contain relevant information, cannot judge quality or interpret data easily, not cost effective, not comprehensive). In addition, few participants had received training for on-line searching and none had it maintained. Participants of the questionnaire survey reported, however, that such databases are useful, that the data are easy to interpret and that one participant had received training for searching and had this maintained.

A5.4 Concept of computerised database or an information unit

Participants of both surveys (94% interview, 83% questionnaire) reported that they would like access to an information unit. A similar high number of participants reported that they would like access to a computerised database (94% interview, 68% questionnaire).

A5.5 Present Information sources satisfactory?

In general it appears that participants (70% interview, 65% questionnaire) are not satisfied with their information sources. Perceive improvements include accessibility, interpretation and reduce sources that need to be consulted, but increase relevance.

A6. FUTURE INFORMATION REQUIREMENTS

The majority of participants felt that their requirement for information will increase in the future with the introduction of new legislation or changes in NRA policy (83% interview, 70% questionnaire).

APPENDIX B

AN EXAMPLE OF THE QUESTIONS ASKED DURING THE INTERVIEW SURVEY

NRA ECOTOXICOLOGICAL DATABASE SPECIFICATION STUDY (A12/91/1):

PRO FORMA FOR INTERVIEWS

DATE:

REGION:

SECTION 1: ABOUT THE INTERVIEWEE

1.1 Name: ....

1.2 Job title: ....

1.3 Position in the NRA from Regional General Manager: ....

1.4 Description of responsibilities: ....

1.5 Length of time working at this job: ....

1.6 Toxicology training (external or internal): ....

SECTION 2: PRESENT USE OF TOXICITY DATA

2.1 GENERAL REQUIREMENTS

2.1.1 Incident management, consent setting (planned discharges) and strategic policies appear broadly to be the three main areas of information requirement within the NRA. Do you agree with this? **YES/NO**. What operational or strategic areas are you involved with?

....

2.1.2 Is there a set procedure for obtaining and using toxicity information? **YES/NO** If yes, could you outline the action plan?

....

2.1.3 How frequently do you require toxicity data?

....

2.1.4 How quickly do you need this data? (for each different type of task)

....

2.1.5 How important is data quality for each operational task that you are involved with?

....

2.1.6 How important is the amount and detail of toxicity data for each operational task that you are involved with?

....

2.1.7 Is presentation of data important to you? (show examples)

....

2.1.8 Is the toxicity data that you use stored for future reference? **YES/NO** If yes how? (filed, database, etc.)

....

2.1.9 Is this data disseminated within/between regions? **YES/NO** If yes, how often? (daily, weekly, monthly)

....

2.1.10 Do you obtain data for yourself or are separate NRA personnel responsible for this?

....

2.1.11 Do external organisations ever provide you with toxicity data? **YES/NO**. If yes who are they?

....

2.1.12 Do any other members of your group use toxicity information? **YES/NO**. If yes, how many use it?

....

2.2 SPECIFIC REQUIREMENTS FOR TOXICITY DATA

2.2.1 What are the different sorts of toxicity data that you use to solve each type of task that you are responsible for? (Acute: LC50, EC50; Chronic, sublethal; Species)

....

2.2.2 Are there any other sorts of data that you use? (Identification, fate and behaviour, physical, chemical, etc., health and safety, regulations on handling and use, guidelines, etc.)

....

2.2.3 What types of data would you like to have access to in order to improve or satisfy your requirement for data? (i.e. incident reports, field data)

....

2.2.4 Do you interpret the data yourself? **YES/NO**. If yes, do you find that there is little time in which to complete this task? Do you use internal or external contacts for guidance?

....

2.2.5 What do you understand by an LC50? How would you translate it to the environment?

....

2.2.6 Do you feel that there are any problems with the data that you use? (Not evaluated, interpreted, etc.)

....

2.2.7 Could you give an example of how toxicity data has been used in your management of everyday tasks?

....

SECTION 3: SOURCES OF INFORMATION USED BY NRA

3.1 What sources of information do you use to obtain toxicity data? (internal; external; computer; text, etc.)

....

3.2 Do you communicate with equivalent staff in other regions to obtain data or to establish how a similar situation has been handled? Or do they come to you?

....

3.3 Is current awareness for ecotoxicology maintained by your department? If so, how?

....

3.4 Do you feel that there is a need for current awareness to be improved? **YES/NO** If yes, how?

....

3.5 Do you use on-line databases?

....

3.6 How many different databases are used?

....

3.7 How many times do you access these databases a month?

....

3.8 Do you find them useful? **YES/NO**. If no, explain why?

....

3.9 Is the data easy to interpret? **YES/NO**

....

3.10 Have you received training for on-line searching? **YES/NO** Is it maintained?

....

3.11 Would you prefer this "information gathering" to be carried out by an information unit?

....

3.12 Would you find a computerised pollution database on chemical substances useful in your day to day management of operational tasks? **YES/NO** If not, why not?

....

3.13 Do your information sources satisfy your information needs? How could they be improved?

....

SECTION 4: FUTURE REQUIREMENTS

4.1 Will legislation, such as the groundwater directive, or changes in NRA policy, such as the approach to consent setting, affect your information requirements? How will they change?

APPENDIX C

AN EXAMPLE OF THE QUESTIONNAIRE USED FOR THE QUESTIONNAIRE SURVEY

NRA ECOTOXICOLOGICAL DATABASE SPECIFICATION STUDY (A12/91/1): QUESTIONNAIRE

SECTION 1: ABOUT YOURSELF

1.1 Name: ....

1.2 Region: ....

1.3 Job title: ....

1.4 What is your position relative to Regional General Manager? ....

1.5 Can you broadly describe your responsibilities? ....

....

1.6 How long have you been doing this job? ....

1.7 Have you received any formal toxicology training (internal or external)? **YES/NO**

1.7.1 If yes, please give details: ....

....

SECTION 2: GENERAL REQUIREMENTS FOR TOXICITY DATA

2.1 Incident management, consent setting (including planned discharges) and strategic policies (including R&D, policy, planning, catchment management, monitoring, EQS derivation, etc.) appear broadly to be the three main areas of requirement for toxicity information within the NRA. Do you agree with this? **YES/NO**

2.1.1 If no, please list additional categories:

....

2.1.2 Which of these areas are you involved with?

....

2.2 Is there a set procedure for obtaining and using toxicity information for each of the areas in 2.1.2? **YES/NO**

2.2.1 If yes, could you outline the action plan?

....

2.3 How frequently do you require toxicity data?

1/DAY	**1/WEEK**	**2/WEEK**
FORTNIGHTLY	**1/MONTH**	**<1/MONTH**
NEVER		

2.4 How quickly do you need toxicity data? (Please indicate for each different task listed in 2.1.2)

Incident Management

IMMEDIATELY	**<24 HOURS**	**2 - 7 DAYS**
1 - 4 WEEKS	**5 - 8 WEEKS**	**>8 WEEKS**

Consent Setting

IMMEDIATELY	**<24 HOURS**	**2 - 7 DAYS**
1 - 4 WEEKS	**5 - 8 WEEKS**	**>8 WEEKS**

Strategic Policies

IMMEDIATELY	**<24 HOURS**	**2 - 7 DAYS**
1 - 4 WEEKS	**5 - 8 WEEKS**	**>8 WEEKS**

2.5 How important is interpreted and assessed data for each operational task indicated in 2.1.2?

Incident management

VERY IMPORTANT   IMPORTANT   NOT A MAJOR CONSIDERATION

Consent Setting

VERY IMPORTANT   IMPORTANT   NOT A MAJOR CONSIDERATION

Strategic Policies

VERY IMPORTANT   IMPORTANT   NOT A MAJOR CONSIDERATION

2.6 How important is the amount and detail of toxicity data for each operational task listed in 2.1.2?

Incident management

VERY IMPORTANT   IMPORTANT   NOT A MAJOR CONSIDERATION

Consent Setting

VERY IMPORTANT   IMPORTANT   NOT A MAJOR CONSIDERATION

Strategic Policies

VERY IMPORTANT IMPORTANT NOT A MAJOR CONSIDERATION

2.7 Is presentation of data important to you? **YES/NO**

2.7.1 Which of the formats listed below are of most use when dealing with each of your operational tasks indicated in 2.1.2?

A. SUBSTANCE PROFILE

B. SHORT ADVISORY/REPORT

C. DETAILED REPORT

Pollution Incident: ....

Consent Setting: ....

Strategic Policies: ....

2.8 Is the toxicity data that you use stored for future reference? **YES/NO**

2.8.1 If yes, how is it stored?

COMPUTERISED DATABASE HARDCOPY FILING MICROFICHE OTHER (please specify)

....

2.8.2 Is the stored data indexed by substance? **YES/NO**

2.8.3 If no, how is it stored?

....

2.9 Is toxicity data ever disseminated to NRA personnel within your region? **YES/NO**

2.9.1 If yes, how often?

DAILY WEEKLY MONTHLY LESS THAN ONCE A MONTH

2.10 Is toxicity data ever disseminated to NRA personnel at different NRA regions? **YES/NO**

2.10.1 If yes, how often?

DAILY WEEKLY MONTHLY LESS THAN ONCE A MONTH

2.11 Is the dissemination of data based on a formal directory of interests/expertise? **YES/NO**

2.12 Do external organisations ever provide you with toxicity data? **YES/NO**

2.12.1 If yes, which organisations do you use?

. . . .

2.13 Do any other members of your group obtain or use toxicity information? **YES/NO**

2.13.1 If yes, how many use it?

. . . .

SECTION 3: SPECIFIC REQUIREMENTS FOR TOXICITY DATA

3.1 Which of the different sorts of toxicity data listed below do you use for each operational task listed in 2.1.2?

Incident Management:

Acute: **LC50** **EC50**

Chronic: **LETHAL** **SUBLETHAL**

Species: **FISH** **INVERTEBRATES** **PLANTS**
COMMERCIAL (SHELL) FISHERIES

Standards: **EQS**

Others (i.e. bioaccumulation, body burdens, etc.):

. . . .

Consent Setting

Acute: **LC50** **EC50**

Chronic: **LETHAL** **SUBLETHAL**

Species: **FISH** **INVERTEBRATES** **PLANTS**
COMMERCIAL (SHELL) FISHERIES

Standards: **EQS**

Others (i.e. bioaccumulation, body burdens, etc.):

. . . .

Strategic Policies:

Acute: **LC50** **EC50**

Chronic: **LETHAL** **SUBLETHAL**

Species: **FISH** **INVERTEBRATES** **PLANTS**
COMMERCIAL (SHELL) FISHERIES

Standards: **EQS**

Others (i.e. bioaccumulation, body burdens, etc.):

....

3.2 Which of the data listed below do you use in addition to that in 3.1?

IDENTIFICATION **FATE AND BEHAVIOUR** **HEALTH AND SAFETY**
BIOLOGICAL MONITORING **OCCURRENCE/USE**
OTHER (Please specify):

....

3.3 What types of data would you like to have access to in order to improve or satisfy your requirement for data?

INCIDENT REPORTS (NATIONAL) **CONSENTS (NATIONAL)**
BIOLOGICAL MONITORING DATA **OTHERS (please specify):**

....

3.4 Do you interpret the data yourself? **YES/NO**

3.4.1 Do you find that you have problems interpreting or evaluating toxicity data? **YES/NO**

3.4.2 Is time a problem for this task? **YES/NO**

3.4.3 Are there any other problems with the interpretation of data? **YES/NO**

3.4.3.1 If yes, what are they?

....

3.4.4 Do you use internal or external contacts for guidance? **YES/NO**

3.5 What do you understand by an LC50?

....

3.5.1 How would you apply it to a real situation?

....

SECTION 4: SOURCES OF INFORMATION USED BY NRA

4.1 What sources of information do you use to obtain toxicity data?

INTERNAL **EXTERNAL** **COMPUTER** **TEXT**

4.2 Do you communicate with equivalent staff in other regions to obtain data or to establish how a similar situation has been handled? **YES/NO**

4.2.1 Do they come to you? **YES/NO**

4.3 Is current awareness of ecotoxicology maintained by your department? **YES/NO**

4.3.1 If so, how?

JOURNALS **BULLETINS** **ABSTRACTS** **CURRENT CONTENTS** **OTHERS** (please specify):

4.4 Are there any problems with your present method of maintaining current awareness? **YES/NO**

4.4.1 If yes, what are they?

....

4.5 Do you use on-line databases? **YES/NO**

4.6 How many different databases do you use?

1 **2 - 3** **4 - 5** **6 - 7** **8 - 9** **>10**

4.7 How many times do you access these databases a month?

<1 **1 - 5** **6 - 10** **11 - 15** **16 - 20** **>20**

4.8 Do you find on-line databases useful? **YES/NO**

4.8.1 If no, can you explain why?

....

4.9 Is the data from on-line databases easy to interpret? **YES/NO**

4.10 Have you received training for on-line searching? **YES/NO**

4.10.1 Is training maintained regularly? **YES/NO**

4.11 Would you prefer your "information gathering" requirement to be carried out by an information unit? **YES/NO**

4.12 Would you find a computerised pollution database on chemical substances useful in your day to day management of operational tasks? **YES/NO**

4.12.1 If no, please specify why not?

4.13 Do your information sources satisfy your information needs? **YES/NO**

4.13.1 How could they be improved?

SECTION 5: FUTURE REQUIREMENTS

5.1 Will legislation, such as the groundwater directive, or changes in NRA policy, such as the approach to consent setting, affect your information requirements? **YES/NO**

5.1.1 How will they change?

....

APPENDIX D

MERITS OF EXISTING DATABASES AND DATABANKS AND THEIR ROLE IN PROVIDING TOXICITY INFORMATION, AND THE ADVANTAGES AND DISADVANTAGES OF DEVELOPING AN INTERNAL SYSTEM COMPARED WITH AN EXTERNAL SYSTEM

CONTENTS

D1. INTRODUCTION

Databases and databanks, on which individuals and organisations could search for information, have been available for approximately 30 years. These computers can be located anywhere in the world and data, in most cases, can be accessed using remote terminals and telephone lines, for an appropriate fee and searching charge. Other types of databases or databanks are located within organisations and are used as part of an information service. A list of on-line databases and databanks and those available via information services are listed in Appendix A - D of NRA Report 254/1/A (Baker *et al* 1991).

D2. MERITS OF EXISTING DATABASES AND DATABANKS

D2.1 Frequency of information updates

The existing types of databases and databanks listed in Appendix A - D of NRA Report 254/1/A (Baker *et al* 1991) are all centralised sources of environmental information that are frequently updated.

The frequency of information updates appear to be related to the function of the database or databank, the amount of relevant information published and the number of publication sources scanned by the database/bank producer. Consequently databases or databanks providing information on a wide subject area are updated more frequently than those providing information on a limited number of subjects.

In general databases appear to be updated more frequently than databanks. CHEMICAL ABSTRACTS, AQUALINE, BIOSIS and POLLUTION ABSTRACTS are all updated 24 times per year. Smaller databases such as ASFA or databanks such as INSTAB are updated less frequently (12 times per year) and specific databanks such as DATALOG are only updated twice a year (Baker *et al* 1991).

D2.2 Access to, availability of and retrieval of information

With the appropriate facilities, access to databases and databanks is straightforward.

On-line computer data sources are accessed by using terminals and telephone lines; PC, mainframe or CD-ROM databases are accessed by using appropriate computing hardware/software; and databases or databanks maintained within certain organisations (e.g. WRc, IFE) can only be accessed via that organisation.

Access to databases and databanks 24 hours a day is likely only to be guaranteed by PC and CD-ROM databanks or databases. On-line computer retrieval systems and, to a lesser extent, databases located within organisations are not necessarily accessible at all times. Maintenance of on-line databases, during which information is not available, can be carried out at any time (usually on a Sunday) and can pose problems to users if the host is located in a different time zone to the UK.

There appear to be few organisations in the UK that supply toxicity data (e.g. BIBRA, Poisons Unit, WRc) as part of an external service. Fewer still appear to provide this:

(i) as a 24 hour service; and

(ii) for environmental toxicity data.

Despite the need for occasional maintenance, such services should still be in a position to answer urgent requests for information.

Retrieval of information from information services is straightforward and is usually by telephone, fax or letter. Effective retrieval of information from on-line databases and databanks, however, can only be achieved through training, which must be regularly maintained. Retrieval of information from PC or CD-ROM databases is largely straightforward, although a basic knowledge of database/bank searching techniques is advisable.

D2.3 Cost

Retrieval of information from on-line databases and databanks can be expensive. The cost includes an annual subscription fee and appropriate searching charges. These charges are published by database or databank hosts and are usually in the form of a connect fee, and in some cases, an additional fee for printing each record whilst on-line.

Searching for data on on-line computer retrieval systems can be a lengthy process and there are features (e.g. repetition, speed of data retrieval) about certain databases which increase the time and therefore, cost of searching. Costs can be reduced by using certain database hosts (e.g. DIALOG, STN) that operate time saving search strategies or by restricting searching of database/banks located abroad (e.g. America) to a specific time of day (e.g. the morning for UK users), when there are likely to be few users retrieving data and searching is therefore quicker.

There is no connect charge for retrieval of information from PC, mainframe or CD-ROM databases. However, updates must be purchased regularly to maintain a complete database.

Organisations that offer commercial toxicity information services principally supply data on a subscription basis (e.g. WRc). Additionally a number of organisations provide toxicity information but do not offer a commercial service. In such cases information is provided on an ad hoc basis (Baker *et al* 1991).

D3. THE ROLE OF DATABASES AND DATABANKS IN PROVIDING TOXICITY INFORMATION

Toxicity information retrieved from existing databases and databanks is not intended to answer operational problems and considerable interpretation is required before this can be achieved. This is due, in part, to the function of the database/bank before it became commercially available. The majority of environmental databases/banks are not intended primarily to provide toxicity data, which may constitute only a small portion of the database/bank.

D3.1 Subject coverage

In general databases available nowadays cover a wide subject area of which toxicology forms a very small part. CHEMICAL ABSTRACTS contains 8 million records which cover the broad area of chemistry and chemical information. The presence of a particular substance on this database will not necessarily imply that there are toxicological data present and consequently time can be wasted when searching.

Water related databases are available which are more specific to NRA's information requirement, but these are small in comparison to the large databases (e.g. CHEMICAL ABSTRACTS). Despite the specificity of these databases (e.g. AQUALINE), ecotoxicology still forms only a small part.

Databanks appear to be a relevant source of information for toxicology. A few provide information on a number of environmental subjects (e.g. INSTAB, ECDIN) and there are databanks which are subject specific (e.g. AQUIRE provides data on aquatic toxicity).

Databases and databank producers use a selection of sources to extract relevant published documents for inclusion. Consequently it is unlikely that any computer data source will be completely comprehensive and, since each producer uses a slightly different selection of sources, a number of databases may need to be searched to obtain a fully comprehensive picture of the toxicity information available for a substance.

D3.2 Quality of information

Existing databases provide information on the bibliographic details of a published document and, in the majority of cases, also an abstract. Databanks similarly provide information on bibliographic details and an abstract, although some databanks provide information in substance profiles (e.g. CHRIS).

A database abstract of a published document differs significantly from a databank abstract in its presentation of information. Database abstracts provide a summary of the published document and the information presented within it is not controlled, i.e. relevant information may or may not be present. In contrast information within databank abstracts is controlled and data are presented in a standard format (Baker *et al* 1991).

The quality of data contained within published documents is assessed by a limited number of databanks (e.g. AQUIRE). No comparable data quality assessment is carried out on databases. Data assessment of published documents is important in databases and databanks, since the user has some confidence of the data presented and can make decisions upon it, without the need to obtain a full copy of the study.

D4. BENEFITS AND DISADVANTAGES OF DEVELOPING AN INTERNAL SYSTEM COMPARED WITH AN EXTERNAL SYSTEM

D4.1 Central source of information

A newly established in-house system is unlikely to act as a central source of information. Such a system would initially suffer from low compound coverage and its users could frequently find that information on certain substances is not available. Consequently additional external sources of information would be needed to satisfy user's requirements. However, in time the system will overcome these problems and develop into a valuable central source of information.

In contrast an appropriate external service would have access to established in-house databases and databanks, and to a number of external data sources. It could therefore, act immediately as a central source of toxicity information to NRA personnel.

D4.2 Ownership

Establishing an in-house system would allow NRA to become more independent in its requirement for toxicity information and also allow it to alter the information content according to any change in its toxicity requirement. However, an external service, although not owned by NRA, could also provide information according to the NRA's changing requirement.

D4.3 Access and availability

Access to either an in-house or external service is likely to be uncomplicated. The database proposed for NRA is intended to be available 24 hours a day, with "down time" for maintenance kept to a minimum.

External services are able to provide toxicity data during working hours, with only a very few offering a 24 hour service. The databases used by such organisations, like all databases and databanks, require maintenance. In the case of WRc maintenance is infrequent, but does occur and during these short periods information can still be provided from backup sources. The performance of other services, however, is unknown.

D4.4 Updates

The proposed in-house database would be updated regularly (e.g. 2 to 4 times a year), but less frequently than some commercial databases (e.g. AQUALINE, CHEMICAL ABSTRACTS), since the amount of new ecotoxicological data published is unlikely to justify the cost of frequently producing and supplying new updates. An external service, as a consequence of using frequently updated databases is likely to have more up to date information available than the NRA in-house database. Consequently it would be beneficial for the NRA to establish links with additional data sources.

D4.5 Information

Speed of information retrieval

An in-house computerised system would provide information immediately to personnel with a short term requirement for data (e.g. those involved with pollution incidents, consent setting, monitoring, catchment management). An external service could also provide basic data immediately (e.g. for a pollution incident), but an impact assessment required to establish a discharge consent would require longer to compile.

Substance coverage

An in-house system when first established is likely to have a poor substance coverage compared an established external service, but this would improve with time.

Relevance of information

The proposed NRA in-house system is intended to contain information specifically required by NRA personnel. All external services gather data on a range of subject areas. Only those services able to tailor their toxicology information to the requirements of NRA staff should be selected.

Awareness of ecotoxicology

The widespread knowledge of the existence of an in-house system and ease of retrieving toxicity data from it are likely to increase awareness on the application of ecotoxicology throughout the NRA. Although access to an external system would be similarly straightforward, users might be discouraged from contacting an external service with "general interest" enquiries.

Presentation

Presentation of the correct amount and detail of toxicity data is important to users of an in-house system or external service, since it allows problems to be resolved without the need for further interpretation. Both the in-house system and external system could present data to users according to their needs, but an external service, at the same time, could offer advice concerning the type of information of most use to help resolve each user's enquiry.

Quality of data

Both an in-house system and an external service would contain assessed and interpreted data. In both cases users could have confidence in the data they were using to resolve problems.

D4.6 Cost

The cost of establishing and maintaining an in-house system, in comparison to using an external system, will be high. It is important to consider whether its use can justify its cost.

D5. CONCLUSION

The merits of databases and databanks are numerous. These computer retrieval systems provide a central source of information that is frequently updated. These systems vary in size and cover a range of subjects relevant to NRA's information requirement. However, their availability is not always guaranteed, neither is their quality or usefulness of information, and searching can be costly.

The advantages and disadvantages of establishing an in-house system as opposed to an external system have been presented in Section 4.2.3. An in-house system would allow the

NRA to become more independent in its requirement for information and is also likely to increase general awareness and application of ecotoxicology throughout the NRA. However, both an in-house and an external system would have several important points in common (e.g. ease of access and data retrieval, available 24 hours a day, provide relevant up to date assessed information) and there are comparatively few features of an in-house system (e.g. speed of retrieval) that would give it a clear advantage over an external system. Consequently the advantages of establishing an in-house system, its level of use and the considerable cost implications require careful consideration before implementation.

APPENDIX E

DERIVATION OF ENVIRONMENTAL QUALITY STANDARDS

CONTENTS

E1. INTRODUCTION

An Environmental Quality Objective (EQO) can be defined as the requirement that a body of water should be suitable for a use identified by the competent authority. An Environmental Quality Standard (EQS) is that concentration of a substance which should not be exceeded if the objective is to be met, i.e. if the identified water use is not to be compromised. A variety of "uses" to which EQSs can be applied have been identified for fresh and saline surface waters in the UK, Table A2.1.

Table E1.1 Identified water uses in the UK (Gardiner and Mance 1984)

Water Use	Freshwater	Saltwater
Abstraction to potable supply - direct	Y	N
Abstraction to potable supply - with impoundment	Y	N
Protection of aquatic food for human consumption	Y	Y
Protection of aquatic life	Y	Y
Irrigation of crops	Y	N
Livestock watering	Y	N
Industrial abstraction	Y	Y
Recreational use (water contact activities)	Y	Y
Aesthetic acceptability	Y	Y

The philosophy behind the EQO/EQS approach in the UK, and its advantages and disadvantages, have been discussed elsewhere (WRc 1976, Otter 1979, Price and Pearson 1979, Agg and Zabel 1989, Crane *et al* 1991) and will not be reconsidered here. Essentially EQSs are useful tools in the control of water pollution because they protect against all sources of contamination (point and diffuse) and because they can be tailored to specific water uses.

A number of EQSs have been established by the European Commission (EC) following provisions laid down in the Dangerous Substances Directive (CEC 1976a). The aim is to ensure that priority (List I) contaminants do not reach a level in surface waters at which they will be detrimental to aquatic communities in both the short- and long-term. In the UK additional EQSs have been established by WRc (on behalf of the Department of the Environment) for a number of metals, pesticides and organic chemicals which are not included on List I. EC and UK EQSs are regulatory tools derived to ensure protection of the aquatic environment, and ultimately are given legislative status. They can be used specifically to assist with:

(i) the establishment of effluent discharge consents;

(ii) control of, and prosecution following, pollution incidents; and

(iii) control of uses leading to diffuse inputs of surface water contaminants.

Most EQSs are designed to protect aquatic communities. However, for certain chemicals other water "uses" may be particularly important. For example, the NRA have attempted to establish EQSs for nitrogen- and phosphorus-based nutrients to prevent eutrophication of surface waters (Cartwright and Painter 1991). EQSs for such "other" uses are considered only briefly here, in Sections E1.1 to E1.2, whilst Section E2 discusses the derivation of EQSs for the protection of aquatic life.

E1.1 Abstraction to potable supply

A number of standards for drinking water and water abstracted from potable sources have been laid down in the EC Directives on Drinking Water (CEC 1980) and Surface Water Abstraction (CEC 1975), and the UK is obliged to comply with these. When considering a substance which is not covered by these Directives the approach used in the UK is to review the literature on mammalian and human toxicology, and consider this in parallel with any relevant guideline values developed by competent authorities such as WHO. These guidelines, where they exist, may then be adopted as EQSs or may be made more stringent to allow for special circumstances applying to the UK situation. In the absence of such guidelines, it is unlikely that any EQSs will be established, although a SNARL (suggested no adverse response level) may be proposed. In addition to a consideration of human health the concentration of a chemical that leads to tainting, odour or other aesthetic problems needs to be considered.

E1.2 Protection of aquatic food for human consumption

Edible shellfish and fish should be adequately protected by EQSs derived for the protection of aquatic life (see Section E2). However, there may be situations where chemical contaminants are accumulated by edible aquatic organisms without causing them harm, but these may lower the quality of the product (e.g. by tainting or by compromising the health of human consumers). In such cases it is necessary to consider bioaccumulation potential and toxicity to humans, with particular emphasis on vulnerable groups (e.g. infants) and dietary composition. It is unlikely that an EQS will be derived for this use in the absence of supporting guidelines from a competent authority, such as WHO, but where statutory limits already exist (e.g. the UK's Lead in Food Regulations 1979, and relevant EC Directives, CEC 1978, 1979), these may be adopted as EQSs.

E1.3 Irrigation of crops

EQSs for the protection of aquatic life are based on the chemical's toxicity to all types of aquatic organisms, including plants. Thus waters complying with such EQSs should not prove detrimental to plant health if used for irrigation purposes. However, consideration must also be made of the risk of contamination of groundwaters (which may be abstracted for potable supply), accumulation in soils, other sources of the chemical, and the potential for transmission of the chemical into plant products destined for human consumption. MAFF have provided guidance for a variety of chemicals (MAFF/ADAS 1980), but no EQSs have been established.

E1.4 Livestock watering

It is assumed that water of sufficient quality for potable supply should also be suitable for livestock watering. As with the protection of aquatic life for human consumption (Section E1.2), bioaccumulation potential and organoleptic tainting thresholds need to be considered. Information and guidance related to EQSs for livestock watering have been sought from the MAFF/ADAS Central Veterinary Laboratory, but in most cases it has not been possible to establish EQSs.

E1.5 Industrial abstraction

The wide variety of water quality required by different industrial sectors means that no general EQSs can be applied for industrial water use. Where process water comes into contact with food or drink it is recommended that it meets the EQSs derived for potable waters. Certain other uses may also require water of particularly high quality; for example a low level of organic contaminants is desirable in water used by the micro-electronics industry. However, on the whole EQSs are not established for waters abstracted for industrial.

E1.6 Recreational use (water contact activities)

Some guideline and mandatory values for bathing and immersion sports are provided in the EC Bathing Water Directive (CEC 1976b). Where no guidelines exist consideration is given to the potential risks to human health associated with swallowing contaminated water or with topical contact. Consequently, it is usual for any EQSs for recreational use to be based on the corresponding EQSs for potable water.

E1.7 Aesthetic acceptability

Aesthetic appreciation is generally a relatively insensitive water use when considering chemical contamination, and EQSs for the protection of freshwater life (and those proposed for potable supply or recreational uses, where applicable) will normally be sufficiently stringent to protect this use also. Only those chemicals that result in oily films, discoloration or odour problems need separate consideration, and as yet no EQSs have been established on an aesthetic basis.

E2. DERIVATION OF EQSs FOR THE PROTECTION OF AQUATIC LIFE

As discussed in Section E1, EQSs for the protection of aquatic life are established as national or international guideline values to be given regulatory force. Thus it is essential that they are established with sufficient confidence to ensure that they are not too stringent or too lax, which could have adverse consequences for either dischargers or aquatic ecosystems. This need for confidence necessitates a large database of chemical and ecotoxicological information, which can be used to determine a chemical's environmental fate and toxicity, and thus assess the risks. In many cases the database for a particular chemical is inadequate to enable EQSs to be objectively derived, and no standards can be proposed without further testing being undertaken.

As shown in Figure E1, there are a number of important stages in the derivation of EQSs for the protection of aquatic life, which may be summarised as follows (Crossland 1986, Agg and Zabel 1989):

(i) Sources and Contamination (Identify the potential sources and likelihood of the chemical entering watercourses);

(ii) Determine the fate of the chemical in the aquatic environment;

(iii) Determine Lowest/No Effects Concentration (Identify the lowest credible adverse effect concentration, or highest no effect concentration, for the most sensitive aquatic organisms);

(iv) Extrapolation (Establish a preliminary standard that should not adversely affect biota, by extrapolation from the concentration derived in (iii));

(v) Validation (Validate the preliminary standard by comparison with field monitoring data);

(vi) Conduct further investigations if there are any discrepancies, and repeat process (i) to (v) as necessary.

These operations and the data requirements for each are outlined in Sections E2.1 to E2.5.

E2.1 <u>Sources and contamination</u>

Production, use and occurrence data

A knowledge of a chemical's major uses can be used in conjunction with its physico-chemical characteristics and environmental fate data (see below) to determine the main routes by which it will enter water. For example, an industrial intermediate is more likely to arise primarily from point sources, whereas a herbicide will arise mostly from diffuse sources.

Estimates of the amounts of a chemical produced, transported and used in the UK enable the scale of potential contamination of surface waters to be more fully assessed. Consideration of the effectiveness of industrial effluent treatment and sewage treatment will assist with this quantification.

Reported concentrations in wastewaters, groundwaters, surface waters (fresh, estuarine and marine), potable waters, and precipitation/bulk deposition provide useful information on the degree of contamination of waters. In addition, such data can be used to validate predictions made on the environmental fate and behaviour of the chemical (see below), and to determine the relative importance of various sources of input (e.g. wastewaters versus atmospheric deposition). Reported concentrations in UK surface waters are particularly important because they can be compared with proposed EQS values as part of the validation process (see Section E2.5) and as a means of risk assessment.

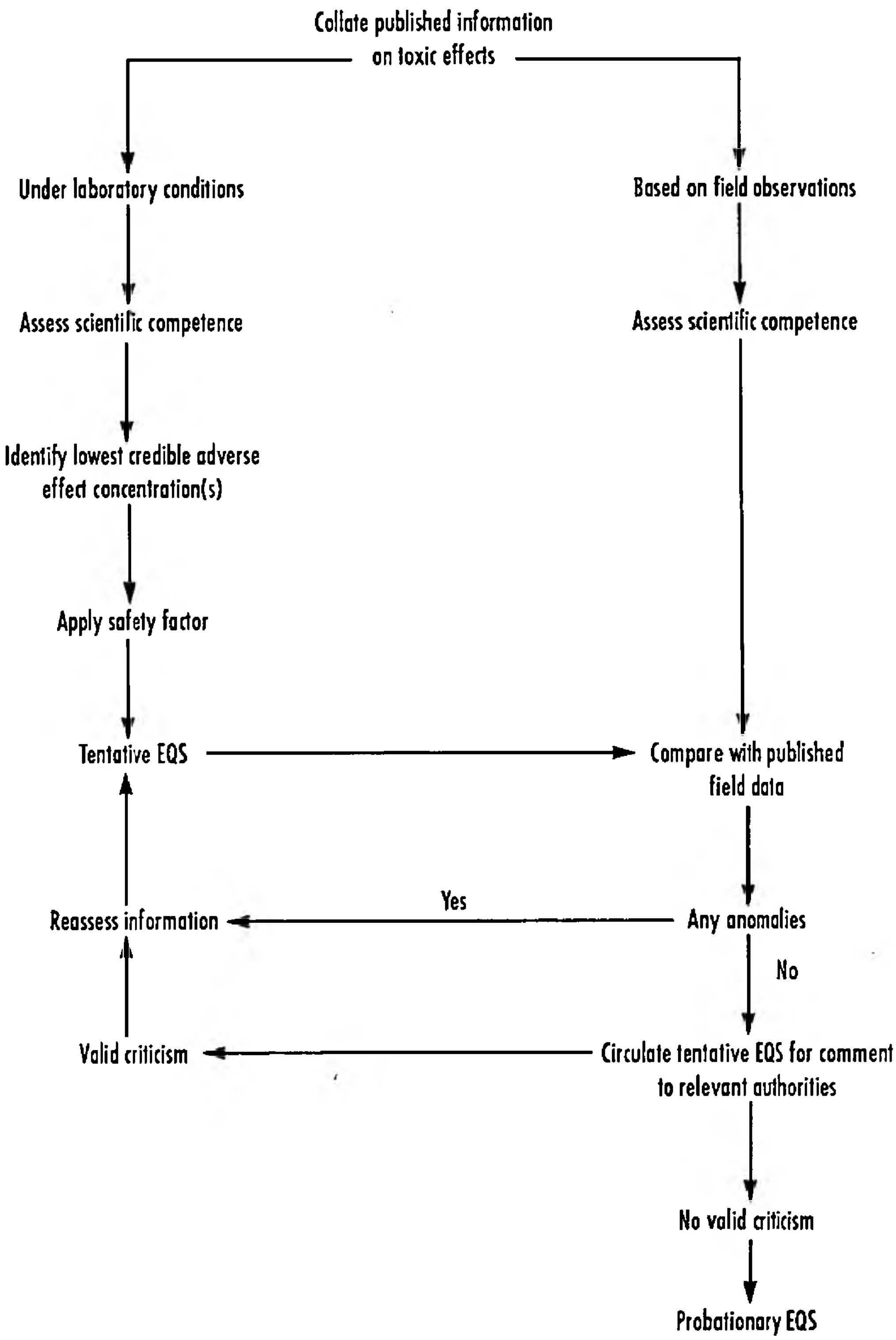


Figure E1 Schematic flow chart for the derivation of environmental quality standards

Fate and behaviour data

An understanding of a chemical's fate and behaviour in the environment can provide useful indicators as to how it will partition in the environment. This will enable some predictions on the likelihood of the chemical entering surface waters, the main routes and temporal nature of such entry, and whether input is likely to be local or widespread.

Fate and behaviour are considered more fully in Section E2.2.

E2.2 Fate

Physico-chemical data

It is important to have reliable values for those physico-chemical parameters which play a particularly important role in a chemical's fate in the environment, especially in water. These parameters are:

(i) Solubility;

(ii) Melting and boiling points;

(iii) Volatility (Henry's Law constant);

(iv) Octanol-water partition coefficient (Kow or Kop), octanol-carbon partition coefficient (Koc); (can be used as indicators of sorption potential in soil and water, and of bioaccumulation potential in aquatic organisms).

These characteristics will (a) determine the behaviour of the chemical in experimental situations, and (b) enable some prediction of the chemical's movement and partitioning in the environment.

It is important to know how the chemical is likely to behave under experimental conditions so that results from toxicity studies can be properly assessed. In particular chemicals with low solubility, high volatility or high sorption potential may present problems associated with preparation of solutions or maintenance of appropriate exposure concentrations, and test design should compensate for this.

Fate and behaviour data

The physico-chemical data considered above will only allow an approximation of how a chemical will behave and partition in the environment. In order to understand this better it is essential to have information (preferably from field studies) on:

(i) Volatilisation and subsequent atmospheric deposition;

(ii) Leaching from soils;

(iii) Sorption to soils and aquatic sediments;

(iv) Speciation in water;

(v) Abiotic degradation processes in the atmosphere, soil and water;

(vi) Biodegradation in soil and water;

(vii) The identity and nature of the main abiotic and biotic degradation products.

It is not possible to develop a list of such data required for the derivation of an EQS. Rather it is a case of using whatever appropriate studies are available. Ideally such information will make it possible to predict:

(i) The likelihood of the chemical entering surface waters, the main routes of such entry, and whether such entry will be sustained or occur in pulses (see also Section E2.1);

(ii) Whether input is likely to be local or widespread (see also Section E2.1);

(iii) The persistence of the chemical in the environment in general, and water in particular, and thus whether aquatic organisms will incur acute or chronic exposure;

(iv) The complexation and speciation, and thus the bioavailability of the chemical to aquatic organisms;

(v) The potential toxic effects of degradation products.

Thus it is possible to ascertain whether a chemical is likely to contaminate water and if so to determine the approximate extent and duration of such contamination.

E2.3 Determine lowest/no effects concentration

Laboratory toxicity studies

In general the likelihood of an EQS value being appropriate increases with the size, reliability and relevance of the toxicological dataset from which it is derived. Therefore, it is essential when attempting to derive an EQS that all available toxicity data are collated and critically assessed in order to determine their reliability and relevance to the aquatic environment. In general toxicity tests that meet the criteria given in Table E2.1 are more reliable and more relevant than those that do not.

Table E2.1 Features of toxicity tests that increase their reliability and relevance

A. Increased Reliability

1. Dosing

- Suitable control, with carrier solvents if used.
- Minimum of three treatments, one at a concentration predicted to cause no effects.
- Concentration intervals less than an order of magnitude.
- Control and treatments all duplicated.
- Exposure maintained at a reasonably constant level (unless specifically investigating effects of intermittent or fluctuating exposure), e.g. flow-through rather than static test.

2. Test Organisms

- Organisms' age, size, sex and health are appropriate.

3. Test Conditions

- Appropriate stocking density of test organisms.
- Extraneous sources of stress eliminated.
- Exposure is long-term, preferably over at least one generation of the test species.

4. Analysis

- Exposure concentrations analysed, at least at start, end and some point in middle, using appropriate method.
- Chemical and physical attributes of test media are measured, e.g. temperature, pH, salinity, hardness, type of test water.

5. Interpretation of Results

- Organisms' response shown to be concentration dependent.
- Endpoint is understood, e.g. mortality, growth or reproduction.
- Statistically significant difference shown between exposure and control.
- All the above features are reported.

B. Increased Relevance

1. Test Organisms
   - Test species is indigenous to the UK, or at least is temperate.
   - Test species is likely to be sensitive, e.g. an alga if testing a herbicide.

2. Conditions

- Appropriate feeding régime.
- Chemical and physical attributes of test media are appropriate, e.g. temperature, pH, dissolved oxygen, salinity, hardness, type of test water.
- Physical conditions mimic as near as possible environmental conditions, e.g. light and temperature.

A particularly important consideration is whether the results are based on nominal or analysed exposure concentrations. For substances that are insoluble, volatile, readily sorbed, or unstable in water the use of nominal concentrations means that the results often cannot be considered sufficiently reliable for use in deriving an EQS, because they may differ widely from actual exposure concentrations (through careless or inaccurate preparation of stock solutions or serial dilutions, or through dissipation of the test chemical during the test). It is also important to ensure that the concentration is maintained throughout the exposure (unless specifically investigating the effects of a variable concentration). Therefore, if the chemical is liable to dissipate under the particular exposure conditions employed, it is essential to renew the test solution (using a flow-through or semi-static design).

By reviewing all available data on a chemical it should be possible to gain an understanding of its uptake, site of attack within the organism, and mode of toxic action, and thus to predict which types of organisms are most likely to be sensitive to it (e.g. invertebrates to insecticides, or fish to non-specific narcotics). It is particularly important to be able to make this prediction for chemicals which do not have a large toxicity dataset available, in order to identify whether there are critical gaps in the data. If particularly sensitive taxons are not adequately represented by the available data they must be accounted for when determining the preliminary standard (by use of a larger safety factor).

A recent OECD workshop attempted to develop an appropriate extrapolation method to derive environmental concern levels for chemicals, based on aquatic toxicity data. Part of this process was to identify the minimum toxicity information considered necessary to enable such an extrapolation to be made with confidence, i.e. what constituted a "comprehensive" dataset. This was based in part on the US EPA's guidelines for deriving water quality criteria (Stephan *et al* 1985), and as a minimum should include:

(i) Reliable acute toxicity data for at least 1 species from each of at least 8 taxonomically distinct Families of aquatic organisms, including at least 1 species of fish, at least 1 species of daphnid, and (if there is evidence for phytotoxicity) at least 1 species of plant;

(ii) A test for microbial function, (although the actual test to use and how to interpret it could not be specified);

(iii) Chronic data for at least 1 of the most acutely sensitive species;

(iv) Multiple tests with non-target organisms that are taxonomically proximate to target organisms for biologically active chemicals (such as insecticides).

In addition some multi-species (microcosm or mesocosm) data would be available. As a minimum requirement, such multi-species studies should:

(i) Include at least one fish species;

(ii) Include components that represent basic ecosystem properties (e.g. photosynthesis, nutrient cycling);

(iii) Be maintained for a duration that reflects the chemical's persistence and the organisms' lifecycles;

(iv) Incorporate a test system that is of an appropriate size for the organisms used;

(v) Include certain minimum design features, (e.g. use of controls, multiple tests concentrations, replication, and others as considered in Table E3.1).

The OECD working group considered multi-species studies essential because they predict effects that single species studies cannot, such as interspecies interactions, ecosystem process responses, ecosystem recovery, and cumulative effects of multiple contaminants and of other stresses.

This OECD approach is more structured than that currently used for EQS derivation in the UK, where no minimum data requirements established but all available toxicity data are reviewed. When no EQS can be set because the data are considered inadequate, this decision is somewhat subjective and a more defensible approach should be adopted. In reality, the data requirements for establishing an EQS should be more rigorous than the OECD dataset because the aims are different in the two approaches:

(i) The OECD dataset relates to the derivation of an environmental concem level from concentrations shown in tests to be toxic (i.e. a level at which a small proportion (usually 5%) of aquatic organisms (either individuals or species) might incur harm);

(ii) Contamination at or below an EQS should result in no significant adverse effects on exposed aquatic ecosystem, and as such should be based on concentrations shown to have no adverse effects on any aquatic organisms.

Thus, whilst the OECD dataset is designed to include species broadly representative of most aquatic species, the EQS dataset should ensure that all types of organisms and ecosystems, particularly those most sensitive to the chemical under investigation, are adequately represented.

Field toxicity studies

Well conducted field tests, which imitate real environmental situations, are generally more relevant than laboratory studies because conditions such as temperature, light and pH are appropriate, exposed organisms are often indigenous to local water bodies, and usually more than one species is studied and inter-species interactions caused by the test chemical (such as changes in dominance) may be detected. However, such studies are normally conducted in man-made ponds or streams, and it is not possible to say with certainty that conditions in these are representative of the real aquatic environment. Aquatic enclosures, (created, for example, by corralling off an area of a lake with plastic sheeting), may appear slightly more realistic than artificial ponds but also have uncertainties associated with them (for example, they increase the surface area available for colonisation by sedentary organisms, may alter the micro-climate or may contain leachable substances that affect the ecosystem).

There are certain circumstances in which laboratory tests might be more useful than field tests. For example: the toxicity of metals such as chromium and lead varies with water hardness, and this effect can be better investigated in the laboratory; and additional stresses such as competition that are variable and may have a variable effect of sensitivity to chemical contamination can be eliminated in the laboratory.

Data from field exposure studies are therefore an important tool when deriving an EQS, but should not be considered in isolation.

Bioaccumulation studies

Results from bioaccumulation (from surrounding media) studies can often be predicted from simple physico-chemical measurements such as Kow values (see Section 2.2). However, at best such predictions can only give an idea of the order of magnitude of bioaccumulation, and also do not take account of biomagnification (from food). Experimental study of these processes enables a consideration of body burdens to be made, and thus allows predictions of possible long-term deleterious effects, which is particularly important if no chronic toxicity data are available. For example, a 24 hour LC50 of 5 mg/l water may be equivalent to a level of 1 mg/kg in tissue; if a long-term BCF of 10 000 is determined then the lethal body burden may be achieved by chronic exposure to only 0.0001 mg/l. Therefore, if a chemical is significantly bioaccumulated or biomagnified (e.g. trichlorobenzenes, Crane *et al* 1988) allowance should be made when determining a preliminary standard (by incorporating an additional safety factor, see Section E2.4).

E2.4 Extrapolation processes

The primary purpose of evaluating all the available laboratory and field toxicity data is to identify the most sensitive aquatic organisms, and to establish for these the lowest credible concentration having a significant adverse effect, or the highest concentration having no effect. A safety factor is then usually applied to this concentration to arrive at a preliminary EQS. This safety factor allows for uncertainties associated with:

(i) Biological variability (both intra- and inter-species, and including the existence of more sensitive life-stages);

(ii) Stochasticity;

(iii) Extrapolating from the laboratory to the real environment;

(iv) Unsuitable test end-points (e.g. LC50s) for deriving a no effect level;

(v) Gaps in the dataset.

The safety factor used depends on the data to which it is being applied, typically in the UK:

- 100 to an acute lethal effects level;
- 10 to a chronic, sublethal effects level;
- (occasionally) 1 to a reliable chronic no effects value from field studies in natural water bodies.

If the toxicity data are reliable and relevant, there is less uncertainty associated with identifying sensitive taxons and determining a lowest effect level. Thus chronic data are more useful than acute data, particularly when attempting to protect against long term exposure (as is the case for most chemical contaminants), and whenever possible are given preference over acute data. Unfortunately many of the data that are available in the literature are derived from acute laboratory studies employing standard test species, many of which have little relevance to UK waters (such as bluegill sunfish). Uncertainty inherent in such data includes:

(i) Uncertainty in extrapolating from acute effects concentrations to chronic effects concentrations;

(ii) Uncertainty extrapolating from artificial, controlled laboratory conditions to variable environmental conditions;

(iii) Uncertainty in extrapolating from effects on a few test species exposed in isolation to complex aquatic ecosystems comprising many biologically diverse organisms; and

(iv) Uncertainty regarding whether standard test species adequately represent the most sensitive organisms, particularly for biologically active substances such as insecticides.

Consequently it may not be possible to identify a lowest effect level, and no reliable EQS can be established. In such situations further toxicity testing should be initiated to ensure that the required data are made available. The DoE has recently carried out such an exercise for chloronitrotoluenes.

Derivation of safety factors

The appropriateness or otherwise of the above safety factors can be justified, at least in part, as follows:

(i) Acute-chronic ratios

When comparing acute LC50 or EC50 values with chronic LOEC or NOEC values for otherwise similar studies (i.e. same species, same test conditions), the following appear to hold true (US EPA 1984):

- the acute:chronic ratio is within about two orders of magnitude for 95% of substances;

- the acute:chronic ratio is within about an order of magnitude for 50% of substances.

Therefore for an "average" substance a factor of 10 applied to the lowest acute value should give a reasonable prediction of the lowest chronic effects value or the no effect value.

(ii) Variability and uncertainty

A factor of 10 is considered desirable to predict a supposedly "safe" environmental concentration from a chronic effects level or highest no effect level. This is in part to allow for other species being more sensitive than those tested (Cairns 1986). The US EPA (1984) presented evidence from three studies investigating the difference between species sensitivities, by comparing their acute LC50s to a number of chemicals. Much variability was found, but in general a factor of 2.4 to 48.9 applied to a single "typical" LC50 would encompass 50% to 95% of the lower LC50s for that chemical, depending on the range of species investigated. Könemann (1984) conducted a similar but smaller investigation and found relative susceptibilities ranging from 1.0 to 6.3 for a wide range of organisms (from bacteria up to amphibians). Based on these studies a factor of an order of magnitude would appear to be appropriate to allow for inter-species variability.

Ideally the extrapolation to a preliminary standard should be based on a chronic no effects concentration, but in practise, (when a highest no effect concentration is not available), it is often based on a chronic effect level. Clearly there is some discrepancy in applying the same safety factor to two different types of toxic end-point, i.e. effects versus no effects. However, given the approximations inherent in the derivation of this safety factor, and in the extrapolation process as a whole, this non-rigorous approach is considered acceptable in circumstances when no effect concentrations are not available.

OECD extrapolation guidelines

A recent OECD workshop held in Washington DC early in 1991 attempted to develop a suitable extrapolation model for use when a comprehensive toxicity dataset (see Section E2.3) is available (OECD 1991). This procedure related to extrapolation to a concern level; i.e. a level at which a small percentage of aquatic organisms might incur harm, whereas EQSs are established at a level that should result in no significant adverse effects on any aquatic organisms. However, although the endpoint of the extrapolations may be slightly different these are largely defined by the original data being extrapolated. The actual extrapolation procedures are comparable because there are similar uncertainties inherent in both approaches. The OECD workshop concluded that extrapolation from a comprehensive dataset should employ the following factors:

(i) 100 to the lowest (of many) acute values (but can be increased if the acute:chronic toxicity ratio is particularly large);

(ii) 10 to the lowest chronic values derived from partial or whole lifecycle studies (where the extrapolation factor allows for laboratory conditions being optimal whereas the environment has stress factors, for the existence of more sensitive species and other toxins in the environment, and for extrapolation from partial to whole lifecycles);

(iii) 1 to no effects values from field studies (e.g. artificial streams), as long as the most sensitive taxons are included.

These extrapolation factors are essentially the same as the safety factors considered above. However, the OECD place greater emphasis on the extrapolation factor of 1 applied to no effect concentrations from field studies. The OECD extrapolation assumes that these test systems are representative of the ecosystem they are mimicking, and also that there are no large differences between different ecosystems. In the UK it is felt that this assumption cannot be made. Thus this approach would only be taken if there was a large database of corroborated information on multi-species field studies, including data derived from natural water bodies (rather than artificial mesocosms). This different view arises partly from the different aims of the OECD and UK extrapolation processes, discussed above.

E2.5 Validation of EQSs

Once a preliminary standard has been suggested its relevance needs to be confirmed. This is done by comparison with any available field monitoring data on the concentrations found in the aquatic environment and any effects these have on the biota (see Section E2.1). Only if such monitoring data do not contradict the preliminary standard is it proposed as an EQS. Unfortunately in many cases there are no, or inadequate, field monitoring data to confirm the relevance of a preliminary EQS. In such situations it may be possible to carry out some validation by using the results from field toxicity tests carried out in natural water bodies (unless these data have been used to derive the preliminary standard in the first place). Because there is a degree of uncertainty associated with most field tests they must be thoroughly evaluated before they can be used. It must also be recognised that this not a proper validation process and should only be used in the absence of field monitoring data.

E3. CONCLUSIONS

The derivation of EQSs involves:

(i) Identification of the potential sources and likelihood of contamination of watercourses;

(ii) Developing an understanding of the chemical's behaviour in the aquatic environment;

(iii) Identification of a lowest credible adverse effect level (or a highest no effect level) for particularly sensitive aquatic organisms;

(iv) Application of an appropriate safety factor to this level;

(v) Validation by comparison with field monitoring data.

The data requirements that enable each of these operations to be carried out with confidence have been detailed in the previous discussion. The essential point when deriving EQSs is that uncertainties must be minimised, particularly those associated with gaps in the toxicity data, the reliability (quality) of the toxicity data, and the relevance of the results to the real environment. Sources of uncertainty and means of increasing the reliability and relevance of experimental studies have been considered in detail.

EQSs are based primarily on toxicity data, but to minimise the uncertainties associated with them it is necessary to have a good understanding of the chemical being considered. This enables the design of toxicity tests to be assessed, and allows the results to be related to the chemical's fate in the environment. It may also enable identification of the types of organisms likely to be particularly sensitive.

The safety factors used when extrapolating from toxicity data to a preliminary EQS have an apparently arbitrary basis but can actually be justified, at least in part, on scientific grounds. It is considered that the uncertainties inherent in EQS derivation negate any arguments for developing more precise safety factors.

A reliable EQS can only be derived if there is reliable and relevant toxicity information available for a number of distinct taxons. The OECD has proposed a minimum comprehensive dataset to be used in extrapolation processes similar to EQS derivation. This is more structured but less rigorous than the dataset required for EQS derivation, but can be considered as a starting point when considering these data requirements. For most substances the data currently available are inadequate to enable EQSs to be derived with certainty. Future ecotoxicological testing needs to address this problem by ensuring that the data produced are reliable and relevant, and by considering the development of more appropriate toxicity test procedures.

APPENDIX F

A PROPOSED SCHEME FOR DERIVING "LIKELY SAFE ENVIRONMENTAL CONCENTRATIONS" (LSECs)

CONTENTS

F1. INTRODUCTION

F1.1 The requirement for a "likely safe environmental concentration"

One of the major problems associated with the derivation of EQS values is that frequently there are insufficient toxicological data available to draw valid conclusions. Due to the national importance of such criteria it is imperative that they should be the best possible value based on the available data. If a minimum dataset does not exist, the proposed standard may be too stringent or too lax and lead to serious consequences for either dischargers or aquatic communities. When available data do not allow acceptable confidence in an EQS, the only acceptable alternatives are either to obtain more information or simply not derive a criterion (Stephan *et al* 1985). Due to limited resources and the requirement for large databases containing acute, chronic and field toxicity data, many chemicals are still without EQS values. This presents a problem for regulatory agencies when setting discharge consents.

The National Rivers Authority currently has 28 days in which to determine a consent after the nature of the discharge has been established. In the absence of EQS values, any relevant toxicity data must be processed to determine an estimated safe level (hereafter referred to as a "likely safe environmental concentration" (LSEC)) for any potentially hazardous chemical present. It is acceptable that there is more uncertainty associated with LSEC values as they are not intended to have as much regulatory impact as EQS values.

F1.2 Definition of an LSEC

At present, the definition of an LSEC is purely narrative, i.e. it is a concentration in the receiving water which if not exceeded is assumed to adequately protect the well being of aquatic organisms and the ecosystem as a whole.

It is the aim of this section to establish a method for deriving numerical criteria to satisfy this definition, with which the NRA can establish discharge consents.

F1.3 The concept of a minimum dataset

One of the primary considerations when setting EQS or LSECs is to select data for species which are particularly sensitive to the toxicant in question. By ensuring the protection of these species, the rest of the indigenous biota unlikely to be affected. Often there is a difference of several orders of magnitude between species sensitivities to a particular toxicant and so it is important to have confidence in the selection of a suitable species. This can only be achieved by studying a wide range of sensitivities; the more acute data that are used, the greater the confidence in the selection. In the EPA's National Guidelines (Stephan *et al* 1985), a minimum of eight species from eight different families is recommended for setting national water quality criteria. When deriving safe concentrations, this amount of data is often not available. It is important therefore, to determine the levels of uncertainty associated with smaller datasets.

Following the EPA's recommendations, Kimerle *et al* (1985), carried out an analysis of species sensitivity ranges under acute exposure to 82 chemicals. Relationships between the LC50 value for the most sensitive species and those for four of the most commonly tested species (daphnids, fathead minnow, bluegill and rainbow trout) were investigated. When the data for three of these species were used collectively, it was found that the lowest LC50 value could be predicted within one order of magnitude for 98% of the chemicals studied. This predictability did not improve substantially when using all four species or when using different combinations of species. The EPA has since recommended that the use of three species is adequate to eliminate much of the uncertainty associated with inter-species differences in sensitivity, and the selection of species is not important as long as they are chosen from ecologically diverse taxa (US EPA 1985). This level of uncertainty is acceptable for the derivation of LSECs and a minimum dataset of acute data for three species is therefore proposed.

F1.4 The use of application and assessment factors

Application factors

Toxic effects often occur over extended time periods and at lower concentrations than those predicted by the results of acute toxicity tests. Since a "safe" environmental concentration must allow for continuous exposure in the receiving water, an application factor must be applied to extrapolate from acute lethality to chronic sublethal effects levels. The application factor used for this purpose is the acute to chronic ratio (ACR) which is the ratio of the LC or EC50 value to the laboratory determined "no observed effects concentration" (NOEC). This ratio varies between species and for different toxicants and should ideally be calculated from available data on acute and chronic effects on the same species tested under the same conditions. However, if such data are limited, an ACR value of 10 will be used in the proposed strategy as recommended by the OECD Workshop (1991) and the US EPA (1985). (Note, however, that persistent chemicals may have ACRs as high as 100 and if this is suspected then further tests must be carried out.)

Assessment factors

When limited data are available, uncertainty is high and the use of assessment or safety factors is recommended to estimate environmental concern levels (the concentration of a chemical at which ecosystems are estimated to be adversely affected) from acute or chronic effects data (OECD 1991). The value of these factors depends on the quality and type of the data available.

F1.5 Concern levels or safe levels

The definition of a safe level implies that the concentration should be "safe" unless exceeded. Unlike the concern level which is derived from effects data and gives a concentration below which ecosystems are safe, the safe level should be derived from chronic "no effects" levels to give a concentration at which ecosystems are safe (OECD 1991).

One of the major problems associated with limited datasets is that there are unlikely to be sufficient chronic no effect data available from which to derive a safe level. In this case, it may be acceptable to use the concern level (as determined by the OECD Preliminary Assessment Guidelines), instead of a "safe" concentration. The main assumption would be that as long as concentrations are maintained at or below concern levels then they are adequately protective of aquatic organisms. This assumption may be reasonable when considering the uncertainty inherent in the handling of limited datasets and the application of assessment factors.

The US EPA have proposed guidelines for the estimation of safe levels when data are insufficient to derive national criteria (US EPA 1987). In the following sections this procedure is compared with the OECD method for deriving concern levels. The two methods, both requiring minimum datasets containing acute lethal data for three species, are also compared to the EPA's procedure for establishing national criteria when more comprehensive datasets are available.

Section F5 considers possible strategies for prioritising and determining safe concentrations for new and untested chemicals which have no toxicological database.

F2. DERIVATION OF LSECs

F2.1 Data requirements

As discussed above, the minimum dataset from which an LSEC should be derived contains acute lethal data for three species from three different families. The US EPA (1987) recommend the use of one fish species, one crustacean and one other invertebrate, preferably in the phylum Mollusca or another family of Arthropoda. Although data for plants and algae are useful, they are not required here as it appears that for many chemicals (with the exception of herbicides) plants are adequately protected when aquatic animals are protected. It is generally accepted that freshwater data can be used to derive saltwater criteria if there are no data available and it is thought that the sensitivities of saltwater species to a particular toxicant will not differ substantially from freshwater species (US EPA 1987, OECD 1991). Data for non-indigenous species should not be used unless other data are insufficient.

Any data must be critically assessed to determine their reliability in the same way as for the derivation of EQS values. Apart from obvious considerations such as unmeasured exposure concentrations and irrelevant endpoints, test data should not be used if the organisms were fed during the test (unless the data indicate that food did not affect the toxicity) or if unusual dilution water was used (e.g. when the total carbon or particulate matter exceeded 5 mg/l).

F2.2 Derivation Methods

Method 1 - EPA Guidelines

These methods are based on the principles set out in the US EPA National Guidelines (Stephan *et al* 1985) (Method 1(a)) and the Guidelines for Deriving Advisory Concentrations (US EPA 1987) (Method 1(b)).

(i) Method 1(a). For datasets containing acute toxicity values for four or more species.

- When more than one acute value is available for a species, the geometric mean is used to calculate the species mean acute value (SMAV). The geometric mean is used because species sensitivity distributions are more likely to be closer to log normal than normal. It is important to check the agreement of all data within and between species and if any results are questionable, they should not be included in the SMAV.

- If data are available for more than one species within each genus then the genus mean (GMAV) is calculated as the geometric mean of the SMAVs.

- A final acute value (FAV) is then calculated in the following way:

  - Assign ranks, R, to the GMAV values from 1 (for the lowest) to "N" (for the highest). If two or more GMAV values are identical, arbitrarily assign successive ranks to them.

  - Calculate the cumulative probability, P, for each GMAV value as R/(N+1).

  - Select the four lowest GMAV values.

  - Using the selected GMAV and P values, calculate:

$$s^2 = \frac{\Sigma((\ln GMAV)^2) - ((\Sigma(\ln GMAV))^2/4)}{\Sigma(P) - ((\Sigma(\sqrt{P}))^2/4)}$$

$$L = (\Sigma(\ln GMAV) - S(\Sigma(\sqrt{P}))/4)$$

$$A = S(\sqrt{0.05}) + L$$

$$FAV = e^a$$

- The FAV must then be divided by an acute to chronic ratio (ACR) to extrapolate to a final chronic value. If acute and chronic data are available for at least three species then an ACR can be calculated on the basis of geometric means. However, this situation is unlikely when deriving LSECs and a value of 10 is used, as explained in Section F1.4.

- The final chronic value forms part of the National criteria set by the EPA and here will be termed the LSEC.

(ii) Method 1(b). For datasets containing acute toxicity values for three species.

- The GMAV values are derived as above.

- An advisory acute value is then calculated by dividing the lowest GMAV by an appropriate application factor. This factor depends on the number of GMAVs that are available (which in this case should be three) (Table F2.1) and has been derived in order to give final values which would be expected if the above calculation had been used.

Table F2.1 Application factors for deriving an advisory acute value

Number of GMAVs	Factors
3	11.0
4	10.0
5	9.0
6	8.0
7	7.0

- The advisory acute value obtained from this calculation is divided by an ACR value of 10 (unless a more realistic value can be derived experimentally) to give an advisory chronic value which will be termed the LSEC.

Method 2 OECD concern levels

This a simple method based on the Guidelines for preliminary effects assessment outlined by the OECD Workshop 1991. It involves applying an assessment factor of 100 to the lowest LC or EC50 value in a dataset containing values for at least three species. The factor takes into account an ACR of 10 and therefore would be reduced to 10 if applied to chronic effects data. If more than one acute value is available for a species then the geometric mean should be used in extrapolation.

F3. VALIDATION OF DERIVATION METHODS

F3.1 Applying a dataset

A dataset taken from Appendix 2 of the EPA National Guidelines (Stephan *et al* 1985) can be used to compare the methods outlined above (Table F3.1).

Table F3.1 Dataset taken from EPA National Guidelines

Rank	MAV	lnMAV	$(\ln MAV)^2$	P=R/(N+1)*	$\sqrt{P}$
4	6.4	1.8563	3.4458	0.44444	0.66667
3	6.2	1.8245	3.3290	0.33333	0.57735
2	4.8	1.5686	2.4606	0.22222	0.47140
1	0.4	-0.9163	0.8396	0.11111	0.33333
Sum:		4.3331	10.0750	1.11110	2.04875

NOTES * N = Total number of MAVs in dataset = 8

Example Calculations using data from Table F3.1.

(i) Method 1 (a).

$$s^2 = \frac{10.0750 - (4.3331)^2/4}{1.11110 - (2.04875)^2/4} = 87.134$$

$s = 9.3346$

$L = [\ 4.3331 - (9.3346)(2.04875)]/4 = -3.6978$

$A = (9.3346)(\sqrt{0.05}) - 3.6938 = -1.6105$

$FAV = e^{-1.6105} = 0.1998$

$ACR = 10$

$$LSEC = \frac{FAV}{ACR} = \frac{0.1998}{10} = 0.00199$$

(ii) Method 1(b).

Lowest GMAV value = 0.4

Application factor (for three GMAVs) = 11

ACR = 10

$$LSEC = \frac{0.4}{110} = 0.00364$$

(iii) Method 2.

Lowest GMAV value = 0.4

Assessment factor = 100

$$LSEC = \frac{0.4}{100} = 0.004$$

F4. CONCLUSIONS

Methods 1(b) and 2 (based on three species datasets) make use of similar application factors and give consistent results. Safe levels are slightly lower than concern levels, but at the level of uncertainty associated with limited datasets the difference between the two values is insignificant. This validates the proposed assumption that the terms "concern level" and "safe level" can be used interchangeably.

Method 1(a) has a more technical basis and is associated with the least uncertainty, therefore it is reasonable to assume that the value obtained from this method is the most realistic. As this method can only be carried out with a minimum of four species and becomes more accurate with experimentally derived ACR values, the optimum dataset for setting LSECs will be defined as containing acute lethal data for at least four ecologically diverse species and both acute and chronic data for at least three species.

LSEC values derived by Method 2 are lower than those derived by Method 1(a). Because there is more uncertainty associated with the former, it is acceptable that it should be a conservative estimate.

F5. PRIORITISATION AND DERIVATION OF LSECs FOR CHEMICALS WITH NO AVAILABLE DATA

F5.1 General

Where no test data are available it is important to determine a prioritisation procedure to identify those chemicals which require further assessment. The chosen procedure must be standard, rapid, sensitive, widely recognised, cheap and mostly available "off the shelf". One test which meets most of these criteria is the Microtox test based on the bioluminescence response of *Photobacterium phosphoreum*. The sensitivity of the bacterium is similar to that of more typical test organisms for many toxicants. However, it is less sensitive to many inorganics and effluents with a high proportion of insecticide, herbicide, pharmaceutical, textile or highly lipophillic components (Crane *et al* 1991). For such components it will be necessary to forego the screening procedure and initiate single species acute testing required for the derivation procedures above. For other components, for example most organic compounds, the Microtox test can be used as cheaper and more simple way of prioritisation.

F5.2 Microtox prioritisation

Results of the Microtox test are expressed in the form of an EC50 value which is divided into 100 to convert into toxic units (TU). (This step is carried out to avoid confusion due to the inverse relationship between the measure of toxicity and toxicity itself.) The resulting value is then adjusted using appropriate application and assessment factors to determine the potential chronic toxic impact on aquatic communities in receiving waters. The following factors are used:

(i) Species sensitivity factor (SS)

As only one test is being used to set a prioritisation value, a factor is required which takes into account the differences in sensitivity between species. A factor of 10 is usually appropriate (Hunt 1989).

(ii) Acute to chronic ratio (ACR)

As discussed above, this factor is required when extrapolating from acute to chronic effects data and usually has a value of 10, unless a more accurate value can be derived experimentally.

(iii) Worst case dilution factor (WCDF)

The environmental exposure of any chemical is variable at different discharge sites, due to changes in the flow rate of the effluent and receiving water. Instead of measuring or estimating the variable exposure state at each, which would require statistical analysis and dynamic modelling, it is easier for the purpose of screening to base criteria on a steady state exposure condition, usually an estimate of the presumed "worst case". The "worst case" condition assumes a low critical receiving water flow and an average effluent flow. By basing criteria on these assumptions it is unlikely that unacceptable effects will occur below this concentration in any body of water.

For the purposes of screening, the 5 and 10 percentile weekly average river flows, used by the EPA to assess chronic toxicity in stressed and unstressed receiving waters are appropriate (Hunt 1989).

The EC50 value expressed in toxic units and the application factors are then used in the following equation, taken from the interim protocol for discharge consent by direct toxicity assessment (Hunt 1989).

$$\text{Estimated Chronic In-Stream Toxicity (ECIST)} = \text{EC50} \times \text{ACR} \times \frac{\text{SS}}{\text{WCDF}}$$

Priority for further toxicological assessment must be given to those chemicals which have ECIST values exceeding 0.1 TU. For less hazardous chemicals showing ECISTs of less than 0.1 TU, provisional LSECs may be set on the basis of Microtox data alone. This involves the application of an assessment factor to the acute EC50 value before it has been converted to toxic units. The OECD workshop (1991) recommends use of an assessment factor of 1000 when only one acute toxicity value is available. However, because of the great uncertainty associated with such a large factor, it must be stressed that only those toxicants showing ECISTs of less than 0.1 TU should undergo LSEC derivation in this way.

F5.3 Further toxicological information

Single species testing

For the LSEC derivation procedures above, a minimum of three acute lethality tests are required, determining lethal or effective concentrations for 50% of individuals (LC50 and EC50 respectively) of three ecologically diverse species.

Standard test species are easier to use than species resident in the area of a discharge. This is mainly due to availability and uniformity of age of the animals, and availability of appropriate test guidelines. Standard species will be representative of the expected impact on resident species as long as a range of sensitivities is assessed and a sensitive species is chosen (US EPA 1985). As mentioned in Section F2.1, algal and plant test data are not required unless the toxicant is a byproduct or component of herbicide. (If necessary algal test species might include *Chlorella vulgaris* (freshwater) and *Phaeodactylum tricornutum* (marine)).

Although toxicity tests using lethality as an endpoint are simple, cost-effective and reproducible, the application of a standard acute to chronic ratio to obtain chronic effects levels, is associated with a degree of uncertainty. Acute tests are used in the derivation of LSECs purely because this type of data is the most readily available. In the absence of substantial chronic data from which to derive an LSEC value, it is important to at least ensure that the ACR value is as realistic as possible. The optimum dataset should therefore include acute and chronic values for the same species in order that an ACR can be derived for every chemical tested. The following species are the most commonly used for acute and chronic tests, and guidelines are available for both procedures.

Table F5.1 Commonly used species and available guidelines for deriving LSECs

Organism	Freshwater	Marine
Invertebrate	*Daphnia magna* (OECD, EPA) *Daphnia pulex* (EPA)	*Crangon crangon* *Mysidopsis bahia* (EPA)
Fish	*Oncorhynchus mykiss* (OECD, EPA, EC)	*Cyprinoden variegatus* (EPA)

Microcosms

A microcosm is defined as a multispecies test system in which more than one species of plant or animal are exposed to a contaminant in order to investigate the direct or indirect effects of pollution. One of the major advantages of such an approach is that it takes into account the environmental fate of a contaminant and the variability of exposure concentrations due to factors such as partitioning between different compartments. The integration of environmental fate and toxic effects measurements cannot be achieved with single species tests. Examples of systems in which both fate and effects can be studied include experimental ponds and streams, lake and marine enclosures and marine land-based tanks (Crane 1990).

Another major advantage of the microcosm approach is that it may be more reliable at predicting responses at higher levels of biological organisation than single species tests. When deriving LSEC values it is important to take into account both variability of environmental exposure and effects on higher levels of organisation. However, one of the major disadvantages of microcosm systems is that they tend to be costly. Therefore they should only be used in cases where there is a small margin of safety between the derived LSEC value and the expected environmental concentration, and insufficient data exist for further assessment leading to the derivation of an EQS value.

F5.4 Validation of LSECs

The only way to test the protective capacity of an LSEC is to carry out long-term, sublethal toxicity tests at the concentration itself. If chronic effects such as growth, development or reproductive impairment are seen, then the toxicant requires further investigation.

F6. CONCLUSIONS

The minimum dataset from which an LSEC can be derived contains acute lethal data for three species taken from ecologically diverse taxa. The lowest LC or EC50 is then divided by an assessment factor of 100 in order to obtain a concern level below which an ecosystem can be assumed to be "safe".

The optimum dataset from which an LSEC can be derived contains acute lethal data for a minimum of four species, and both acute and chronic data for a minimum of three species. The four lowest species mean acute values are used in the equation recommended by the US EPA for use in deriving National Criteria. The final value is then divided by an acute to chronic ratio preferably derived from experimental data. This gives an LSEC value at or below which an ecosystem can be assumed to be "safe".

Where no data are available the Microtox test can be used to prioritise those toxicants for which the method is sensitive, such as most organics. This procedure gives rise to "Estimated Chronic In-Stream Toxicity" (ECIST) values expressed in toxic units (TU). For toxicants showing ECIST values of less than 0.1 TU an LSEC value can be derived by dividing the EC50 value (before it has been converted to toxic units) by an assessment factor of 1000. This gives a concern level below which an ecosystem can be assumed to be "safe".

For those toxicants which have ECIST values exceeding 0.1 TU or for which the Microtox test is considered to be insensitive, acute lethal tests must be carried out on at least three species from ecologically diverse taxa. This is the minimum dataset required for the derivation of an LSEC, above.

Where possible, chronic tests should be carried out on the same species as acute tests so that acute chronic ratio (ACR) values can be derived for each chemical. This reduces the uncertainty which is associated with applying a standard ACR value.

When the margin of safety between the derived LSEC and the expected environmental concentration is small and there are insufficient data for further toxicological assessment, microcosm tests should be carried out with systems more closely approaching environmental conditions.

When the margin of safety between the derived LSEC and expected exposure is small and there is more toxicological information available, further investigation must be carried out with a view to deriving EQS values.

If the concentration of a chemical in the receiving water of a discharge is equal to or below the LSEC value for that chemical, there is probably no cause for concern about its effects on aquatic organisms. If the receiving water concentration is above the LSEC, then the NRA must set more stringent discharge consents to ensure adequate protection.