# A REVIEW OF AVAILABLE INFORMATION SOURCES FOR ASSESSING THE HAZARDS AND RISKS OF CHEMICAL SUBSTANCES IN THE ENVIRONMENT

Recommendations for the acquistion of certain sources of environmental data

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#### **EXECUTIVE SUMMARY**

The NRA has a requirement for environmental data to support certain operational activities, such as consent setting, catchment planning and managing pollution incidents. One of the roles of the Environmental Toxicology Unit of the National Centre for Toxic and Persistent Substances (TAPS) is to advise operational staff throughout the regions on the environmental hazard/risk of chemical substances. In order to do this effectively, access is required to quality assessed environmental data. The aim of this review was therefore to identify and critically assess information sources in computer and text format, that primarily provide data relating to substance identification, ecotoxicity and fate/behaviour in the environment.

Trials were conducted on numeric and text databases available in CD-ROM/diskette format or through connection to on-line hosts via telecommunication networks, to assess available systems for usefulness and value for money. On the basis of these exercises certain CD-ROM/diskette products as well as various text books have been acquired. In addition, recommendations have been made for the acquisition of certain other data sources and for access to on-line database hosts via connection to telecommunication networks such as BT or the Internet.

#### 1. INTRODUCTION

There are many sources of environmental information and data available to NRA that could assist staff in a variety of operational scenarios. However, these sources are apparently not exploited to their maximum potential. In 1991, WRc was commissioned to review sources of environmental information available to NRA (R&D Note 12 - Baker et al 1991) in an attempt to rectify this situation. The basic conclusion of the review was that acquisition of environmental data was most effective through the use of WRc's Environmental Toxicology Advisory Service (ETAS). This led to an increased reliance by Regional staff on ETAS to assist in routine operations. However, because this route of access to information was not standardised or conducted through a central body, over-reliance on the service caused considerable duplication of effort.

Consequently, a new scheme was initiated whereby staff requiring environmental data had first to liaise with an appointed Regional contact, who would then, if necessary, contact the Environmental Toxicology Unit of the NRA National Centre for Toxic and Persistent Substances (TAPS) at Reading. This group would then consult their own sources to see if similar work had previously been conducted by ETAS for NRA, thereby avoiding duplication of effort. This scheme is still in operation and only where no data are available do NRA now contact ETAS for further information.

This system has eliminated unnecessary duplication of work and the numbers of enquiries referred to ETAS have dramatically reduced. However, there is still a need to gain access to a wide range of quality data sources that are currently unavailable to the TAPS Environmental Toxicology Unit and other interested groups. The aim of this report is to review up-to-date sources of environmental information/data (primarily concerning substance identification, toxicity and fate/behaviour in the aquatic environment), both in printed and computer formats, and can therefore be regarded in many ways as an update of R&D Note 12. In addition, many key issues concerning computer databases that are often confused have been clarified.

It should be noted that a separate review has been commissioned through the NRA R&D Programme that aims to broadly identify all data sources currently exploited by NRA across all functions, with a view to providing guidance when making future purchases. However, this review adopts a more specific approach than that of the former, in order to address the requirements of the Environmental Toxicology Unit of TAPS, so that it may fulfill its role as a provider of environmental data and advice more effectively.

A comparison has also been made between the use of computer databases either in CD-ROM/diskette format or through the use of on-line hosts accessed via telecommunication networks. This has been achieved by trialing databases accessed via the two types of system. Following these exercises, recommendations have been made for the acquisition of certain computer and printed data sources, based on considerations of usefulness and cost.

The report has been divided into the following Sections:

- (i) Computer databases
  - Overview of principles and search techniques
  - Quality implications

- Advantages and disadvantages of use of CD-ROM/diskette formats against the use of on-line hosts
- Specific examples of useful databases
- (ii) Other information sources
  - Printed texts
  - External services
- (iii) Discussion and recommendations for acquisition of best data sources to maximise efficiency in retrieval of quality data
- (iv) Appendices
  - Full details of useful computer databases including those not reviewed in main body of the report
  - Details of text sources
  - Details of external information services

#### 2. COMPUTER DATABASES

#### 2.1 INTRODUCTION

Commercial computer systems on which individuals and organisations can search bibliographic records or data held on large computers, have been available for the last 30 years. These systems can be located anywhere in the world and are accessed via remote terminals and telecommunication networks, usually for a small subscription fee and appropriate searching charges. In addition, some information held on these systems is available on CD-ROM or diskette for an annual subscription fee. The advantages and disadvantages of the different formats is discussed more fully in Section 3. Most databases are straightforward to access, although some knowledge is required in order to maximise the efficiency with which data are retrieved. However, basic searching procedures are easily learnt and many training courses exist to help with advanced techniques.

Databases contain information obtained from a wide variety of sources, including papers of conferences, foreign research, published journals/books and unpublished material. There are many thousands of commercially available databases, some of which contain information relating to substance identification, fate/behaviour and ecotoxicity in the aquatic environment. The most useful of this group are outlined in Section 3, with full details of other relevant databases given in Appendices A and B.

Available databases vary in their coverage of environmental information and in the way they are structured. N.B. In the WRc report (Baker et al 1991 - R&D 12), a clear distinction was made between 'databases' and 'databanks', where databases were defined as those systems containing bibliographic text records and databanks as systems containing environmental data extracted from original documents. These definitions have also been made by Richardson (1986). However, the distinction is somewhat confusing since, both systems can be searched in very similar ways and it is only the degree of detail that varies. In addition, the distinction does not appear to have been made elsewhere, although recently the terms 'textbases' and 'databases' have been used (Thames Water Library, Pers. Comm., 1995). To avoid confusion, the different systems will referred to as either 'text databases' or 'numeric databases' throughout this review.

#### 2.2 TEXT DATABASES

The majority of environmental text databases are not intended to provide specific data on substance identification, fate/behaviour and ecotoxicity, and such data may only contribute to a small proportion of the database, which may have a very broad coverage of environmental information. For example, the popular database 'Chemical Abstracts' available through a number of on-line hosts contains over 12 million records relating to all aspects of chemical science. To retrieve a set of data relating to, for example, the toxicity of a particular substance to aquatic organisms requires a set of search terms using Boolean Logic. At the most basic level this might be something along the lines of 'COPPER AND TOXIC? AND (FISH OR INVERTEBRATE?)', which are used to search certain fields of the database records (e.g. BIBliography, ABstract, Basic Index, etc).

Text databases are not the best sources of information if environmental data are required rapidly.

Few abstracts (if abstracts are provided; not all databases do so) contain the level of detail that is usually required and the original document may need to be consulted. Complete documents are not available on-line or on CD-ROM/diskette and so need to be acquired, usually through an institution such as the British Library (around £4-£6 per document). In addition, some abstracts may be taken from obscure or foreign journals, further adding to the delay in obtaining specific data on a substance. However, due to the large numbers of records on text databases, they are a very good source of information if a comprehensive search of all available literature is required on a particular chemical and if time is not a limiting factor. Otherwise, they can be used to support data obtained from numeric databases.

#### 2.3 NUMERIC DATABASES

Numeric databases tend to be devoted to a particular topic area such as ecotoxicology or environmental fate and behaviour of substances and contain actual data extracted from original documents. As a consequence they sometimes contain fewer records than text databases, although they are an extremely valuable source of immediately available data.

Information contained in numeric databases is retrieved and viewed in much the same way as in text databases, with the exception that more extensive use is made of field searching. For example, the United States Environmental Protection Agency (USEPA) produces a very useful database called the Aquatic Information Retrieval system (AQUIRE), available on-line and more recently on diskette, which contains over 100,000 records on over 5,000 substances. Each record on this database holds the summarised information extracted from an ecotoxicological study in fixed fields. In other words, numeric values relating to aspects of the study (e.g. CAS number, chemical name, species, certain test conditions, route of exposure, end-point of toxicity, etc) can be searched individually or combined to further refine the retrieved dataset.

#### 2.4 QUALITY ASSESSMENT OF DATA

There is no indication to suggest that information within most databases has been assessed for quality before it's entry onto the system. It seems likely that abstracts and data taken from published journals and other sources are placed onto databases regardless of quality. A few numeric databases incorporate a 'quality score' for studies from which data are taken, although no database appears to exclude data from poorly conducted studies. This is probably for the best as data of low quality are usually better than no data at all.

The USEPA numeric databases AQUIRE, ENVIROFATE and ISHOW use pre-defined guidelines for quality assessment of studies from which data are extracted and a measure of reliability is assigned to each record. In this way the database user has a certain degree of confidence in the data.

In order to assess the quality of information in text databases it will probably be necessary to obtain the original document from a supplier such as The British Library. Even having done this, it is not always possible to thoroughly assess the quality of a study due to occasional inadequate reporting of study details by the author(s).

## 3. EVALUATION OF DATABASES IN EITHER CD-ROM/DISKETTE FORMATS OR 'ON-LINE' THROUGH THE USE OF TELECOMMUNICATION NETWORKS

As has already been mentioned, computer databases can be accessed "on-line" via telecommunication networks or through the use of CD-ROMs/diskettes. In order to determine which approach is likely to be of most practical use to the TAPS Environmental Toxicology Unit, several selected systems were trialed and critically assessed. This involved contacting appropriate producers of CD-ROMs/diskettes and on-line databases. It should be noted that the following organisations were contacted but did not respond to a request for information; The Organisation, for Economic Cooperation and Development (OECD) (Paris), TDS Numerica (US) and Cambridge Scientific Abstracts (US).

This section gives a general introduction to the use of CD-ROMs, diskettes and on-line systems and summarises the findings of the trial exercises.

#### 3.1 CD-ROMS/DISKETTES

#### 3.1.1 Introduction

CD-ROMs are virtually indestructible and are a convenient tool for the retrieval of information. All that is needed is a standard IBM compatible or Macintosh personal computer and a CD-ROM drive. A single CD-ROM (Compact Disc Read Only Memory) can store nearly a quarter of a million pages of text on a single disc - the equivalent of 1,500 diskettes. Therefore, even databases containing millions of records can be stored and searched in their entirety on a small number of discs.

#### 3.1.2 The trials

The following CD-ROMs were assessed in the exercise:

The Environmental Chemicals Data Information Network (ECDIN, produced by Springer Verlag), Aquatic Sciences and Fisheries Abstracts, Biological Abstracts, Chem Bank, EINECS-plus, POLTOX I-III (all marketed by SilverPlatter), Hazardous Materials, Pollution Control and the Environment and Regulatory Compliance (all part of the CASurveyor series produced by The Chemical Abstract Service), Environmental Chemistry and Health and Environmental Management (produced by DIALOG OnDisc) and CHEMTOX (produced by Resource Consultants Inc.).

In addition, the following diskettes were trialed:

The Environmental Fate Databases (EFD) and estimation programs produced by Syracuse Research Corporation (SRC), Material Safety Datasheets (MSDS) produced by Sigma-Aldrich, EXICHEM produced by the Organisation for Economic and Cooperation and Development (OECD) and CHEMDATA produced by the UK National Chemical Emergency Centre.

N.B. For the purposes of this review costs given as US dollars have been converted into pounds sterling.

#### Advantages:

Having conducted the trials, the main advantage of CD-ROM was found to be ease of use and clarity of display. This was particularly true for those systems that used search software compatible with Microsoft Windows. For example, WINSpirs, the software package supplied by SilverPlatter with all their CD-ROM databases, allows the user to build up a search strategy that is clearly laid out in a series of steps. Any of these stages can be used or modified at any time. The records that are retrieved in a search are also very clearly laid out in a format that can be predefined by the user. Retrieved records can be 'marked' for future downloading or printing. In addition, the software incorporates some fairly powerful tools such as an index, a thesaurus and an 'Auto Subject Look Up' that allows the user to identify similar search terms that might also be of use. The search software provided with CASurveyor databases operates in a similar way.

The databases produced by DIALOG OnDisc suffer as they currently operate in a DOS environment only. This means that while still easy to use, the displays are less clear as the user is forced to shuttle back and forth between different menus to view records in different formats. However, both DOS and Windows products are quick to install and to search for information, allow easy browsing of retrieved records and selection for down loading/printing, and make use of extensive HELP facilities at any time without interrupting the search.

#### Disadvantages:

The main drawback to the use of CD-ROMs/diskettes is their relatively high cost, with most on the market priced between £600 and £2,600 for an annual subscription, which generally only includes updates for 1 year. Furthermore, the provision of quarterly updates can lead to a cumbersome pile of CDs for the larger databases, all of which may need to be searched separately in order to retrieve the desired information. While it is true to say that the use of CD-ROMs/diskettes do not incur the fees associated with on-line searching, the latter tend to be relatively low (around £33-£160/hour) and are available on a 'pay-as-you-use' basis (see Section 3.2.1).

#### Specific numeric databases:

Of the trialed databases themselves, the numeric databases are likely to be of more use than the text databases, as they act as an immediate source of data. By far the most useful systems trialed were the Aquatic Information Retrieval system (AQUIRE) produced by USEPA and the Environmental Chemicals Data and Information Network (ECDIN) produced by the Commission of the European Communities (CEC). AQUIRE contains quality assessed ecotoxicity data extracted from published studies, while the ECDIN database gives physico-chemical properties, ecotoxicity, production and legislation details for over 120,000 existing chemicals (see Appendices A and B for full details). These databases have now been purchased and are routinely used by the TAPS Environmental Toxicology Unit.

The numeric database CHEMBANK produced on CD-ROM by SilverPlatter, was also found to

be particularly useful for the provision of substance identification details (CAS number, synonyms, structures, etc), ecotoxicity data (although more extensive coverage is given to mammalian toxicity data), risk assessment and advice on what to do to minimise hazards in pollution situations (e.g. spillages during transport). This database (which costs £1,271 for an annual subscription) contains the files RTECS, OHM-TADS, CHRIS and HSDB, all of which are also available on-line (SilverPlatter, Pers. Comm., 1995). The Material Safety Datasheets CD-ROM produced by Sigma-Aldrich provides similar information to CHEMBANK (although with a greater bias towards mammalian toxicity and occupational safety) for over 70,000 chemicals. The cost of this product is £975 for an annual subscription.

Some of the Environmental Fate Databases (EFD) produced on diskette by SRC, were found to be very comprehensive and good value for money. Of these, the databases CHEMFATE and BIODEG are likely to prove particularly useful as they provide substance identification details, physico-chemical values and transformation rates in a variety of environmental compartments for 1,700 and 700 chemicals respectively. The respective costs of these databases are £1,000 and £333. The EFDs DATALOG and BIOLOG are slightly more expensive (£1,600 and £530) and provide bibliographic records (up to 200,000 on DATALOG covering 13,000 chemicals) that have been identified as containing environmental fate and exposure information. However, the records themselves do not contain actual data and so these databases are of less immediate use.

In addition to the EFDs, SRC also produce estimation programs on diskettes for the prediction of certain physico-chemical parameters and environmental transformation rates based on chemical structures and experimental data. In the trials, these programs were found to be extremely useful, particularly LOGKOW which estimates octanol-water partition coefficients for organic chemicals using an atom/fragment contribution method. This program also contains a database of 9,500 experimental values for validation of predicted data. The LOGKOW program (which is only £400) is particularly useful for the prediction of chemical toxicity when using Quantitative Structure Activity Relationships (QSARs), as this approach requires Log Kow values. Other programs produced by SRC estimate probability of biodegradability in the environment, water solubilities, melting and boiling points, vapour pressures, Henry's Law Constants, Log Koc's and hydrolysis rates. All cost around £130-£260 (SRC, Pers. Comm. 1995).

Two numeric databases that should prove extremely useful when they have been released are the aquatic toxicity database produced on diskette by the European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC) and the European Union/OECD database IUCLID (The International Chemicals Information Database). The ECETOC database is currently available in text format and contains quality assessed ecotoxicity data for over 2,000 chemicals. A 'non-confidential' version of IUCLID will be available on CD-ROM and will contain data relating to substance identification, physico-chemical properties, ecotoxicity, mammalian toxicity, occupational safety and production volumes of existing chemicals. The non-confidential version will have manufacturers data removed from the system before release (M.Thomas, DoE, Pers. Comm. 1995).

In addition to the above, the TAPS Environmental Toxicology Unit has access to CHEMDATA produced by the AEA National Chemical Emergency Centre at Culham, Oxon. This database currently contains information on emergency procedures in case of spillages, fires, etc, First Aid and occupational safety information. Furthermore, a project has been initiated by NRA and NCEC

to incorporate ecotoxicity profiles for priority substances onto the system.

The only trialed numeric database that was found not to be of much practical use was EINECS-plus (produced on CD-ROM by SilverPlatter). This database contains substance identification information for over 100,000 chemicals listed on the European inventories of existing and new substances (EINECS and ELINCS). However, only CAS numbers and IUPAC names tend to be given for the majority of chemicals, with no other relevant information.

#### Specific text databases:

The text databases trialed are likely to be of less use than the numeric databases as the abstracts provided did not usually contain the level of detail required. Furthermore, the text databases were usually very broad in content, covering a variety of environmental topics, of which substance identification, fate/behaviour and ecotoxicity only contributed a small fraction to the whole. In addition, acquisition of more than one or two of these databases is probably not cost-effective as there is likely to be a considerable amount of overlap with regard to identical records being covered on the different products. However, of the trialed systems POLTOX (Volumes I-III) and Aquatic Sciences and Fisheries Abstracts (ASFA) produced on CD-ROM by SilverPlatter contained the most records relating to substance identification, ecotoxicity and fate/behaviour in the environment. The costs of these products are £1,265, £721, £938 and £2,627, respectively (SilverPlatter, Pers. Comm. 1995).

In addition to the above, trials were conducted on the OECD database EXICHEM (free to OECD member countries). While this database (in diskette format) does not give environmental data per se, it gives details of work (with contacts) currently underway in OECD countries on existing chemical substances.

#### 3.2 ON-LINE SYSTEMS

#### 3.2.1 Introduction

Much of the information held on CD-ROM products outlined above is also available through connection to on-line 'hosts' via telecommunication networks. Hosts' are computers that contain a variety of databases or 'files' that can be searched from a remote PC or terminal. In order to do this a modem (Hayes or compatible) is required to enable the remote PC to communicate with the host computer via British Telecom (GNS Dialplus) or Mercury telephone lines. Alternatively, connection can be made via the Internet. The use of the Internet has several distinct advantages, including access to various environmental bulletin boards (e.g. HMIPs board) and global communication facilities to other scientists and regulators. If using a PC some communications software is also required. For example, STN EXPRESS, the software produced by The Scientific and Technical Information Network (STN), not only allows communication with the modem but also offers a range of features, including easier searching and viewing facilities (similar to those offered by CD-ROM software such as WINSpirs), downloading/printing facilities and extensive Help facilities. Microsoft Windows is required to operate STN EXPRESS and similar communications packages.

#### 3.2.2 The trials

For the purposes of this review, no on-line databases have been trialed due to the lack of facilities. However, the author has experience in searching several databases on all the main hosts. In addition, contact has been made with the following hosts for details of current databases and prices:

The Scientific and Technical Information Network (STN), Chemical Information Systems (CIS), DIALOG, DATASTAR, QUESTEL-ORBIT and the European Space Agency Information Retrieval Service (ESA-IRS).

#### Advantages:

The main advantage of on-line databases is their extensive coverage. Since the information contained on the majority of CD-ROM products are subsets taken from on-line databases, the on-line user has access to the same information as held on CD-ROM with the added advantage of additional material (some products only contain a few years worth of records) and other databases held on the host. Furthermore, the user does not (usually) need to make an annual subscription in order to receive updates, as on-line databases are updated as a continuous process. Many databases held by an on-line host can be searched simultaneously increasing the number of relevant records retrieved. The problem of information overlap encountered when searching multiple text databases on CD-ROM, is avoided when conducting such 'multi-file' searches on-line by the use of powerful 'duplicate remove' commands.

In order to use on-line databases effectively some basic knowledge of Boolean Logic is required (i.e. AND, NOT, OR, etc), although this is easily acquired and many training courses are held to instruct users in the more advanced techniques. In addition, all the main on-line hosts operate Help Desks in the UK that can quickly be contacted for further assistance, an option that is not usually available when using CD-ROM packages.

#### Disadvantages:

There appear to be few disadvantages in the use of on-line systems. An obvious one is a failure in the telecommunications link which can happen from time to time. However, this is rarely a problem and when it does occur, is not persistent. In addition the display of information retrieved on-line is not always as clear as when using CD-ROM, although the use of communications packages such as STN EXPRESS overcomes this problem.

#### Costs:

The cost of using on-line databases varies from host to host. Some, although not all, charge an annual subscription fee (around £30-£200), a connect fee (around £13-£130/hour), a display fee (usually up to £0.7/record) and sometimes search term costs (approximately £0.07/term). A 'typical' search on STN Chemical Abstracts and CIS AQUIRE for the toxicity of a particular substance to aquatic organisms might be around £60 and £20, respectively. Additional costs include start up fees (around £20), documentation (around £30), software (STN EXPRESS is

£160), connection to BT, Mercury or Internet (BT GNS Dialplus is £60 plus £5/month and around £2/hour of usage) and the cost of a modem (around £300-£500).

#### Specific on-line numeric databases:

There are many thousands of on-line databases. Those relevant for the acquisition of environmental data are given in Appendix A. As outlined in Section 3.1.2, the numeric databases are likely to be of more immediate use than the text systems, although on-line text databases are likely to be more useful than their CD-ROM counterparts, due to the much wider coverage on-line.

The most useful numeric databases are STN REGISTRY for substance identification, CIS ENVIROFATE and STN BEILSTEIN for physico-chemical properties and environmental transformation rates and CIS AQUIRE for aquatic toxicity data. Other useful numeric databases supplying similar information are HSDB, OHM-TADS and CHRIS, all of which are accessed via CIS (see Appendix A for full details). The Syracuse Environmental Fate Databases mentioned in Section 3.1.2 can be accessed via TDS NUMERICA, although details of this host were not received.

#### Specific on-line text databases:

By far the most useful text database is Chemical Abstracts which can be accessed via several hosts. This database contains over 12 million records on all areas of chemical science, including chemical toxicity and fate/behaviour in the environment. In addition, it covers the majority of journals that are included in other useful text databases such as Pollution Abstracts and Aquatic Sciences and Fisheries Abstracts, although all can be searched simultaneously and duplicates removed as already described.

#### Comparison of hosts:

There is some overlap regarding databases covered by different hosts. For example, Chemical Abstracts can be found on STN, DIALOG, ESA-IRS and Orbit. However, only STN is licensed to print the full abstract of each record, while the other hosts are only permitted to provide the user with the bibliographic portion of the record (i.e. Journal, title, author, etc). Furthermore STN is also one of the less expensive options when using this database. For example, the connect fee for STN Chemical Abstracts is £19 as compared to the £80 for connection through DIALOG.

It is therefore apparent that some on-line hosts are more cost-effective and supply more information than others. Experience has shown STN to be a good source for both text and numeric databases, while CIS is particularly useful for the acquisition of quality assessed data from numeric databases.

#### 3.3 SUMMARY OF TRIAL EXERCISES

The above trials and investigations have shown that CD-ROM is a very convenient way of accessing information, very easy to use and requires little additional software or hardware.

However, the products can be expensive, with the majority costing around £600-£2,600 for an annual subscription, and require frequent updates leading to cumbersome piles of backlog CDs.

On-line databases require some additional equipment (e.g. communications software, modem, etc) but their use is not as expensive as purchase of CD-ROM products. Experience has shown that a typical search on STN Chemical Abstracts and CIS AQUIRE for aquatic toxicity data might be around £60 and £20, respectively. Furthermore the user need not worry about updates as this is a continuous process to on-line systems. Some knowledge of Boolean Logic is required to use on-line databases, although basic search techniques are quickly learnt. The searching of multifile text databases is also more efficient on-line as duplicates are more easily identified and removed.

Of the trialed databases it is apparent that the numeric type will be of more immediate use to the TAPS Environmental Toxicology Unit, as they quickly provide the necessary data for environmental hazard/risk assessments of chemicals. The best of this group include AQUIRE (diskette/on-line), ECDIN (CD-ROM/on-line), EFDs (diskettes/on-line), CHEMBANK (CD-ROM/on-line), REGISTRY (on-line) and BEILSTEIN (on-line). Abstracts of published scientific papers contained within text databases do not usually contain the level of detail required and so the original document must usually be obtained (£4-£6 from The British Library, 1-2 weeks delay). However, some such databases have a very large number of records and so can still be of use if time constraints are not an issue. For example, the best of this group, Chemical Abstracts (on-line) contains over 12 million records. These text databases are more effectively used on-line due to the larger number of records available through host systems.

It is apparent that some on-line hosts are more cost-effective and supply more information than others. Experience has shown STN to be a good source for both text and numeric databases. It is less expensive than its largest rival DIALOG and is the only host permitted to display abstracts from the Chemical Abstracts file. CIS is particularly useful for the acquisition of quality assessed data from numeric databases.

## 4. OTHER SOURCES OF ENVIRONMENTAL DATA/INFORMATION

Sources of information other than computer databases can be divided into printed texts and external services.

#### 4.1 PRINTED TEXTS

Printed texts (and microfiche records) can be divided into three categories; books, reports and journals. Useful book sources are those that contain substance profiles which give details of substance identification, physico-chemical properties, ecotoxicology and other useful environmental data on a selected group of chemicals. Various examples are given in Appendix D, although some important ones include The Dictionary of Substances and their Effects (DOSE), The Handbook of Environmental Data on Organic Chemicals, The Handbook of Environmental Fate and Exposure Data (Volumes IV), and The Pesticide Manual (incorporating The Agrochemicals Handbook).

Published reports and reviews on the effects of chemicals in the environment are generally produced by regulatory and other scientific bodies such as the Water Research Centre (WRc), the Department of the Environment (DoE), the National Rivers Authority (NRA), the United States Environmental Protection Agency (USEPA), the Canadian Council of Ministers for the Environment (CCME), the World Health Organisation (WHO), etc. These usually take the form of a 'position document' reviewing all available literature on a specific substance or group of substances (see Appendix D for full details of some examples). However, such reviews only exist for substances of particular environmental concern and are unlikely to be available for more obscure chemicals due to the paucity of published information.

Scientific journals are more useful as a means of maintaining current awareness than as a ready source of environmental data, unless journal papers are being searched via a computerised indexing system (e.g. on-line text databases) using appropriate search terms.

#### 4.2 EXTERNAL INFORMATION SERVICES

Several organisations exist (other than the TAPS Environmental Toxicology Unit) that are able to provide environmental data and advice. Most organisations provide information during working hours and the time taken to produce such information can vary from a few minutes to several weeks, depending on the urgency and nature of the enquiry.

For many years NRA relied on WRc's Environmental Toxicology Advisory Service (ETAS) for the provision of quality information and advice. WRc still offer this service to NRA through their newly created National Centre for Environmental Toxicology. However, as outlined in the introduction to this review, the TAPS Environmental Toxicology Unit is now the main group for the provision of more routine data and advice to operational staff throughout the regions.

A relatively new service that WRc offers in addition to ETAS is SARTOX. This service provides estimated physico-chemical values, environmental transformation rates and toxicity data, based

on chemical structures and properties.

Another information service that the Environmental Toxicology Unit has recently made use of, is that provided by Zeneca's Environmental Laboratory in Brixham, Devon. This service uses on-line databases such as CIS AQUIRE in order to meet the requirements of its clients.

Other services are provided by the United Nations Environment Program (UNEP), the Freshwater Biological Association (FBA) and the Institute of Freshwater Ecology (IFE). Full details of all the above services are given in Appendix E.

### 5. DISCUSSION AND RECOMMENDATIONS

#### 5.1 GENERAL PROJECT DISCUSSION

The NRA has a requirement for environmental data to support certain operational activities, such as consent setting, catchment planning and managing pollution incidents. One of the roles of the Environmental Toxicology Unit of the National Centre for Toxic and Persistent Substances (TAPS) is to advise operational staff throughout the regions on the environmental hazard/risk of chemical substances. In order to do this effectively, access is required to quality assessed environmental data. The aim of this review was therefore to identify and critically assess information sources in computer and text format, that primarily provide data relating to substance identification, ecotoxicity and fate/behaviour in the environment. Recommendations for the acquisition of certain data sources have been made on the basis of these exercises.

Computer databases can be divided into two types; numeric and text. Numeric databases contain actual data (sometimes quality assessed, although not always) extracted from original documents, while text databases consist of bibliographic records which sometimes include the abstracts of published papers. Due to the nature of the work carried out by the Environmental Toxicology Unit, numeric databases are likely to be of more immediate use as they quickly provide the data necessary for assessing the environmental hazard/risk of chemicals. Text databases are likely to be less useful in the short term as abstracts rarely provide the level of detail required and acquisition of original documents will usually be necessary (can take from 1-2 weeks through the British Library). However, due to the large number of records on text databases they are a good information source if a comprehensive search of all available literature is required and time is not a limiting factor. Otherwise, they can be used to support data obtained from numeric databases.

Computer databases can be accessed on-line via telecommunication networks or through the use of CD-ROM/diskettes. In order to assess which approach is likely to be of most practical use, trials have been conducted on a variety of numeric and text databases available in both formats. The trials revealed that the only real advantage of CD-ROM is its ease of use and clarity of display (particularly true when used in a Windows environment). However, CD-ROM products tend to be relatively expensive, with most on the market priced between £600 and £2,600 (Biological Abstracts is £21,634) for just one years subscription. In other words, if the user does not continue to subscribe, updates in the form of additional CD's will not be received. For this reason, CD-ROM/diskette formats are most practical for the use of infrequently updated numeric databases (e.g. the USEPA aquatic toxicity database, AQUIRE), particularly if it is essential that access to the database is always guaranteed (occasionally not the case when on-line).

The main advantage of connection to on-line hosts is the extensive collection of databases available to the user at a relatively low cost. Experience has shown that a typical search on STN Chemical Abstracts and CIS AQUIRE for aquatic toxicity data on a single chemical might be around £60 and £20, respectively. Much of the information contained on CD-ROM, particularly within text databases, are subsets taken from their much larger on-line counterparts (e.g Chemical Abstracts on-line through STN contains over 12 million records). The on-line user therefore has access to all the information held on CD-ROM and more, without the concern over acquisition of updates. Some additional equipment is required to go on-line (e.g. communications software, modem, etc), although this is relatively inexpensive. In addition, some communications software

such as STN Express makes connection, searching and viewing as easy as when utilising CD-ROM search software.

Accessing environmental data through on-line hosts is therefore generally preferable to using CD-ROM/diskettes, especially for bibliographic text databases. However, utilising numeric databases on CD-ROM/diskette can be practical as these formats provide a source of data that can be searched rapidly and are completely portable.

Sources of environmental information other than computer databases consist of printed texts and external services. Useful text sources include reference books, reports and journal papers that contain data relating to substance identification, ecotoxicity and fate/behaviour in the environment. The most useful external information service available is that offered by WRc. However, since the TAPS Environmental Toxicology Unit is the main group for the provision of more routine data and advice to operational staff throughout the regions, WRc is now generally contacted only when enquiries cannot be dealt with internally.

#### 5.2 DISCUSSION AND RECOMMENDATIONS

In order to effectively fulfil it's role as an information and advisory centre, the TAPS Environmental Toxicology Unit requires access to good quality data sources. The aim of this review has been to address this issue and to make recommendations for the acquisition of certain sources.

At the most basic level, this entails acquiring the more useful reference text books that contain substance identification, physico-chemical properties, ecotoxicity and environmental fate/behaviour information. The Environmental Toxicology Unit already has access to, among others, the following important sources; The Dictionary of Substances and their Effects (DOSE), The Handbook of Environmental Data on Organic Chemicals, The Handbook of Environmental Fate and Exposure Data (Volumes I-IV), The Pesticide Manual (incorporating the Agrochemicals Handbook) and the Merck Index.

Useful reports and reviews include the Environmental Hazard Assessments produced by the Building Research Establishment (BRE) for the Department of the Environment (DoE), Environmental Quality Standard (EQS) reports produced by WRc, Environmental Health Criteria (EHC) documents produced by the World Health Organisation (WHO) and technical reports produced by the European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC). The Environmental Toxicology Unit routinely receives the former two as soon as current reports are produced, while only a selection of useful EHC documents have been acquired. It is therefore recommended that the most up to date EHC publication list is reviewed and useful reports (around £5-£15) ordered from Her Majesty's Stationary Office (HMSO). Furthermore, the ECETOC publication list should be scanned for useful technical reports. These can be ordered at a cost of BF2,000, but are free to members. It may therefore be advantageous for NRA to join this important organisation. Details of membership are currently being pursued.

In addition to the above, regulatory bodies such as the United States Environmental Protection Agency (USEPA) and the Canadian Council for Ministers of the Environment (CCME) produce useful ecotoxicity reviews, Water Quality Criteria documents and other reports relating to

large number of numeric and text databases that the user can search simultaneously. To subscribe to CIS there is an annual subscription fee of £200 and the use of AQUIRE is charged at a rate of £50/hour. The main advantage of connection to this host is that the user has access to other databases that would be otherwise unavailable. For example, CIS also hosts the database ENVIROFATE (£50/hour), that contains experimental data extracted from quality assessed studies measuring physico-chemical properties and environmental degradation rates. In addition, CIS also hosts the databases that make up the CD CHEMBANK, thus making expensive annual subscriptions for this product unnecessary.

As well as connection to CIS, it is also recommended that connection is made to STN (no annual subscription fee) and that the communications software STN Express (£160) is purchased (this is also compatible with CIS). Connection to this host would not only provide access to the massive identification and physico-chemical property numeric databases, REGISTRY and BEILSTEIN, but also to Chemical Abstracts, probably the most useful chemical text database available on-line. Furthermore, access to all the major databases from which information is taken to produce the most useful CD-ROM products, would also be available (e.g. Pollution Abstracts, Aquatic Sciences and Fisheries Abstracts, etc), without the concern over acquisition of updates (this is a continuous process on-line).

The use of some databases through STN appears to be cheaper than through its closest rival, DIALOG. For example, the connect fee for STN Chemical Abstracts is £19/hour (a typical search for aquatic toxicity data on a single chemical might be around £60, including all display and search costs) as compared to the £80 just for connection on DIALOG. In addition, only STN is licensed to print the full abstract of each record, while the other hosts are only permitted to provide the user with the bibliographic portion of the record (i.e. Journal, title, author, etc). In any case, the Library at NRA Head Office in Bristol already has access to the main competitors of STN, namely DIALOG, DATASTAR, ORBIT and ESA/IRS, but not STN itself (or CIS).

Many of the above databases and other software packages can be used from either Windows or DOS platforms. However, some (e.g. STN Express) operate in a Windows environment only, and besides, Windows makes the use of these systems considerably more user-friendly. It is therefore strongly recommended that the Environmental Toxicology Unit maintains and enhances its current Windows capabilities.

#### 5.3 SUMMARY OF RECOMMENDATIONS

The recommendations made in Section 5.2 for the acquisition of certain data sources can be summarised as follows. The list does not include those useful sources that the Environmental Toxicology Unit already has access to or has recently acquired as a result of this review (e.g. ECDIN and AQUIRE on CD-ROM/diskette).

1. Obtain the necessary equipment to access on-line hosts. This will include a modern (£300-£500), communications software (£100-£200) and connection to British Telecom GNS Dialplus (£60 plus £5/month and around £2/hour of usage). Alternatively, connection could be made via the Internet. This route would allow the user to search environmental bulletin boards and to communicate globally with other regulators and scientists.

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Migh

- Purchase the communication software, STN Express (£160) and subscribe to The Scientific and Technical Information Network (STN) in order to allow access the following on-line databases; REGISTRY, BEILSTEIN, Hazardous Substances Databank, Chemical Abstracts and many other systems. Full details on the content of these databases are given in Appendix A.
- Subscribe to Chemical Information Systems (CIS) (£200/annum) in order to allow access the following on-line databases; AQUIRE, ENVIROFATE, ISHOW, OHM-TADS, CHRIS and CESARS (all charged at a rate of £50/hour). Full details on the content of these databases are given in Appendix A.
- Obtain the following environmental fate databases and estimation programs produced on diskette by Syracuse Research Corporation; CHEMFATE (£1,000), BIODEG (£330), CHEMBASE (£500), LOGKOW (£400), WS/KOW (£470/£70), HENRYS LAW CONSTANT PROGRAM (£270), BIODEGRADATION PROBABILITY PROGRAM (£270), PC-HYDRO (£30), PC-KOC (£30), DATABASE OF SMILES NOTATIONS (£200/£70) and EPI INTERFACE (£130). Full details of these systems are given in Appendix B1.1.3.
  - 5. Purchase other CD-ROM/diskette products as seem necessary in line with the on-going work of the TAPS Environmental Toxicology Unit.

### REFERENCES

Baker, M.G.C., Rogers, H.R., Johnson, C., Fawell, J.K. and Wright, K. (1991) Fate and behaviour of contaminants in the aquatic environment: A review of the sources of information, NRA R&D Note 12. WRc Report No. NR2726.

Richardson, M. (1986) Retrieval of data. In: *Toxic hazard assessment of chemicals*. pp15-48. Edited by Mervyn Richardson, The Royal Society of Chemistry.

Young-Marcaccio, K. (Ed.) (1994a) Gale directory of databases. Volume I. On-line databases. Gale Research Inc. Detroit, US.

Young-Marcaccio, K. (Ed.) (1994b) Gale directory of databases. Volume II. CD-ROM, diskette, magnetic tape, handheld and batch access database products. Gale Research Inc. Detroit, US.

# APPENDIX A ENVIRONMENTALDATABASESAVAILABLE THROUGH ON-LINE HOSTS

It is not practical to list all databases that are available through on-line hosts since they number in their thousands. Instead, details are given of selected systems (broadly listed in order of potential usefulness) considered to be of most relevance to staff involved in pollution control. The accuracy of the figures quoted are approximately correct at the time of writing (March 1995) but depend largely on the source from which they are taken. However, it should be noted that most databases are updated relatively frequently. For example, an additional 2 million records were added to the 'Chemical Abstracts' database between 1991 and 1994.

Those databases that are also available on CD-ROM/diskette are crossed referenced to Appendix B.

In referring to the records contained in Appendix A, the following abbreviations apply:

SF - Subscription fee per year

ST - Search fee per term

DF - Display fee per record

CF - Connect fee per hour

Where one of these charges is not indicated, the fee does not apply.

#### A1 NUMERIC DATABASES

#### A1.1 SPECIFIC NUMERIC DATABASES

These databases give numeric values that relate to a specific environmental topic area. For example, the database AQUIRE gives numeric values relating to the toxicity of pollutants to aquatic organisms.

#### A1.1.1 Substance identification

Substance identification is also broadly given in other categories of database

Name: REGISTRY

Produced by: Chemical Abstracts Service (CAS)
Contact: See STN contact (Appendix C)

Content: Chemical names, CAS numbers, synonyms and structures.

Can be used with CA (see Section A2)

Quality assessment: No

Number of substances: 16 million
Number of records: 16 million
Time span: 1957 to date

Updates: Weekly (8,000-14,000 records)

On-line availability: STN (CF £19, ST £16.80-30.50, up to DF £3.11)

Alternative formats: Not applicable Reference: STN (Pers. Comm.)

#### A1.1.2 Physico-chemical properties

Name: BEILSTEIN

Produced by: Beilstein Information Systems, Germany

Contact: See STN contact (Appendix C)

Content: Substance identification, structures and Physico-chemical

properties

Quality assessment: No

Number of substances:
Number of records:
Continue span:
Not known
6.2 million
1779-1993
Updates:
Periodically

On-line availability: STN (CF £35, ST £1.95, DF £3.51), DIALOG (SF £30,

CF £147, DF £7.5-£40)

Alternative formats: Excerpts on CD-ROM (see Appendix B) and

as a printed handbook

Reference: STN, DIALOG (Pers. Comm.)

Information System for Hazardous Substances in Water

(ISHOW)

Produced by:

USEPA

Contact:

Tel: 0101(202)260-4610 (producer)

Content:
Quality assessment:

Physico-chemical properties (Annex)

Number of substances:
Number of records:

5,400 5,400

Time span: Updates:

1970-1983 Periodically

On-line availability:

CIS (SF £200, CF £50)

Alternative formats:

Not applicable

Reference:

CIS (Pers. Comm.), Young-Marcaccio (1994a)

Name:

**CHEMEST** 

Produced by: Contact:

Technical Database Service (TDS)
Tel: 0101(212)245-0044 (producer)

Content:

Fax: 0101(212)247-0587 (producer)
Physico-chemical properties for use in environmental risk

assessment

Quality assessment: Number of substances:

Not known Not known

Number of records: Time span: Updates:

Not known
Periodically as data become available

On-line availability:

TDS (SF £100, CF £100)

Alternative formats:

Not applicable

Reference:

Young-Marcaccio (1994a)

#### A1.1.3 Environmental fate and behaviour of substances

Name:

**Environmental Fate (ENVIROFATE)** 

Produced by:

USEPA

Contact:

Tel: 0101(202)260-3810 (producer)

Content:

Physico-chemical properties and environmental transformation rates extracted from published literature

(see Annex)

Quality assessment:

Yes 800

Number of substances:

15,000

Number of records: Time span:

1970-1991 Periodically

Updates:
On-line availability:

CIS (SF £200, CF £50)

Alternative formats:

Not applicable

Reference:

CIS (Pers. Comm. 1995), Young-Marcaccio (1994a)

Produced by:

Contact:

Environmental Fate Databases

Syracuse Research Corporation (SRC) Tel: 0101(315)426-3200 (producer)

Fax: 0101(315)426-3429 (producer) Content: Four inter-related files that provide physico-chemical

properties and environmental transformation rates (see

Annex)

Quality assessment: Yes

Number of substances: up to 13,800 Number of records: up to 218,000 Time span: Not known

**Updates:** Quarterly On-line availability: TDS (SF £17, CF £100)

Alternative formats: Diskette (see Appendix B) Reference: Syracuse (Pers. Comm. 1995), Young-Marcaccio (1994a)

#### A1.1.4 Ecotoxicology of chemical substances

Name: Aquatic Information Retrieval (AQUIRE) Produced by: **USEPA/Computer Science Corporation** 

Contact: Tel: 0101(218)722-0075 (producer)

Content: Data extracted from aquatic toxicity studies (see Annex)

Quality assessment: Yes Number of substances: 5,600 Number of records: 114,000 Time span: 1970-1992

**Updates:** Approximately every 2 years

On-line availability: CIS (SF £200, CF £50) TDS (SF £170, CF £113)

Alternative formats: Diskette (see Appendix B)

Reference: CIS (Pers. Comm. 1995), Young-Marcaccio (1994a)

#### A1.2 GENERAL NUMERIC DATABASES

Each of these databases give numeric values that relate to various topic areas concerning chemical pollutants and environmental protection. For example, the database CHRIS gives details of chemical names, synonyms, physico-chemical properties and biological/fire hazard potential.

Name: Environmental Chemicals Data Network (ECDIN) Produced by: Commission of the European Communities (CEC)

Contact: Tel: Italy 0332 789720 (producer) Fax: Italy 0332 789963 (producer)

Content: Substance identification,

Physico-chemical properties, ecotoxicity, production,

legislation

Quality assessment: Yes Number of substances: 122,400 Number of records: 122,400 Time span: 1970 to date

Updates: Periodically as data become available On-line availability:

Alternative formats: CD-ROM (see Appendix B)

Reference: CEC (Pers. Comm. 1995), Young-Marcaccio (1994a)

Name: Hazardous Substances Databank (HSDB) Produced by: US National Library of Medicine (NLM)

Contact: Tel: 0101(301)496-1131 (producer)

Content: Substance identification,

Physico-chemical properties, ecotoxicity, environmental fate and behaviour, safety and handling, legislation and

analytical methods

Quality assessment: Not known Number of substances: 4,400 Number of records: 4,400

Time span: Current information

Updates: As required

On-line availability: STN (CF £16, ST £0.08, DF £0.11),

DATA-STAR (SF sFR 80, CF sFR 1.32/min, DF sFR 0.8),

DIMDI

Alternative formats: CHEMBANK on CD-ROM (see Appendix B)

Reference: DATA-STAR, STN (Pers. Comm. 1995), Young-

Marcaccio (1994a)

Name: European Directory of Agrochemical Products

Produced by:

Royal Society of Chemistry

Tel: (01223) 420066 (producer)

Fax: (01223) 423623 (producer)

Content: Substance identification,

Physico-chemical, toxicity, production and analytical data

Quality assessment:

Number of substances:

Number of records:

Time span:

Updates:

Not known
26,000
26,000
1984 to date
Biannual

On-line availability: DIALOG (SF £30, CF £160, DF £3.70)

Alternative formats:

Reference: RSC (Pers. Comm. 1995), Young-Marcaccio (1994a)

Name: Oil and Hazardous Materials Technical Assistance Data

System (OHM-TADS)

Produced by: USEPA

Contact: Tel: 0101(202)260-4610 (producer)

Content: Substance identification,

Physico-chemical and toxicological properties for use in

hazard assessment

Quality assessment:YesNumber of substances:1,402Number of records:1,402

Time span: 1950 to date

Updates: Periodically as data become available

On-line availability: CIS (SF £200, CF £50)

Alternative formats: On CHEMBANK CD-ROM (see Appendix B)
Reference: CIS (Pers. Comm. 1995), Young-Marcaccio (1994a)

Name: Chemical Hazards Response Information System (CHRIS)

Produced by: US Coast Guard

Contact: Tel: 0101(202)267-2611 (producer)
Fax: 0101(202)247-4085 (producer)

Content: Substance identification

Physico-chemical properties and biological/fire hazard

potential for use in spill situations (see Annex)

Quality assessment:Not knownNumber of substances:1,210Number of records:1,210Time span:Not known

Updates: Periodically as data become available

On-line availability: CIS (SF £200, CF £50)

Alternative formats: On CHEMBANK CD-ROM (see Appendix B)

Reference: CIS (Pers. Comm. 1995), Young-Marcaccio (1994a)

Produced by:

Registry of Toxic Effects of Chemicals (RTECS)

National Institute for Occupational Safety and Health,

USA

No

Contact:

Content:

See STN contact (Appendix C)

Chemical names, CAS numbers, synonyms and mammalian

toxicology/human health information

Quality assessment: Number of substances:

Number of records:

Time span: **Updates:** 

On-line availability:

Alternative formats:

Reference:

300,000 1986 to date

120,000

Quarterly

STN (SF £31, ST £0.13, DF £1.22), DIALOG (SF £30, CF £40, DF £0.4)

On CHEMBANK CD-ROM (see Appendix B)

STN, DIALOG (Pers. Comm.)

Name:

Chemical Evaluation Search and Retrieval System

(CESARS)

Produced by:

Contact:

Michigan State Dept. of Natural Resources Tel: 0101(517)373-2190 (producer)

Fax: 0101(517)373-9958 (producer)

Content:

Substance identification,

Physico-chemical and toxicological data extracted from

literature (see Annex)

Quality assessment: Number of substances:

Number of records:

Time span:

**Updates:** 

On-line availability:

Alternative formats:

Reference:

Yes 370

370 (up to 120 items in each record)

1962 to date

Periodically as data become available

CIS (SF £200, CF £50)

Not applicable

CIS (Pers. Comm. 1995), Young-Marcaccio (1994a)

Produced by: Contact:

Content:

Quality assessment:

Number of substances:

Number of records: Time span: Updates:

On-line availability: Alternative formats:

Reference:

MRCK

National Inst. for Occupational Safety and Health (US)

Tel: See CIS contact

Fax: See CIS contact
Substance identification,

Physico-chemical and mammalian toxicological data.

Corresponds to printed Merck index

No >10,200 >10,200

Not known
Twice per year

CIS (SF £200, CF £60), ORBIT (CF £43, DF £0.46)

Not applicable

CIS, ORBIT (Pers. Comm. 1995)

#### A2 TEXT DATABASES

These databases contain information relating to substance identification, ecotoxicity and fate/behaviour of chemicals in the environment, often as part of a broader subject coverage as a whole. Environmental data is sometimes available within a bibliographic or abstract record, although it is often necessary to acquire the original document.

Name:

Produced by: Contact:

Content:

Quality assessment:

Number of substances:

Number of records: Time span:

Updates:

On-line availability:

Alternative formats:

Reference:

Chemical Abstracts (CA)

Chemical Abstracts Service (CAS)
See STN contact (Appendix C)

Abstracts from world literature on all areas of chemistry, including environmental fate/behaviour and ecotoxicology

(see Annex)

No

Not applicable >12 million

1967 to date

Biweekly (20,000 records)

STN (CF £19, ST £0.06, DF £1), DIALOG (SF £30, CF

£80, DF £0.80),

ESA-IRS (CF £11.54, DF £0.96), Orbit (CF £10) CD-ROM as CASurveyor (see Appendix B) DIALOG, STN, ESA-IRS (Pers. Comm. 1995)

Name:

Produced by: Contact:

Content:

Quality assessment:

Number of substances: Number of records:

Time span:

Updates:

On-line availability:

Alternative formats:

Reference:

CAOLD

Chemical Abstracts Service (CAS)
See STN contact (Appendix C)

Abstracts from world literature on all areas of chemistry, including environmental fate/behaviour and ecotoxicology

No

Not applicable

695,000 1957-1967

Not applicable

STN (CF £19, ST £0.06, DF £1)

STN (Pers. Comm. 1995)

Produced by: Contact:

Content:

**CAPREVIEWS** 

Chemical Abstracts Service (CAS) See STN contact (Appendix C)

Current awareness. Abstracts from world literature on all areas of chemistry, including environmental fate/behaviour

and ecotoxicology. Will ultimately be on CA

Quality assessment:

Number of substances:

Number of records:

Time span: Updates:

On-line availability:

Alternative formats:

Reference:

Not applicable

100,000 Current

No

Daily

STN (CF £19, ST £0.06, DF £1)

STN (Pers. Comm. 1995)

Name:

Produced by: Contact:

Content:

Quality assessment:

Number of substances: Number of records:

Time span:

**Updates:** 

On-line availability:

Alternative formats:

Reference:

Pollution Abstracts

Cambridge Scientific Abstracts (CSA) Tel: 0101(301)961-6750 (producer) Fax: 0101(301)961-6720 (producer)

Abstracts from world literature on environmental

pollution, including effects and control

No

Not applicable 195,000 1970 to date

Monthly (1,200 records)

STN (CF £57, ST £0.06, DF £0.53), DIALOG (SF £30,

CF £40, DF £0.75),

ESA-IRS (CF £7.76, DF £1.09)

POLTOX I-III on CD-ROM (see Appendix B)

DIALOG, STN, ESA-IRS (Pers. Comm. 1995), Young-

Marcaccio (1994a)

Produced by:

Contact:

Content:

Quality assessment: Number of substances: Number of records:

Time span: Updates:

On-line availability:

Alternative formats:

Reference:

Produced by:

Contact:

Content:

Aquatic Sciences and Fisheries Abstracts (ASFA)

United Nations Food and Agriculture Organisation (FAO)

Tel: 010 06 57971 (producer) Fax: 010 06 57973152 (producer)

Abstracts from world literature on management of aquatic resources, ecology, biology and pollution (see Annex).

No

Not applicable

475,000 1978 to date Monthly

STN (CF £57, ST £0.06, DF £0.53), DIALOG (SF £30,

CF £60, DF £0.6).

ESA-IRS (CF £7.76, DF £1.09), DIMDI, CAN-OLE.

CD-ROM (see Appendix B)

DIALOG, STN, ESA-IRS (Pers. Comm. 1995), Young-

Marcaccio (1994a)

Name: **BIOSIS Previews** 

BIOSIS, US

Tel: See STN contact (Appendix C)

Abstracts from world literature on all areas of biology

including toxicology and pollution

Quality assessment:

Number of substances: Number of records:

Time span: **Updates:** 

Not applicable

9.3 million 1964 to date

Weekly

On-line availability: STN (CF £61, DF £0.52), DIALOG (SF £30, CF £40, DF

£0.75), ESA-IRS (CF £11.14, DF £1.09), DIMDI, CAN-

OLE.

Alternative formats: Biological Abstracts on CD-ROM (see

Appendix B)

Reference: DIALOG, STN, ESA-IRS (Pers. Comm. 1995)

Produced by:

Contact:

Content:

Quality assessment:

Number of substances: Number of records:

Time span: **Updates:** 

On-line availability:

Alternative formats:

Reference:

LIFESCI

Cambridge Scientific Abstracts (CSA)

See STN contact (Appendix C)

Abstracts from world literature on biology, medicine,

ecology and some aspects of agriculture

No

Not applicable

1.3 million

1978 to date

Monthly

STN (CF £50, ST £0.06, DF £0.44)

CD-ROM (see Appendix B) STN (Pers. Comm. 1995)

Name:

Produced by:

Contact:

Content:

Quality assessment:

Number of substances:

Number of records:

Time span:

**Updates:** 

On-line availability:

Alternative formats:

Reference:

JICST-E

Japan Information Centre of Science and Technology

See STN contact (Appendix C)

Abstracts from Japanese literature on all areas of

chemistry, including environmental fate/behaviour and

ecotoxicology

No

Not applicable

2.0 million

1985 to date

Biweekly

STN (CF £51, DF £0.34)

STN (Pers. Comm. 1995)

Produced by:

Contact: .

Content:

Quality assessment: Number of substances:

Number of records:

Time span: Updates:

On-line availability:

Alternative formats:

Reference:

Name:

Produced by: Contact:

Content:

Quality assessment:

Number of substances: Number of records:

Time span:

Updates:

On-line availability:

Alternative formats:

Reference:

AQUALINE

WRc plc, UK

Tel: 01793 511711 (producer) Fax: 01793 511712 (producer)

Abstracts from world wide literature. Water treatment and

supply. Waste

water/sewage treatment. Pollution of aquatic environment.

No

Not applicable 170,000

1960 to present

Monthly. 10,000 per year Orbit (CF £60, DF £0.75)

CD-ROM (see Appendix B). Current awareness journals

**Aqualine Abstracts** 

Young-Marcaccio (1994a) and WRc (Pers. Comm. 1994)

Oceanic Abstracts (OA)

Cambridge Scientific Abstracts (CSA) Tel: 0101(301)961-6750 (producer) Fax: 0101(301)961-6720 (producer)

Abstracts from world literature on oceanography. Includes

marine pollution and saltwater ecotoxicity data.

No

Not applicable 190,000 1964 to date

Bimonthly (1,750 records)

STN (CF £57, ST £0.06, DF £0.53), DIALOG (SF £30,

CF £40, DF £1.20),

ESA-IRS (CF £7.76, DF £1.09)

STN, DIALOG, ESA-IRS, (Pers.Comm. 1995), Young-

Marcaccio (1994a)

Produced by:

Contact:

Content:

Quality assessment:

Number of substances:

Number of records: Time span:

Updates:

On-line availability:

Alternative formats:

Reference:

Name:

Produced by: Contact:

Content:

Quality assessment:

Number of substances: Number of records:

Time span: **Updates:** 

On-line availability:

Alternative formats:

Reference:

ENVIROLINE

Congressional Information Services Tel: 0101(301)654-1550 (producer)

Fax: 0101(301)657-3203 (producer)

Abstracts from world literature on environment and management of natural resources, air, water and noise

pollution. Environmental impact of chemicals

No Not applicable

187,000 1975 to date Monthly

DIALOG (SF £30, CF £40, DF £0.50),

ESA-IRS (CF £11.14, DF £0.73), Orbit (SF £100, CF

£75, DF £0.40),

DATA-STAR, DIMDI CD-ROM (see Appendix B)

DIALOG, ESA-IRS, Orbit (Pers. Comm. 1995), Young-

Marcaccio (1994a)

**CONFSCI** 

Cambridge Scientific Abstracts (CSA)

See STN contact (Appendix C)

Abstracts from unpublished research journals presented at conferences on all areas of science, including life sciences

Not applicable 1.4 million

1973 to date Bimonthly

STN (CF £50, ST £0.06, DF £0.44), DIALOG (SF £30,

CF £40, DF £0.40)

STN (Pers. Comm. 1995)

Produced by:

Contact:

Content:

Quality assessment:

Number of substances:

Number of records: Time span:

Updates:

On-line availability: Alternative formats:

Reference:

Name:

Produced by:

Contact:

Content:

Quality assessment:

Number of substances:

Number of records:

Time span: Updates:

On-line availability:

Alternative formats:

Reference:

DISSABS

University Microfilms Inc

See STN contact (Appendix C)

Abstracts from US university dissertations

No

Not applicable

1.3 million

1861 to date

Monthly

STN (CF £58, ST £0.06, DF £0.26)

STN (Pers. Comm. 1995)

**AQUAREF** 

**Environment Canada** 

Tel: (819)953-1531 (producer)

Fax: (819)997-8701 (producer)

Abstracts from Environment Canada documents and world

wide journals. Water resources and pollution

No

Not applicable

83,000

1970 to present

Bimonthly.

CAN/OLE (CF \$Can. 40)

CD-ROM (AQUAREF) (see Appendix B)

Young-Marcaccio (1994a)

# APPENDIX B ENVIRONMENTAL DATABASES AVAILABLE IN CD-ROM/DISKETTE FORMATS

It is not practical to list all databases that are available on CD-ROM/diskette since they number in their thousands. Instead, details are given of selected packages (broadly listed in order of potential usefulness) considered to be of most relevance to staff involved in pollution control. The accuracy of the figures quoted are approximately correct at the time of writing (March 1995) but depend largely on the source from which they are taken. However, it should be noted that most databases are updated relatively frequently.

Those databases that are also available through on-line hosts are crossed referenced to Appendix A.

In referring to the records contained in Appendix B, the following abbreviations apply:

AS - Annual subscription (includes update discs where applicable) NW - Network annual subscription

Where one of these charges is not indicated, the fee does not apply.

### B1 NUMERIC DATABASES

### B1.1 SPECIFIC NUMERIC DATABASES

These databases give numeric values that relate to a specific environmental topic area. For example, the database AQUIRE gives numeric values relating to the toxicity of pollutants to aquatic organisms.

#### B1.1.1 Substance identification

Substance identification is also broadly given in other categories of database

Name: Beilstein Current Facts in Chemistry (CD-ROM)

Produced by: Microinfo

Contact: Tel: 01420 86848 (producer in UK)
Fax: 01420 89889 (producer in UK)

Content: Substance identification, structures and Physico-chemical

properties

Quality assessment: No

Number of substances: >300,000
Number of records: >300,000
Time span:

Time span: 1990 to date Updates: Quarterly Price: AS £2,565

Alternative formats: Print
On-line availability: STN

Reference: SilverPlatter (Pers. Comm. 1995)

Produced by:

Contact:

Content:

EINECS plus-CD (CD-ROM) SilverPlatter Information Inc.

Tel: 0181 995 8242 (producer in UK) Fax: 0101 995 5159 (producer in UK)

Gives details of chemicals on European Inventory of Existing Chemicals (EINECS) and European List of

Notified Chemical Substances (ELINCS). Includes

chemicals names, CAS numbers and formulae

Quality assessment: No

Number of substances: Number of records:

Time span: **Updates:** Price:

Alternative formats: On-line availability:

Reference:

>100,000 >100,000

Current information

Not known

AS £1,014, NW £1,521

SilverPlatter (Pers. Comm. 1995)

## B1.1.2 Physico-chemical properties of substances

Name:

Produced by:

Contact:

Content:

Quality assessment: Number of substances:

Number of records:

Time span: Updates:

Price:

Alternative formats: On-line availability:

Reference:

CHEMBASE Physical Properties Database (Diskette)

Syracuse Research Corporation (SRC)
Tel: 0101 315 426 3429 (producer)
Fax: 0101 315 426 3429 (producer)

Chemical names, structures and physico-chemical properties

Not known 7,000 7,000

Not known Biannually

£500 (£40/update)

Syracuse Research Corporation (Pers. Comm. 1995)

Name:

Produced by:

Contact:

Content:

Quality assessment: Number of substances:

Number of records:

Time span: Updates:

Price:

Alternative formats: On-line availability:

Reference:

**SOLV-DB** (Diskette)

Syracuse Research Corporation (SRC) Tel: 0101 315 426 3429 (producer) Fax: 0101 315 426 3429 (producer)

Common name/synonyms, physico-chemical properties, environmental fate and health/safety implications of

solvents Not known

321 321

Not known Periodically

£170

Syracuse Research Corporation (Pers. Comm. 1995)

Produced by: Contact:

Content:

Quality assessment:
Number of substances:
Number of records:
Time span:
Updates:

Price:
Alternative formats:

On-line availability:

Reference:

CHEMBASE Chemical Pointer File (Diskette)

Syracuse Research Corporation (SRC) Tel: 0101 315 426 3429 (producer) Fax: 0101 315 426 3429 (producer)

Gives details of US legislative lists for selected chemicals.

Also gives chemical structures

Not known 20,000 20,000 Not known Biannually

£2,000 (£200/update)

Syracuse Research Corporation (Pers. Comm. 1995)

### B1.1.3 Environmental fate and behaviour of substances

Name: Environmental Fate/Exposure Databases (EFEDB)

(Diskette)

Produced by: Syracuse Research Corporation (SRC)
Contact: Tel: 0101 315 426 3429 (producer)
Fax: 0101 315 426 3429 (producer)

Content: Four inter-related files that provide physico-chemical properties and environmental transformation rates

DATALOG:

218,000 records on 13,800 chemicals. Indicates location

of fate/exposure data.

CHEMFATE:
Contains numeric physico-chemical properties for 1,700

commercially significant chemicals (see Annex)

BIOLOG:

45,000 records on 6,500 chemicals. Indicates sources of

microbial toxicity and biodegradation data

BIODEG

Contains actual experimental results on biodegradability of

700 chemicals (see Annex)

Quality assessment: Yes
Number of substances: See above

Number of records:

Time span:

Updates:

See above

Not known

Quarterly

Price: DATALOG £1,600 (£330/update)
CHEMFATE £1,000 (£200/update)
BIOLOG £530 (£80/update)

BIODEG £330 (£50/update)
Alternative formats:

On-line availability: TDS (see Appendix A)

Reference: Syracuse Research Corporation (Pers. Comm. 1995)

Produced by: Contact:

Content:

Environmental Fate/Exposure Estimation Programs

(Diskette)

Syracuse Research Corporation (SRC) Tel: 0101 315 426 3429 (producer) Fax: 0101 315 426 3429 (producer)

See Annex for example outputs

LOGKOW:

For estimation of logKow values (£400)

DERMAL:

Estimates dermal absorption of organic compounds (£470)

£70 with LOGKOW)

WS/KOW:

Estimates water solubility from LogKow (£470, £67 with LOGKOW)

ATMOSPHERIC OXIDATION RATE PROGRAM:

Estimates gas-phase reaction rate between organic chemicals and hydroxyl radicals (£267)

MPBPVP:

Estimates melting point, boiling point and vapour pressure of organic compounds (£130)

HENRYS LAW CONSTANT PROGRAM:

Calculates Henry's law constant (£267)

**BIODEGRADATION PROBABILITY PROGRAM:** 

Calculates probability of a chemical biodegrading either rapidly or slowly under aerobic conditions (£267)

PC-HYDRO:

Calculates hydrolysis rates and half-lives for esters, carbamates, halomethanes and alkyl halides (£267)

PC-KOC:

Calculates soil or sediment adsorption coefficient (£267)

**DATABASE OF SMILES NOTATIONS:** 

Contains 29,000 SMILES notations for use with the above programs (£200, £67 with any of the above)

**ESTIMATION PROGRAMS INTERFACE (EPI):** 

Interface that allows easier use of the above programs. Also allows use of the WVOL and STP programs for the estimation of volatilisation rates from water and sewage

treatment plant fugacity, respectively (£130)

Not applicable Not applicable

Not applicable

Not applicable

Not applicable

See above

Alternative formats: On-line availability:

Quality assessment:

Number of records:

Number of substances:

Reference:

Time span:

**Updates:** 

Price:

Syracuse Research Corporation (1995)

# B1.1.4 Ecotoxicology of chemical substances

Name:

Produced by:

Contact:

Content:

Quality assessment: Number of substances:

Number of records: Time span: Updates:

Price:

Alternative formats:

On-line availability:

Reference:

AQUIRE (Diskette)

Spectrum Research Inc.

Tel: 0101 218 525 5322 (producer) Fax: 0101 218 525 6472 (producer)

Data extracted from aquatic toxicity studies (see Annex)

Yes 114,000 5,600 1972-1992 Biannual

'Express' service: AS £730 (£460 per update). 'Normal'

service: AS £1,700 (£146 per update)

CIS (see Appendix A)

Spectrum Research Inc. (Pers. Comm. 1995)

#### B1.2 GENERAL NUMERIC DATABASES

Each of these databases give numeric values that relate to various topic areas concerning chemical pollutants and environmental protection. For example, the database CHRIS gives details of chemical names, synonyms, physico-chemical properties and biological/fire hazard potential.

Name: ECDIN (CD-ROM)
Produced by: Springer Verlag

**Contact:** Tel: 01420 86848 (producer)

Fax: 01420 89889 (producer)

Content: Substance identification,

Physico-chemical properties, ecotoxicity, production,

legislation

Quality assessment:YesNumber of substances:122,400Number of records:122,400Time span:1970 to date

Updates:YearlyPrice:£1,935

Alternative formats:

On-line availability: DIMDI (see Appendix A)

Reference: CEC, Springer Verlag (Pers. Comm. 1995)

Produced by:

Contact:

Content:

CHEMBANK (CD-ROM)

SilverPlatter Information Inc.

Tel: 0181 9958242 (producer in UK)

Fax: 0181 9955159 (producer in UK)

Made up of 5 important databases:

HSDB:

Substance identification,

Physico-chemical properties, ecotoxicity, environmental

fate and behaviour, safety and handling, legislation and

analytical methods OHMTADS:

Substance identification,

Physico-chemical and toxicological properties for use in

hazard assessment

CHRIS:

Substance identification.

Physico-chemical properties and biological/fire hazard

potential for use in spill situations

RTECS:

Chemical names, CAS numbers, synonyms and mammalian

toxicology/human health information.

IRIS:

Human risk assessment data

No

Up to 120,000

>126,000

1950 to date

Quarterly (5,000 records per year)

AS £1271, NW £1907-£5084

RTECS also available as CCINFOdisc

CIS, STN, DIALOG (see Appendix A)

SilverPlatter (Pers. Comm. 1995), Young-Marcaccio

(1994b)

Quality assessment:

Number of substances: Number of records:

Time span:

Updates:

Price:

Alternative formats:

On-line availability:

Reference:

Produced by:

Contact:

Content:

Material Safety Datasheets (MSDS) (CD-ROM)

Sigma-Aldrich Tel: 0800 717181 (producer)

Fax: 0800 378538 (producer)

Substance identification,

Physico-chemical properties, mammalian toxicity. occupational safety storage details and advice for fire

fighting and prevention of discharges

Quality assessment: Not known Number of substances: >70,000 Number of records: >70,000 Time span:

Not known **Updates:** Not known Price: AS £975,

Alternative formats: On-line availability:

Reference: Aldrich (Pers. Comm. 1995)

Name: CCINFOdisc: Core Series C2 (RTECS)

(CD-ROM)

Produced by: US National Library of Medicine (NLM) Contact: Tel: 0101 301 496 1131 (producer)

Chemical names, CAS numbers, synonyms and manumalian Content:

toxicology/human health information. Corresponds to Registry of Toxic Effects of Chemical Substances

(RTECS)

Quality assessment: No Number of substances: 120,000 Number of records: 300,000

Time span: Current information

**Updates:** Quarterly Price: AS £200

Alternative formats: Also on CHEMBANK

On-line availability: STN, DIALOG (see Appendix A)

Reference: Young-Marcaccio (1994b)

Produced by:

Contact:

Content:

Quality assessment: Number of substances:

Number of records:

Time span: Updates:

Price:

Alternative formats:

On-line availability:

Reference:

The CHEMTOX Database (diskette)

Resource Consultants Inc.

Tel: 0101 615 373 5040 (producer)

Fax: 0101 615 370 4339 (producer)

Chemical names, CAS numbers, synonyms, physicochemical properties, toxicological data and transport

hazard/emergency response data

Not known

7,100

7,100

Current information

Quarterly AS £470

-

Young-Marcaccio (1994b)

### B2 TEXT DATABASES

These databases contain information relating to substance identification, ecotoxicity and fate/behaviour of chemicals in the environment, often as part of a broader subject coverage as a whole. Environmental data is sometimes available within a bibliographic or abstract record, although it is often necessary to acquire the original document.

Name:

Produced by:

Contact:

Content:

Quality assessment:

Number of substances: Number of records:

Time span: Updates:

Price:

Alternative formats:

On-line availability:

Reference:

Name:

Produced by:

Contact:

Content:

Quality assessment:

Number of substances:

Number of records:

Time span:

Updates: Price:

Alternative formats:

On-line availability:

Reference:

POLTOX I (CD-ROM)

SilverPlatter Information Inc.

Tel: 0181 9958242 (producer in UK) Fax: 0181 9955159 (producer in UK)

Abstracts taken from world literature concerning the

detrimental effects of pollution and toxicity of chemicals to

plants, animals and humans

No

Not applicable 800,000

1966 to date Quarterly

AS £1,750, NW £2,188,

Identical records

records contained

similar databases

Various hosts likely to hold databases

within

containing the same records

SilverPlatter (Pers. Comm. 1995)

POLTOX II: EMBASE (CD-ROM)

SilverPlatter Information Inc.

Tel: 0181 9958242 (producer in UK) Fax: 0181 9955159 (producer in UK)

Abstracts concerning the detrimental effects of pollution and toxicity of chemicals to plants, animals and humans,

taken from biomedical and pharmacological journals

No

Not applicable

318,000 1983 to date

Quarterly (30,000 records annually)

AS £721, NW £1,082

Identical records contained within

similar databases

Various hosts likely to hold databases

containing the same records

SilverPlatter (Pers. Comm. 1995)

Produced by:

Contact:

Content:

Quality assessment:

Number of substances:

Number of records: Time span:

Updates:

Price:

Alternative formats:

On-line availability:

Reference:

Name:

Produced by:

Contact:

Content:

Quality assessment:

Number of substances:

Number of records:

Time span:

**Updates:** 

Price:

Alternative formats:

On-line availability:

Reference:

POLTOX III: CAB (CD-ROM)

SilverPlatter Information Inc.

Tel: 0181 9958242 (producer in UK)

Fax: 0181 9955159 (producer in UK)

Abstracts concerning the detrimental effects of pollution and toxicity of chemicals to plants, animals and humans,

taken from agricultural journals

No

Not applicable

157,000

1984 to date

Quarterly

AS £938, NW £1,407

Identical records contained within

similar databases

Various hosts likely to hold databases

containing the same records

SilverPlatter (Pers. Comm. 1995)

CASurveyor (CD-ROM)

Chemical Abstracts Service (CAS)

Tel: 0101 800 753 4227 (producer)

Fax: 0101 614 447 3751 (producer)

Abstracts from world literature on all areas of chemistry

divided into 16 disks on specific areas of research.

HAZARDOUS MATERIALS (1), POLLUTION

CONTROL AND THE ENVIRONMENT (2) and

REGULATORY COMPLIANCE (3) include

environmental fate/behaviour and ecotoxicology

information

No

Not applicable

Not known

1991 to date

Quarterly

1 and 2 (AS £660, NW £1,260), 3 (AS £840, NW £1,300)

CA (see Appendix A)

CAS (Pers. Comm. 1995), Young-Marcaccio (1994b)



Produced by: Contact:

Content:

Quality assessment: Number of substances: Number of records:

Time span: Updates: Price:

Alternative formats:

On-line availability:

Reference:

Name:

Produced by: Contact:

Content:

Quality assessment: Number of substances: Number of records:

Time span: Updates: Price:

Alternative formats:

On-line availability:

Reference:

Aquatic Sciences and Fisheries Abstracts (ASFA)

(CD-ROM)

SilverPlatter Information Inc.

Tel: 0181 9958242 (producer in UK) Fax: 0181 9955159 (producer in UK)

Abstracts from world literature on management of aquatic

resources, ecology, biology and pollution.

No

Not applicable 440,000 1978 to date Quarterly

AS £2,627, NW £5,245-7,881

Identical records contained within similar databases. Parts

of ASFA also on POLTOX I-III STN, DIALOG, ESA-IRS, DIMDI, CAN-OLE (see Appendix A) SilverPlatter (Pers. Comm. 1995)

Environmental Chemistry, Health and Safety (DIALOG

OnDisc) (CD-ROM)

Royal Society of Chemistry (RSC)
Tel: 01865 326226 (producer in UK)
Fax: 01865 326282 (producer in UK)

Abstracts from world literature on effects of chemicals in the environment, including corporate issues and legislation.

No

Not applicable >100,000 1980 to date Quarterly AS £1068

Identical records contained within

similar databases

Various hosts likely to hold databases

containing the same records

DIALOG, RSC (Pers. Comm. 1995)

Environmental Management (DIALOG OnDisc)

(CD-ROM)

Produced by:

Contact:

Cambridge Scientific Abstracts (CSA)
Tel: 01865 326226 (producer in UK)

Fax: 01865 326282 (producer in UK)

Content:

Fax: 01865 326282 (producer in UK)
Abstracts from world literature on environmental sciences

including toxicology, pollution and environmental

to

hold

within

databases

management/action

Quality assessment:

Number of substances: Number of records:

Time span: Updates: Price:

Alternative formats:

On-line availability:

Reference:

aber of substances:

Not applicable >100,000 1984 to date Quarterly AS £1,568

No

Identical records contained similar databases

Various hosts likely containing the same records

DIALOG (Pers. Comm. 1995)

Name:

Produced by:

Contact:

Content:

Quality assessment:

Number of substances:

Number of records: Time span:

Updates: Price:

Alternative formats:

On-line availability:

Reference:

Biological Abstracts (CD-ROM)

SilverPlatter

Tel: 0181 9958242 (producer in UK) Fax: 0181 9955195 (producer in UK)

Abstracts from world literature on all areas of biology including toxicology and pollution

No

Not applicable Not known 1985 to date

Quarterly (260,000 records per year)
AS £21,634, NW £23,013-27,214
Identical records contained

similar databases

BIOSIS on STN, DIALOG, ESA-IRS, DIMDI,

CAN-OLE

SilverPlatter (Pers. Comm. 1995)

Produced by: Contact:

Content:

Quality assessment: Number of substances: Number of records:

Time span: Updates: Price:

Alternative formats:

On-line availability:

Reference:

Name:

Produced by: Contact:

Content:

Quality assessment: Number of substances: Number of records:

Time span: Updates: Price:

Alternative formats:

On-line availability:

Reference:

Oceanographic and Marine Resources (Volume I)

(CD-ROM)

National Information Services Corporation (NISC)

Tel: 0101 410 243 0797 (producer) Fax: 0101 410 243 0982 (producer)

Abstracts from Oceanographic Literature Review and information from UK Oceanographic Institutes and marine laboratories on all areas of oceanography. Some information concerning pollution and effects of chemicals

on saltwater organisms

No

Not applicable 350,000 1975 to date Biannual

AS £646

Identical records contained within

similar databases

Various hosts likely to hold databases

containing the same records NISC (Pers. Comm. 1995)

ENVIROLINE (CD-ROM as part of

ENVIRO/ENERGYLINE Abstracts Plus)
Congressional Information Service (CIS)
Tel: 0101 301 654 1550 (producer)
Fax: 0101 301 657 3203 (producer)

Abstracts from world literature on environment and management of natural resources, air, water and noise pollution. Environmental impact of chemicals

No

Not applicable 165,000 1971 to date Quarterly AS £860

Identical records contained within

similar databases. Also on magnetic tape

DIALOG, ESA-IRS, Orbit (See Appendix A)

Young-Marcaccio (1994b)

Name: AQUALINE ABSTRACTS (CD-ROM)

Produced by: Microinfo

Contact: Tel: 01420 86848 (producer)
Fax: 01420 89889 (producer)

Abstracts from world wide literature. Water treatment and

supply. Waste

water/sewage treatment. Pollution of aquatic environment.

Quality assessment: No

Content:

Number of substances:
Number of records:

Time span:

Not applicable
170,000
1960 to date

Updates: Quarterly (10,000 records per year)

**Price:** AS £1,500

Alternative formats: Identical records contained within

similar databases. Also available as current awareness

abstracts

On-line availability: Orbit (See Appendix A)

Reference: Microinfo (Pers. Comm 1995)

Name: EXICHEM (diskette)

Produced by: Organisation for Economic Cooperation and Development

(OECD)

Contact: Tel: 0171 2768501 (distributor in UK)

Fax: 0171 2768333 (distributor in UK)

Content: Gives details of areas of research (with contacts)

conducted by OECD member countries on existing

chemicals

Quality assessment:Not applicableNumber of substances:Not knownNumber of records:14,540 (1993)Time span:Current information

Updates: Annual

Price: Free to OECD member countries

Alternative formats:

On-line availability:

Reference: Department of the Environment (Pers. Comm. 1995)

# APPENDIX C ADDRESSES AND CONTACT NUMBERS FOR ON-LINE HOSTS

Chemical Information systems (CIS)
Frazer Williams
London House
London Road South
Poynton
Cheshire SK12 1WY
Tel: (01625) 871126
Fax: (01625) 871128

DIALOG/DATASTAR
Knight Ridder Information Ltd
Haymarket House
1 Oxendon Street
London SW1Y 4EE
Tel: (0171) 9305503
Fax: (0171) 9302581

DIMDI (Deutchsches Institut fuer Medizinische Dokumentation und Information Weisshausstrasse 27 P.B. 420580 D-5000 KOELN 41 Tel: 40 221 47241

Tel: 49 221 47241 Fax: 49 221 411429

European Space Agency Information Retrieval System (ESA-IRS)
The British Library
IRS Dialtech
25 southampton Buildings
London WC2A 1AW
Tel: (0171) 3237951
Fax: (0171) 3237954

Questel-Orbit 18 Parkshot Richmond Surrey TW9 2RG Tel: (0181) 3327888 Fax: (0181) 3327449 The Scientific and Technical Information Network (STN)
The Royal Society of Chemistry (RSC)
Thomas Graham House
Science Park
Milton Road
Cambridge CB4 4WF

# APPENDIX D PRINTED TEXTS AS SOURCES OF ENVIRONMENTAL INFORMATION

The following text sources give environmental data (broadly listed in order of potential usefulness) relating to substance identification, fate/behaviour and toxicity in the environment.

Books:

TITLE:

The Dictionary of Substances and their Effects (DOSE).

Volumes I-VII

**AUTHORS:** 

Richardson, M.L. and Gangolli, S. (Eds.)

PUBLICATION DETAILS:

First Editions, 1992-1994, The Royal Society of

Chemistry, Cambridge, UK

**SUBJECTS COVERED:** 

Substance identification, physico-chemical properties, environmental degradation rates, ecotoxicity, mammalian toxicity, occupational exposure and legislation details on

over 5,000 chemicals

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS:** 

Handbook of Environmental Data on Organic Chemicals

Verschueren, K.

TOBLICATION DETAILS.

Second Edition, 1983, Van Nostrand Reinhold Company,

US

SUBJECTS COVERED:

Substance identification, physico-chemical properties, environmental degradation rates, ecotoxicity and mammalian toxicity data for thousands of chemicals

TITLE:

Handbook of Environmental Fate and Exposure Data for

Organic Chemicals

VOL I: Large Production and Priority Pollutants (1989)

VOL II: Solvents (1990) VOL III: Pesticides (1991) VOL IV: Solvents 2 (1993) Howard, P.H. et al (Eds.)

**AUTHORS:** 

PUBLICATION DETAILS: SUBJECTS COVERED:

First Editions, Lewis Publ. Inc., US

Substance identification, physico-chemical properties, environmental fate/behaviour and degradation rates for around 75 chemicals (each volume)

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS:** 

SUBJECTS COVERED:

Handbook of Environmental Degradation Rates

Howard, P.H. et al (Eds.)

First Edition, 1991, Lewis Publ, Inc., US

Predicted environmental degradation rates for around 300

chemicals

TITLE:

**AUTHORS:** 

The Pesticide Manual (Incorporating the Agrochemicals

Handbook)

Tomnlin, C. (Ed.)

**PUBLICATION DETAILS:** 

SUBJECTS COVERED:

Tenth Edition, The British Crop Protection Council, UK Substance identification, physico-chemical properties,

environmental degradation rates, ecotoxicity and

mammalian toxicity data for pesticides

TITLE:

**AUTHORS:** 

PUBLICATION DETAILS: SUBJECTS COVERED:

The Agrochemicals Handbook
The Royal Society of Chemistry

Third Edition, The Royal Society of Chemistry, UK

Substance identification, physico-chemical properties, environmental degradation rates, ecotoxicity and

mammalian toxicity data for pesticides

TITLE:

**AUTHORS:** 

PUBLICATION DETAILS:

SUBJECTS COVERED:

Pesticides 1995. Pesticides approved under the Control of

Pesticides Regulations 1986

Ministry of Agriculture Fisheries and Food (MAFF)

Her Majesty's Stationary Office (HMSO), London, UK

Pesticide product identification and legislation

TITLE:

Guidelines for the Use of Herbicides on Weeds in or near

Watercourses and Lakes

AUTHORS:

PUBLICATION DETAILS:

SUBJECTS COVERED:

Ministry of Agriculture Fisheries and Food (MAFF)

1985, MAFF

Includes ecotoxicity and mammalian toxicity data as well

as guidelines for use

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS:** 

Handbook of Ecological Parameters and Ecotoxicology

Jorgensen et al (Eds.)

First Edition, 1991 Elsevier Science Publ. B.V., The

Netherlands

SUBJECTS COVERED:

Ecology and ecotoxicity data

TITLE:

**AUTHORS:** 

PUBLICATION DETAILS:

SUBJECTS COVERED:

Manual of acute toxicity: Interpretation and Database for 410 chemicals and 66 species of freshwater animals

Mayer and Ellersieck (Eds.)

First Edition, 1986, US Dept. of the Interior, Fish and

Wildlife Service, US

Acute ecotoxicity data

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS:** SUBJECTS COVERED:

Dangerous Properties of Industrial Materials. Volumes I-

Sax, I. and Lewis, Sr., R.J.

Seventh Edition, Van Nostrand Reinhold, New York, US Substance identification, physico-chemical properties, mammalian toxicity and occupational safety details for

thousands of chemicals

TITLE: **AUTHORS:** 

**PUBLICATION DETAILS: SUBJECTS COVERED:** 

Chemical Safety Data Sheets. Vol I-VI The Royal Society of Chemistry The Royal Society of Chemistry

Substance identification, physico-chemical properties, mammalian toxicity, occupational safety and First Aid

details for hundreds of chemicals

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS:** SUBJECTS COVERED:

Water Quality Criteria for Freshwater Fish Alabaster, J.S. and Lloyd, R.

First Edition, 1980, Butterworth & Co., London, UK Ecotoxicity data for fish and suggested Water Quality Criteria for their protection against certain physical and chemical parameters

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS:** SUBJECTS COVERED:

The Merck Index Budavari, S. et al

Eleventh Edition, 1989, Merck and Co. Inc., US Substance identification, physico-chemical properties and

mammalian toxicity data

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS: SUBJECTS COVERED:** 

The Thesaurus of Chemical Products. Volumes I-II Ash, M. and Ash, I. (Eds.)

1986, Chemical Publishing company, Inc., US

Identification of chemicals by trade name and vice versa

TITLE:

**AUTHORS:** 

PUBLICATION DETAILS:

**SUBJECTS COVERED:** 

Surfactants Europa. Volumes I-II

Hollis, G.L.

1982, George Goodwin, London, UK

Identification of surfactants by chemical and trade name

and vice versa. Includes physico-chemical data

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS:** 

**SUBJECTS COVERED:** 

Manual for Spills of Hazardous Materials
Environmental Protection Service, Canada

1984, Technical Service Branch, Environmental Protection

service, Canada

Includes some toxicity, fate and behaviour data for

hazardous materials

TITLE:

**AUTHORS:** 

PUBLICATION DETAILS:

**SUBJECTS COVERED:** 

Handbook of Chemical Property Estimation Methods:

Environmental Behaviour of Organic Chemicals Lyman, W.J., Reehl, W.F. and Rosenblatt, D.H.

1982, McGraw Hill Book Company

Methods for estimating fate of organic compounds

TITLE:

**AUTHORS:** 

PUBLICATION DETAILS:

**SUBJECTS COVERED:** 

CRC Handbook of Chemistry and Physics: A Ready

Reference Book of Chemical and Physical Data

Weast, R.C. (Ed.) 1988, CRC Press, US

Chemical and physical data

TITLE:

**AUTHORS:** 

PUBLICATION DETAILS:

**SUBJECTS COVERED:** 

Nitrification Inhibition in the Treatment of Sewage

Richardson, M.

1985, The Royal Society of Chemistry

Effects of around 300 chemicals on nitrification in various

sewage treatment processes

#### **REPORTS AND REVIEWS:**

It would be difficult to provide details of all useful reports in the public domain. Therefore, some particularly useful sources are summarised below.

As well as the specific reviews outlined below, regulatory bodies in other countries such as the United States Environmental Protection Agency (USEPA) and the Canadian Council of Ministers for the Environment (CCME) produce their own position documents (e.g. Water Quality Criteria) relating to the effects of certain substances in the environment. These bodies have been contacted in order to receive this information.

TITLE:

**AUTHORS:** 

**PUBLICATION DETAILS:** 

SUBJECTS COVERED:

Environmental Hazard Assessments

**Various** 

The Building Research Establishment (BRE) for the

Department of the Environment (DoE)

Large reviews on single or groups of chemicals that include substance identification, physico-chemical properties, ecotoxicity and environmental fate and

behaviour information

TITLE:

**AUTHORS:** 

PUBLICATION DETAILS: SUBJECTS COVERED:

Proposed Environmental Quality Standards for Substances

in Water

Various

WRc for NRA, DoE, SNIFFER and EU

Large reviews on single or groups of chemicals that include substance identification, physico-chemical properties, ecotoxicity and environmental fate and

behaviour information. Includes derivation of an

EOS

THINDS:

**AUTHORS:** 

PUBLICATION DETAILS:

Various Technical Reports

Various

The European Centre foe Ecotoxicology and Toxicology

of Chemicals (ECETOC)

SUBJECTS COVERED:

Large reviews on single or groups of chemicals that can include substance identification, physico-chemical

properties, ecotoxicity and environmental fate and

behaviour information. See Annex for list

TIFILE:

Environmental Health Criteria (International Program on

Chemical Safety)

**AUTHORS:** 

Various

**PUBLICATION DETAILS:** 

The World Health Organisation. Available from HMSO.

See Annex for list

SUBJECTS COVERED:

Large reviews on single or groups of chemicals that sometimes include ecotoxicity and environmental fate and behaviour information. Predominantly concerned with mammalian toxicity and human health/exposure risk

TITLE:

Aquatic Toxicity Data Evaluation. Appendix C: The

Database. Technical Report No. 56

**AUTHORS:** 

**ECETOC** 

PUBLICATION DETAILS: SUBJECTS COVERED:

1993, ECETOC, Brussels

Ecotoxicity data for around 2,000 chemicals. Soon to be

issued as a computer database

# APPENDIX E EXTERNAL INFORMATION SERVICES AS SOURCES OF ENVIRONMENTAL DATA

ORGANISATION:

NRA

CONTACT:

Environmental Toxicology Unit. National Centre for Toxic and Persistent Substances (TAPS)

ADDRESS:

NRA Thames Region, Kings Meadow House, Kings

Meadow Road, Reading, Berks, RG1 8DQ

TELEPHONE:

(01734) 535385

SERVICE OFFERED:

The Unit is able to provide data on the toxicity of substances to aquatic organisms, environmental fate and

details of environmental legislation

ORGANISATION:

CONTACT:
ADDRESS:
TELEPHONE:

WRc National Centre for Environmental Toxicology

Information Services Coordinator

Henley Road, Medmenham, Marlow, Bucks, SL7 2HD

(01494) 571531

**SERVICE OFFERED:** 

This Service provides quality information and advice on the aquatic and mammalian toxicity of substances, fate/behaviour in the environment, information on the effects of substances on sewage treatment processes and details of environmental legislation. In addition, Environmental Quality Standards and Guideline values are proposed for the protection of aquatic organisms, human

health and other amenities

**ORGANISATION:** 

CONTACT: ADDRESS:

Zeneca

Library and Information Section - Dr Sarah Barrett Brixham Environmental Laboratory, Freshwater Quarry,

Brixham, Devon, TQ5 8BA

TELEPHONE:

(01803) 882882

**SERVICE OFFERED:** 

The Information Service offered at this laboratory is able to provide data on the aquatic toxicity of substances

**ORGANISATION:** 

CONTACT:

ADDRESS:

TELEPHONE:

WRc

SARTOX - Dr Chris Watts

Henley Road, Medmenham, Marlow, Bucks, SL7 2HD

(01494) 571531

**SERVICE OFFERED:** 

The service provides data that predict the environmental fate, behaviour and toxicity of substances, based on structure-activity relationships. The predicted data are critically assessed by expert environmental chemists

**ORGANISATION:** 

CONTACT:

ADDRESS:

TELEPHONE:

**SERVICE OFFERED:** 

Freshwater Biological Association (FBA) Head of Library and Information Services

FBA, The Ferry House, Far Sawrey, Ambleside, Cumbria

LA22 OLP

(015394) 42468

This service publishes a current awareness bulletin that lists recent publications in the field of freshwater biology.

the library operates a loan facility

**ORGANISATION:** 

CONTACT:

ADDRESS:

TELEPHONE:

**SERVICE OFFERED:** 

Institute of Freshwater Ecology (IFE)
Head of Library and Information Services

FBA, The Ferry House, Far Sawrey, Ambleside, Cumbria

LA22 OLP

(015394) 42468

The IFE can provide details of publications relating to

pollution.

**ORGANISATION:** 

CONTACT:

ADDRESS:

TELEPHONE:

United Nations Environment Program (UNEP)

Director UNEP/IRPTC

16 Avenue Jean-Trembley, Petit-Saconnex, 129 Geneve,

Switzerland

Geneva 798 84 00

SERVICE OFFERED:

A query-response service operates for chemical substance information, principally through the use of the International Register of Potentially Toxic Chemicals (IRPTC). UNEP supplies chemical profiles on request, for which a fee may be charged depending on the enquiry

ORGANISATION: ADDRESS:

National Chemical Emergency Centre (NCEC)
AEA Technology, F6 Culham, Abingdon, Oxon, OX14
3DB

TELEPHONE:

(01235) 463030

**SERVICE OFFERED:** 

Centre which provides 24 hour advice and assistance to public emergency authorities as part of the chemical industry scheme for assistance in freight emergencies. The service is supported by Central Government and the Chemical Industries Association

ORGANISATION: CONTACT: ADDRESS: TELEPHONE: Plymouth Marine Laboratory (PML) Head of Library and Information Services Prospect Place, West Hoe, Plymouth, PL1 3DH (01752) 222772

**SERVICE OFFERED:** 

Regularly publishes a bibliographic list of current marine pollution research titles. No formal information service exists but environmental data has been supplied on an informal basis