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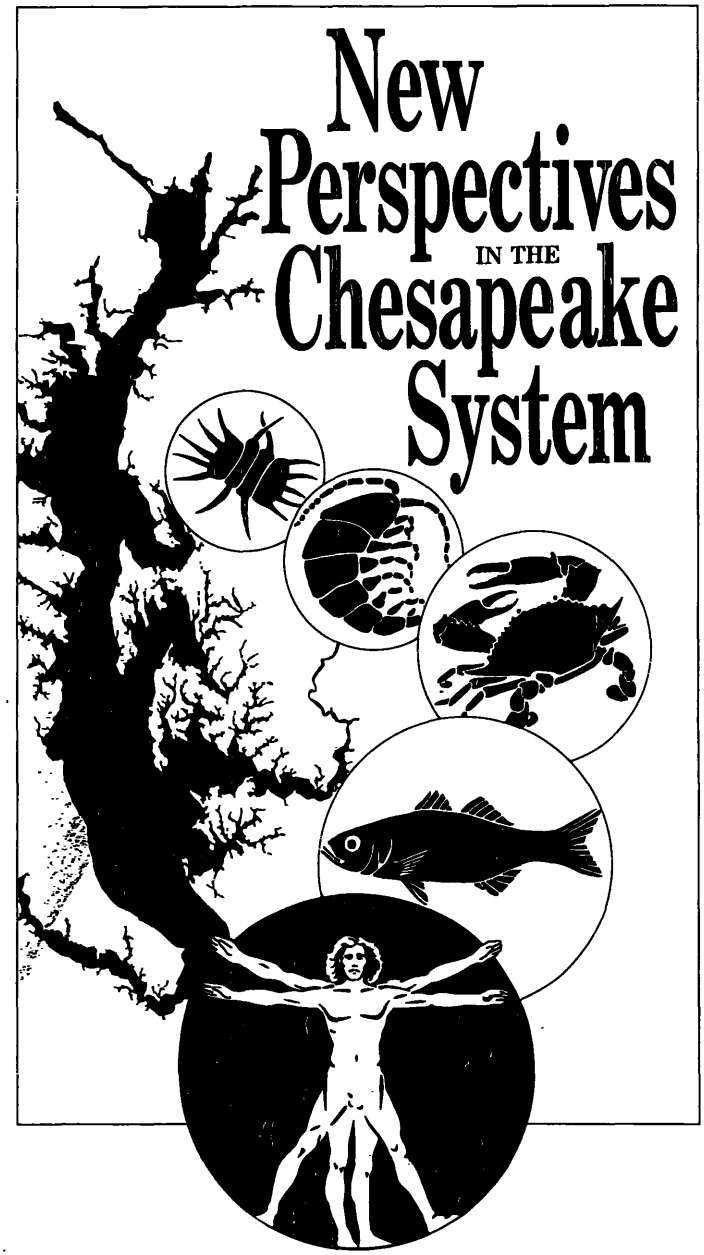

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New Perspectives in the Chesapeake System: A Research and Management Partnership

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Prototype for a Regional Online Toxics Database

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ABSTRACT
An interactive online computerized database for retrieval of chemical analytical information on volatile and extractable organic compounds, and the priority pollutant metals has been developed. Current information about samples from the Chesapeake Bay region in Virginia and Maryland are available. This database stores information on organic compounds in effluent, water, tissue, and sediment in a format which does place restrictions on the number of compounds per sample. It includes various QA/QC items as well as the analyst's assessment of the validity of the data. A variety of keyed retrieval options permits selection of reporting format, and flagging of items exceeding selected limits of concentration. Application includes retrievals for use by managers, and by researchers in planning and interpreting environmental studies related to toxic chemicals.

INTRODUCTION

The traditional chemical environmental database is a collection of records (samples) for a limited list of chemical compounds. This approach is certainly useful for rapid retrieval and statistical manipulation, it presents a severe restriction to the environmental chemist who finds more compounds in a sample, or who is unable to prove absolute identities of certain compounds. There is a large amount of useful information which is lost in traditional databases about many samples because there was only room for a limited number of compounds. Newer chemical databases, usually retrieval systems for powerful instruments such as the gas chromatograph-mass spectrometer (GC-MS), retain all the analytical data which these instruments generate in abundance, and are therefore very useful for purposes of re-examination of specific samples, but are not suited to perform rapid routine searches. Such systems require massive amounts of data storage space, and do not have the ability to store the interpretations made by the analyst. These types of databases represent extremes of a continuum of possible database types. The Virginia Toxics Database is an example of an intermediate system.

The use of computer-based instrumentation in modern broad spectrum chemical analysis of environmental samples not only makes it possible but

important to keep record of unknown and partially identified compounds, as these may well turn out to be later identified as environmentally significant. Some researchers maintain specimen banks of tissue or sediment samples preserved for later analysis in the event new analytical techniques are developed or to test for some compound not originally determined. By similar reasoning, it is important to maintain chemical databases with enough original information to allow re-examination and new interpretations. However, it is detrimental to retain all raw instrumental data for a system with requirements for rapid retrieval.

It is generally true that the most useful databases are those which can be directly accessed by prospective users from their own locations. Current development in microcomputers, telephone modems, and various network systems have made such access quite simple. Environmental chemical databases, particularly those encompassing significant geographic and historic scope, are customarily quite large in size. An online interactive database retrieval program must be efficient both in its search algorithms and in its search protocol, as time expended by the user, long-distance interconnect time, and the actual operations initiated on the host computer can rapidly become prohibitively expensive. The Virginia Toxics Database Retrieval System employs a menu-driven retrieval program, in which series of master and sub-menus offer sets of choices for report formats, samples to be searched, and other limits.

DATABASE FEATURES

Access

The Virginia Toxics Database was originated by cooperative effort between the Virginia Institute of Marine Science (VIMS) and the Virginia Water Control Board (VWCB) as a tool for storage and retrieval of chemical analytical data to be used by the VWCB in the exercise of its toxics management programs. It currently resides on the Prime 9955 Computer at VIMS. Its retrieval program is designed to communicate with a PC microcomputer running a ProComm VT100 terminal emulation program for interactive retrieval sessions and for data uploading or report downloading. The system uses only minimal VT100 capabilities, and works with many similar terminals or emulators. VIMS and VWCB users currently logon directly, or by telephone modem interconnection, but interconnection via network (InterNet or BitNet) is available to authorized users. The database is remotely accessed by the VWCB six regional offices and headquarters office. Analytical data from the State Division of Consolidated Laboratory Services (DCLS) and contract laboratories are uploaded to the database by electronic file transfer (see Fig. 1).

The Database Content

The database currently holds chemical analytical data generated during the period from 1976 to present. The initial input to the database was analytical data on effluent, ambient water, sediment and tissue analyses conducted to assess the effects of point source discharges. This was subsequently expanded to include all historical VWCB toxics data and the previous decade of ambient sediment analyses conducted for several projects by VIMS. Although all data supplied by VWCB was for Virginia rivers and estuaries, many of the VIMS sediment data covered both Virginia and Maryland portions of Chesapeake Bay and tributaries. Currently, the database contains information on over 1200 effluent samples, 650 sediment samples, 150 ambient water samples and 75 tissue samples.

Search Limiting Features

The system first prompts users to select a subset of samples. This keyed retrieval option lets the user select the scope of the retrieval, offering such broad limiting keys as date window or latitude/longitude bounds and sample type (i.e. water, sediment, or tissue), and narrower keys such as river drainage basin or station name. Selection keys are as follows:

- Station name
- VPDES permit #
- Industry type
- Effluent type
- River basin/subbasin

- Sample matrix (effluent, water, sediment, tissue)
-Sponsor organization
-Species
-Date (specify window)
-Location (specify lat/long window)

A second master menu allows the user to select the types of chemical data to be retrieved for a particular sample subset which include:

- Volatile organics data
- Halogenated compounds data
- Extractables organics
-Metals conc. data
- List stations by compound (organics/metals)
-List compounds by station (organics/metals)
-Bioaccumulation potential data (effluents only)

These reports are quite variable in scope, and may range from listing of the sample site names and geographic locations to listings of concentrations of one or more specific compounds. Several report formats are available, including ones suited to exportation to spreadsheet or statistical programs such as SAS or Lotus-1-2-3 on mini- or microcomputers. More than one report format may be selected, and each will be a sub-file in the retrieval report. Each will be limited by subsequent keys that determine which set of samples will be included.Report Header FeaturesA third menu allows customization of report headers, offering a variety of sample and station descriptive items to be included as part of the report. This can be full and expansive, listing all available data, or may be restricted to minimal information such as sample name and sampling date. Options for sample headers are:

- Station name- Hardness
- VPDES permit #- Total organic carbon
- Industry type- Flow (mgd)
- Effluent type- Percent silt + clay
- River basin/subbasin- Percent sand
- Sample type- Percent solids
- Sponsor- Number pooled organisms
- Organism species- Sex
- VWCB regional office acronyn- Length (mm)-Station abreviation- Weight (g)
- Sampling date- Percent lipids
- Latitude/Longitude- Analytical labReport Content Features

Report Content Features

A final master menu or menus if more than one report type was selected, allows additional tailoring of the analytical results in the report, where restrictions on minimum concentration or compound names can be selected, or non-standard information can be requested. Listings of particular subsets of compounds, such as the EPA Priority Pollutant list, can be selected as follows:

- List all peaks (includes unknowns)
- ARI values or HRI values listed- MS - list eight-peak mass spectra
- Totals - list total conc. of resolved compounds
- Priority pollutants only
- Non-priority pollutants only
- Search based on compound name(s)
- Search based on CAS #'s
- Search by ARI or HRI values
-Search for compounds above cutoff conc.
- Octanol/water partition coeff., log P (specify minimum)

A unique feature is the search access to the Relative Retention Indices (RRIs). These index systems, Aromatic Retention Index (ARI) and Halogenated Retention Index (HRI), are particularly useful in labeling entries by a reproducible manner derived from their gas chromatographic behavior under standard conditions, especially the ARI system. Even where compounds cannot be immediately identified by the analyst, the Index value serves as a qualitative descriptive label which can be accessed at a later date. In the cases where new information becomes available, either through analysis of newly obtained reference standards, or by other evidence suggesting probable existence of compounds not previously identified searches for database entries whose RRIs fall within preselected windows corresponding to the new compounds may be easily made. Use of this feature for sediment aromatics has allowed positive identification of several PAHs when authentic standards allowed determination of their Aromatic Retention Indices (ARIs), including the known carcinogen dibenz(a,h)anthracene, in samples analyzed more than eight years earlier.

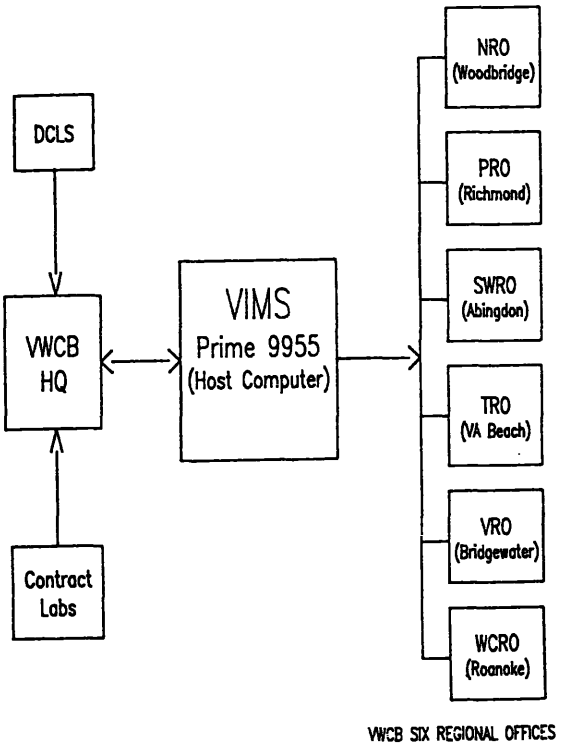

Figure 1. *Configuration of Virginia Toxics Database.*

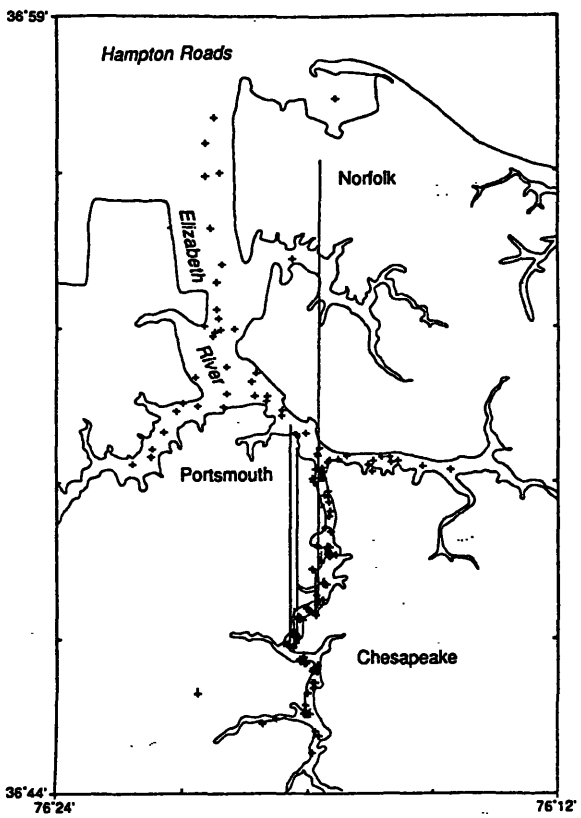

Figure 2. *Results of use of the database to extract information on content and location of sediment samples analyzed in the past decade.*

APPLICATIONS

The Toxics Database has current relevance to scientific investigators and managers who need to know what the prior chemical analytical work in a geographic region reveals. For example, a manager charged with establishing guidelines of acceptable limits of a given set of compounds in environmental samples should be able to rapidly reference all prior analyses which might show past and current levels already found to exist. These data can be applied in concert with toxicity information and water quality standards to pinpoint those geographic regions which may not be in compliance with initially proposed guideline levels, and will suggest courses of action which are feasible. These may include upward revision of guideline levels if current levels are universally higher, targeting of emission of certain compounds, or some sort of remedial or cleanup action. The open format of this Toxics Database means that such searches may be conducted on a wide variety of components, not necessarily limited to priority pollutants or similar restricted 'hit lists'. The simple fact that certain compounds are not listed in analyses in this database does not necessarily imply that such compounds could not have been present, just that they were not detected by the analyst. The proper inference to be drawn from the absence of a particular compound is a direct function of the nature of the compound and analytical protocol. Most results in this database are derived from GC-MS, and absence of a compound likely to be detected by this protocol implies that it was not present in concentration above a specified detection limit. In contrast, a few compounds must be specifically determined by ad hoc analyses (i.e. kepone or TBT), and the absence of these compounds merely implies that no attempt at detection was made. An option for listing sum total of all extractable compounds reported provides a general basis for comparison of samples without direct reference to any compound. Figure 2 is an example of use of the Virginia Toxics Database to abstract total extractable compound concentrations and latitude-longitude information for sediment samples analyzed in the past ten years. The concentrations are presented in analog-scale vertical bars superimposed on a shoreline chart. Similar abstracted data for specific compounds, or for time-series plots could be as readily obtained. For environmental scientists, this database may be searched to retrieve historical data about specific compounds, groups of compounds, or total compound sums in geographic regions. This information is directly useful in selection of sites for conduct of research which is relevant to the levels of toxic components, and for the comparison of the results of such research with them. Researchers customarily collect single sediment or water samples for toxic chemical analysis at the site of their field studies, which is then used in interpretation of their results. Because of considerable small scale variability of micro-environments so sampled, the chemical levels determined in a single sample may be misleading. Most studies, even those intended to measure toxic chemicals, are unable to afford the greater sampling density required to ensure that the sample variance is within acceptable limits. Certain measurements made on field samples of motile organisms are more appropriately compared to a larger average environment, and may not necessarily reflect the coincidental chemical levels measured in a single sediment or water sample. The value of the single analysis is greatly enhanced if it can be put into geographical and chronological perspective by comparison of the results with similar analyses conducted on adjacent and/or time series samples. The greater power derives from the ability to claim that the parameters measured in the current sample are statistically similar to its neighbors in space and time.

Future Additions

The future outlook is to solicit input from more analytical sources, including newly generated information and previously reported data throughout the Chesapeake Bay region, making it a true regional resource, and to provide access to the retrieval system through computer network and telephone connection to researchers and managers on a broad scale.

Acknowledgement

We thank Tracey Harmon and Susan McCoy for their help with manuscript preparation. The Virginia Toxics Database is supported by the Commonwealth of Virginia, Toxics Database InitiativeFig 2. Plot of total extractable organic compounds in sediment samples (n=229) collected from the Elizabeth River system, 1980-1989. Highest vertical bar represents 16,000 ug/g, dry weight.fi