

Online Analytical Chemistry

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Online computer systems provide rapid access to current information. Most importantly, they provide a way to scan the literature for relevant information without spending every waking hour in the library. Given the number of professional journals published in this and other countries and the volume of work performed daily in laboratories all over the world, it can be difficult for the analytical chemist to stay current. Online computer systems do the tedious work for you and do it faster than a human ever could.

The number of online computer systems available to scientists has burgeoned in recent years, and there are many more systems than can be listed in this article. However, many analytical chemists have found certain online systems to be particularly useful: electronic database-searching systems, nationwide computer systems and networks, and computerized bulletin boards.

Database-searching system

The Dialog Information Services system is one of the premier bibliographic database-searching systems. Dialog provides a number of useful features,

including a current awareness service that covers 85 databases.

One of the more useful features is a one-search function that enables users to search up to 20 different databases at once without having to reenter search terms with each database, producing a combined output. The system also has image transfer capability, enabling users to retrieve, display, save, and print graphic representations such as geometric designs and drawings using an IBM-compatible personal computer with a graphics adapter. DialogLink software for IBM PCs is optimized for the Dialog Searching Service

FOCUS

and supports the image transfer protocols as well as dot-matrix and laser printers.

Dialog users manuals, including the DialogLink, are among the most complete manuals available for any computer system. They are indexed, well organized, and easy to use. In addition, Dialog provides a number of special low-cost files (called ONTAP files) that can be quickly searched. Courses on using the system are also available as self-instruction video packages and guidebooks.

Dialog databases that may prove interesting to the analytical chemist include the following.

Analytical Abstracts lists general analytical applications in inorganic, organic, pharmaceutical, environmental, and agricultural chemistry. Analytical Abstracts reviews approximately 1300 journals when producing its database. The database is searchable by chemical names, including synonyms and trade names, and by Chemical Abstracts Service (CAS) registry numbers, titles, and keywords.

CA Search, the CAS database, is indexed from 1967 to the present on the Dialog system. Complete records are available for the 8th through the 12th Collective Indexes. CA Search also provides a current awareness service, keeping chemists up to date on the latest results.

Chemical Engineering Abstracts includes information on processing chemicals, chemical reactions, heating or cooling, and transportation of chemicals. Physical and chemical properties of substances, types of equipment used in handling the materials, and safety information are all found in this database, which covers the period from 1971 to the present.

The Chemical Regulations and Guidelines System contains regulations that have been in effect since October 1982 regarding control of chemical substances. Federal statutes and regulations, guidelines, and standards are included. Every chemical cited in a regulatory document is indexed by name, CAS registry number, and a

chemical role tag that describes the context in which the chemical appears in the applicable regulatory document.

Chemname contains almost 2 million records (from 1967 through the present) that describe chemical substances in CAS registry nomenclature. Chemname is designed to provide substance-searching capabilities on the basis of nomenclature; trade names; synonyms; and substructure-searching techniques such as ring data, element count, and molecular formula.

Chemsis covers more than 5 million substances (indexed from 1967 to the present) that have been indexed only once during a Collective Index period of Chemical Abstracts. Because 75% of all the chemicals cited in the literature are cited only once in a given period, this database can be an important source of information on some of the lesser known chemicals. Chemsis is a nonbibliographic dictionary file.

Chemzero is another nonbibliographic dictionary file that contains chemical substances for which there are no citations in the CA Search files. This database contains more than 1 million substances and covers the period from 1965 to the present.

The **Claims Compound Registry** indexes more than 14,000 compounds and is designed to locate compounds of interest in patent files.

The **Heilbron** chemical properties database is available for searching online indexes, dictionaries of organic compounds, organometallic compounds, antibiotics, and organophosphorous compounds. Chemical substances can be identified by searching physical and chemical properties, including molecular formula and weight; melting, freezing, and boiling points; solubility; relative density; optical rotation; and dissociation constants.

The **Kirk-Othmer Encyclopedia of Chemical Technology** covers a wide range of chemistry, including areas such as agricultural chemicals, drugs, fibers and textiles, food, fossil fuels, glass and ceramics, metals, semiconductors, and electronic materials. All of the tables in the paper version of the encyclopedia are included in this database and are searchable online.

The **Paperchem** database is provided by the Institute of Paper Chemistry for paper chemists. Subjects such as packaging, graphic arts, forestry, carbohydrate chemistry, cellulose, hemi-

cellulose, lignin, and wood extracts are covered by this database. Approximately 50% of the Paperchem records are citations on patent information.

Other databases that may be of interest to analytical chemists include Pollution Abstracts, Water Resources Abstracts, Energy Line, DOE Energy, The World Patents Index, U.S. Patent Abstracts, Medline, The Pharmaceutical News Index, and Scisearch (which provides citation indexing).

The Dialog Computer Service can be reached through its own computer network (called Dialnet) as well as through the national networks Tymnet and Telenet. Dialog is available for users with 300-, 1200-, and 2400-baud modems and can be accessed with MNP error-correction protocols.

Online training and practice files are provided for CA Search, Chemname, Analytical Abstracts, Kirk-Othmer Online, Medline, National Technical Information Service, Scisearch, and The World Patents Index.

Nationwide computer systems and networks

Nationwide computer networks can provide a low-cost means of accessing

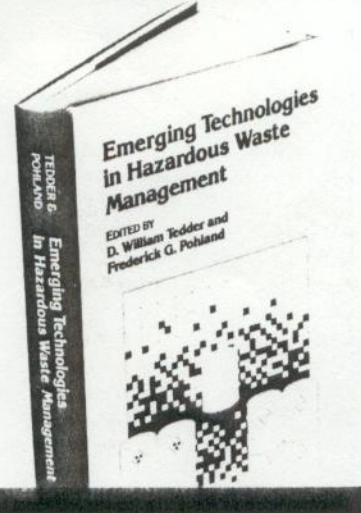
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Emerging Technologies in Hazardous Waste Management

Here is an insightful reference on developing technologies for treating and managing wastewater and solid residuals that are contaminated with hazardous chemicals.

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This concise presentation draws from a variety of science and engineering disciplines with specific emphasis on physical, inorganic/organic, and biological chemistry. It provides an across-the-board perspective of problems and proposed management technologies.

This volume will serve as a useful introduction to hazardous waste treatment for the novice as well as a valuable reference for the technical expert.

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raw computational power and electronic message services. Systems such as CompuServe provide access not only to electronic mail but also to rapid, electronic, and error-free transfer of computer programs and files from one location to another. (Error-free transfer protocols are designed to verify that no interference has occurred that might result in garbled data or program codes.) Using electronic program transfers is usually faster and easier than mailing a diskette or a magnetic tape. CompuServe also includes some online database searching capabilities and sells its own communications programs through which graphics and text can be transferred error free to and from their system.

Self-study courses and classroom training are available for the CompuServe system through private vendors. Although the instruction manuals for CompuServe are less useful than those for Dialog, the CompuServe menu system is strong and requires little additional explanation. CompuServe is highly responsive to its users, and when a particular database is rarely used, it soon becomes unavailable. Databases and functions are continuously added to the system, which complicates the problem of updating manuals. However, CompuServe does provide a monthly magazine, *Online*, which describes the options, databases, and functions currently available. The system also offers a number of national bulletin boards that are similar to the PC-based bulletin boards available almost everywhere.

Electronic bulletin board systems

Most PC-based electronic bulletin board systems (BBSs) are used for electronic mail and for uploading and downloading of archived PC programs. These bulletin boards provide virtually every imaginable type of software available in the public domain (as well as a few pieces of software that are not available in the public domain, although this is illegal). You can't beat the cost of these programs, because most of them are free.

Unfortunately, the programs available on BBSs frequently lack adequate documentation and are at best easy to misuse. At worst, programs obtained from BBSs can be ridden with bugs and even viruses capable of destroying the hard disk data of the computer to which they are downloaded. Persons using electronic bulletin boards to obtain programs should be careful in making selections and should be on the lookout for suspicious program behavior (i.e., program accessing of hard disks when it seems inappropriate or

strange messages popping up at inappropriate times). Few, if any, BBS operators are deliberately hostile, but most operators use little or no user identification or password protection protocols, audit trails are short, and virtually anyone is permitted to upload or download compiled software. As a consequence, the systems can be abused by unscrupulous individuals.

To access a bulletin board, a user needs a modem—generally one capable of a baud rate of 300-2400 (a higher baud rate will save time and reduce telephone bills)—and a communications program. Communications programs can be purchased for approximately \$200. If you can borrow someone else's equipment before you are set up to access BBSs, you can obtain a communications program more cheaply, or for free, directly from a bulletin board. (ProComm, one of the better communications programs, is available on several of the bulletin boards described later in this article.) Communications parameters for most bulletin boards are set to 8 data bits, 1 stop bit, and no parity.

Most programs are squeezed in "archive files" and have the extension ".ARC." An archive file is a package of several programs under one file name that can be downloaded as is, but it must be "unpacked" with a special program. The best unpacking program is PKX35A35.EXE, available on most bulletin boards. This should be the first program copied. There are several different schemes to pack an archive file. PKX35A35.EXE has an advantage over older unpacking programs because it detects the packing method and unpacks accordingly. High telephone bills can be avoided by using local bulletin boards or by registering for Telenet's PC Pursuit, which permits access to any bulletin board in 24 metropolitan areas for an initial \$25 registration fee plus \$25 per month.

One BBS that could be particularly useful to analytical chemists is operated by the Society for Applied Spectroscopy and the Council for Near-Infrared Spectroscopy. The SAS/CNIRS BBS, located at the University of Kentucky, is available for use by members of the SAS and the CNIRS. This system supports electronic mail and is accessible to all users via a telephone line. Academic members can access the bulletin board and files through BITNET.

At present the SAS/CNIRS computer system includes a public bulletin board as well as message boards for users of spectroscopic instrumentation. The computer system provides a file for members of the ASTM E13.03.03 Task Group on Near-Infra-

red Spectroscopy. Files giving electronic mail addresses for users and describing the various programs available are accessible in a directory called [DOWNLOAD]. Programs are available to the public in [DOWNLOAD-PROGRAMS], a subdirectory that contains a source code. (A source code is more difficult to infect with viruses and worms and tends to be more useful to chemists, who often prefer to modify their own software.) In the future the SAS/CNIRS BBS may be used as a clearinghouse for near-IR spectra. These spectra may be uploaded for assembly into a library database that can be distributed to everyone in the JCAMP-DX spectral-exchange format. (For more information, contact SAS/CNIRS BB, c/o JoAnn Brown, 198 Thomas Johnson Dr., Suite S2, P.O. Box 1438, Frederick, MD 21701; (301) 694-8122.)

Other BBSs of interest, and some of their prominent features, include the following.

- The Digital Imagery BBS, (602) 622-8131, provides a message service and file transfers for digital image processing.

- Exec-PC, (414) 964-5169, an extensive general-purpose bulletin board for IBM users, contains more than 50,000 software files, and is accessible through PC Pursuit.

- The File Cabinet, (215) 678-9334, offers a full range of software in more than 7700 files.

- Inventory Factory, (212) 431-1194, another IBM-only general-purpose BBS, has more than 41,000 individual files in 76 different topics. Inventory Factory has an annual subscriber fee of \$100 for unlimited access.

- Killer BB, (817) 824-7881, provides free access to UseNet and a UNIX shell and is capable of programming online in several different languages.

- NOAA BB, (303) 497-5000, contains information on geophysical and solar activity.

- Royalink I, (805) 484-9343, a general-interest BBS, contains more than 900 files, including ProComm.

- Thousand Oaks Technical Database, (805) 493-1495, for IBM users only, operates like DOS. (If you don't know how to use the "change disk" command, consult your MS-DOS manual before attempting to use this BBS.)

- Utilization Exchange, (614) 488-3991, also IBM only, provides limited free access or unlimited access for a \$25 fee. You can see a full listing of files offline by downloading UTILS.ARC.

The landscape of online systems is a constantly changing one. Most analytical chemists will probably come across database searching systems, nation-

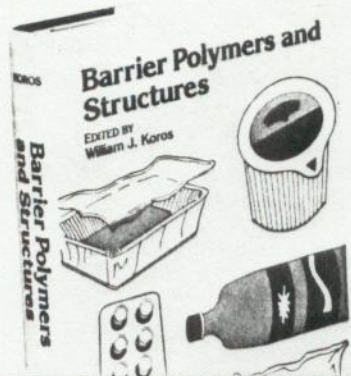
wide computer systems and networks, and electronic bulletin boards at some time in the course of their work. An awareness of the capabilities of these online systems will make the chemist's contact with them a more profitable one.



Elizabeth G. Kraemer received her B.S. degree from Susquehanna University and did graduate work at SUNY—Binghamton before going to the University of Kentucky Chandler Medical Center. She is an experimental psychologist currently working with Robert Lodder on biological applications of near-IR spectroscopy.



Robert A. Lodder received his B.S. (1981) and M.S. (1983) degrees from Xavier University (Cincinnati, OH) and his Ph.D. in analytical chemistry (1988) from Indiana University. He is currently an assistant professor of pharmaceuticals and analytical chemistry at the University of Kentucky. Lodder has explored mathematical solutions to the "false-sample" problem in thought-like processes, the results of which have been applied to product tampering, analysis of complex biological samples by optical methods, and 3D imaging of paintings under restoration. He has received the Tomas Hirshfeld Award in Near-IR Spectroscopy and a Research and Development 100 Award.



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