

ONLINE NETWORKS, INTERNET, AND INFORMATION SERVICES FOR CHEMICAL AND PETROCHEMICAL INDUSTRIES

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Introduction

We are living in the so called, " Information Age ". Information is a vast, dynamic and inexhaustible resource that affects all disciplines and all people. Information by itself has no value. Its value comes from its communication and use. The process of communication information is rendered difficult due to several inherent problems, such as information explosion, inter-disciplinary nature of information, information in numerous sources, geographical, language and other barriers to communication.

Information Technology

In order to overcome these barriers, there exists today a vast array of electronic tools and techniques for accumulating, storing, organising, retrieving, communicating and interpreting information on a world-wide scale, in a volume and at speed and with an accuracy that would have been possible hardly a few years ago.

The advent of the digital computer and the advances in the telecommunication and audio-visual technologies have opened up new possibilities in dealing with problems arising from the collection, organisation and dissemination of a vast amount of information.

while the spectacular growth of the computer and communication technology in the last few decades is notable, what is even more notable is the rapid way these technologies are merging.

Machine readable data bases

Recently various Abstracting and Indexing services started using computers for offering the services cost-effectively and timely. Because of this change, the text is kept on magnetic media capable of being processed, in general, by a computer. The primary purpose was to use this form of material to drive 'drive' typesetting equipment for the production of the printed volumes. During the process, the machine readable records becomes the most useful by-products as data bases, enabling the users to get access to the required information at a faster rate.

Online Systems and Services

The term "online" now embodies many concepts. Literally it means that the user is in contact with the computer through some direct linkage. In practice it implies very much more and is now accepted as being some kind of individual terminal attached to the computer either by a direct line or over the telephone network. Online services can be provided with small or medium sized computers for a few users with limited processing requirements but larger computers are used for services where many users must be served simultaneously. Large amounts of random access memory are used today in the major online systems. Extensive communications capability must exist in any online service that is designed to accommodate a diversity of users. Usually national and international databases can be accessed by one or more of the following communication media, (1) the telex network (2) the automatic telephone network and (3) a specialised (dedicated) data network. For access via telephone circuits, it will be necessary to use a *MODEM (Modulator-Demodulator)* which is a device to convert the digital signal signals coming from the terminal.

Online Networks

The kind of networking which is referred to here is electronic networking that permits sharing and remote use of hardware, software and databases. Cost sharing constitutes one of the biggest advantages of network use of databases. Adequate and affordable communication technology now exists to accommodate the shared use of databases. Communication networks that now exist include government sponsored networks (e.g. *ESANET of European Space Agency*) and commercial networks, such as, *TYMNET, TELENET* and so on).

Database Hosts

DIALOG, DATASTAR, USA; STN, USA; Orbit, USA, etc. are some of the database hosts available for online information retrieval through different telephone networks.

There are different types of information networks existing in our country. The reasons are diversity

caused by the different needs of users, the different types of organisations owning or operating networks, and the emerging new requirements of the office of the future. Some of the existing network in India are given below.

Wide Area Network	Metropolitan Network
NICNET, INDONET, I-NET, INFLIBNET, ERNET, VIDYNET BTNET, SAILNET, BANKNET, NETWORK OF INDIAN AIRLINES, RAILNET, SIRNET, SBINET, OILCOMNET, RABMN	CALIBNET DELNET

I-Net

I-Net is India's X.25 based Packet Switched Public Data Network. It provides high speed connectivity between computers/ terminals. I-Net (Phase I) is now operational in nine cities viz. Delhi, Bombay, Calcutta, Madras, Hyderabad, Bangalore, Pune, Ahmedabad and Baroda. I-Net is based on Packet Switching philosophy with error detection and correction techniques. I-Net is connected both ways to many data network in other countries. I-Net customers can use the networking and database facilities available on the international networks.

Online searching facilities at IPCL Research Centre

Recently IPCL R&D had procured a new PC-AT386, MODEM, I-Net Password, STD Line and DIALOG Password. Using this facility online searching services has been initiated, using DIALOG Host (Knight-Ridder). Dialog has over 450 databases from a broad ranges of disciplines. It is particularly noted for its collection of business, science and technology and intellectual property. It has also Dialmail, Dialog Alert service, Dialorder services etc. The various databases, available in DIALOG useful for retrieval of information in chemical and Petrochemical Industries is given in Appendix-I. Efforts are on to obtain Internet connectivity at our Research Centre in order to further enhance the information accessibility at the global level.

Sample DIALOG SEARCHES

What are possible dangers of chemical Lawn care?

Environmental Bibliography File 68
s Lawn ? and Danger ? and chemical (N) Grass
and Hazard ? and (treatment or care)
Yard and Risk and (weed(N) Kill) ?

? B 68
? S Lawn ? OR Grass OR Yard ?
S1 2359
? S danger OR Hazard OR Risk

S2 8309
? S Chemical (N) (Treatment or Care) OR
Weed (N) Kill?
S3 180
? S S1 and S2 and S3
S4 2
? PR S4/8/1-2.
3.12 Zeolite in polypropylene
CA Seach File 313 1992-1995
? S Zeolite ?
S1 12686
? S Polypropylene
S2 8992
? S S1 and S2
S3 37
PR S3/1/ALL

Internet services/ Facilities

Computers and information technology have made their way into all scientific disciplines, including chemistry. The fast growth and massive production of knowledge in science demand rapid and efficient ways of retrieving. The most important electronic information highway today is the Internet, a world-wide computer network.

Rapid person-to-person communication can be achieved by electronic mail. Internet offers several methods for reaching a ohlarge number of persons, and taking part in 'electronic' scientific discussions with persons all over the world. In addition, ohvarious services exist that enable scientists to retrieve information and computer programs, search databases and exchange information. oneof the advantages of Internet services is that the services are accessible to many people, and that new information is almost instantly available.

A fundamental notion of modern computer technology is the client-server model. The computer program, used to retrieve information from network the is the client. The client is served by a server, which is a remote computer with available information and a computer program running to take care of the exchange of information and data between the client and the server.

Communicating with other scientists

Electronic Mail

One common of person-to-person communication is by means ohof electronic mail. The communication is the fast and the recipient can read the message when time allows, in contrast to telephone communication. This is particularly advantageous for communication between scientists living in very different time zones. In order to use electronic mail one must have a set up of infrastructure, typically handled by the computer centre or equivalent. The user also needs a mail program on his/her computer to be able to send

receive mail. Person-to-person electronic mail is useful for communicating textual information. It is possible to communicate binary data, e.g. computer programs.

Mailing list servers

Another useful way of communicating is person-to-group communication. One method for doing this is by use of a list server. One person volunteers to create and maintain the necessary software to enable to use of a list server. Those who are interested in Participating in such a list send an electronic mail message to the list server maintainer with a request to be added to the list of participants. Mailing list servers have two addresses, one for administrative purposes (e.g. subscription) and one for communicating with the other participants. Messages sent to the list distributed to all participants, and administrative messages are read by the list administrator or are processed automatically by a computer program. Some mailing list are moderated, i.e. one more volunteers read the incoming messages and judge the content for its suitability for distribution to all participants. On other list servers only digests are distributed. Unmoderated and moderated list servers may handle highly specialized scientific discussions.

Table 1. Examples of Electronic Mail Discussion Lists of Interest to chemists.

Administrative Address	Topic
LISTSERV @ PDB.PDB.BNL.GOV	Protein Databank discussion
LISTSERV @ UWF.CC.UWF.EDU	Chemistry Education
CHEMISTRY-REQUEST @OSC.EDU	Computational Chemistry
LISTSERV @ IUBVM.UCSINDIANA.EDU	Chemical Information Sources
ORGREQ @ EXTREME.CHEM.RPI.EDU	Organic chemistry.

News

A better organised but somewhat similar system is called News (also called NetNews and USENET News). For electronic mail the user needs a mail reader as client software, while for news there is a need for another type of client software, the News reader. Such software exist for most modern computer systems. Many News-readers also have the capability to post (send a message) to News groups or one needs a separate computer program for that purpose. It is similar to electronic mail but the recipient is the name of the News group. By using the News client software the user can join any News group available. by using the News system one can answers to problems and discuss advanced topics with participants from all over the world. It is really similar to participate in electronic mailing lists. Each user can read and respond to the News messages

whenever time permits. A very nice feature of many News groups is that volunteers maintain documents with frequently asked questions (FAQS) and answers, so that the discussions in the News group will be on new topics and not ones discussed or answered many times before. It is a good habit to check the FAQ of a News group before posting a question.

Table 2. News Group Related to chemistry

Group Name	Topic
Alt.drugs. Chemistry	Drug Chemistry and synthesis
Bionet. Journals Contents	Table of contents of many Scientific journals.
Bionet. Molec. model	Physical and Chemical aspects of molecular modelling.
Bionet. Xtallography	Protein crystallography
Sci. Chem.	Chemistry and related sciences
Sci. Chem. Electrochem	Electrochemistry
Sci. Chem. Labware	Laboratory equipment
Sci. Engr. Biomed	Biomedical Engineering
Sci. Engr. Chem.	Chemical Engineering
Sci. polymers	Polymer Science
Sci. Techniques. magresonance	Magnetic resonance imaging and spectroscopy.

Information systems

A large number of computers throughout the world have computer programs and information of general interest available. The most popular archives have identical copies several places in the world (mirror sites) to save the Internet from overloading. One should always use the nearest archive if possible, and avoid massive file transfer in the peak hours at the server site.

Accessing File Archives with ftp.

One method of accessing such archives is by using a client program called ftp (file transfer protocol) or similar. Often archives are hierarchically organised in a directory names pub., for public. The

archives are often organised in several sub-directories, e.g. by software category or computer system type. If one wants to contribute software or information to such site, the most common place is in a directory called incoming. One should carefully read the instructions available at most sites before donating data to such archive.

Accessing file archives and services with electronic mail.

Some people do not have access to ftp, and for this and other reasons several archives can be accessed using electronic mail. Users access the archive by sending a message to the archive by using the electronic mail address of the archive. The message is often one or more commands from a limited set of available commands for retrieving help, obtaining a listing of available information and retrieving computer programs and information sources.

A useful service accessible by electronic mail is run by the publisher Springer. A large number of journals have their tables of contents distributed by electronic mail. One can subscribe to this service and receive the table of contents of the journals of interest as soon as they are available, often a couple of weeks before shipping of the printed journal from the publisher. For a small fee, one can also receive abstracts in his electronic mailbox. The journal tables of contents are also distributed to the News group, which also contains a number of other journal tables of contents.

Table 3. Archives Reachable by ftp and Electronic Mail

Address of archive	Directory	Description	Mail server Address
nic.funet.fi(128.214.6.100).	/pub/sci/ch chem.	chemistry archives computer programs.	Mail server @ftp.funet.fi
osc.edu(128.146.5)	/pub/chem.	computational chemistry mail mailing list (CCL)Archives.	Mail serv @ Osc.edu.
ftp.pdb.bnl.gov. (130.199.144.1).	/afc	Brookhaven National Laboratory, the protein Databank.	
Physics.arizona.edu	/afc	Buckminster fullerene bibliography.	

Accessing archives and information using gopher.

A more sophisticated method of accessing remote file archives is by using a system called gopher. In many cases the necessary client program is also

called gopher. Gopher presents a menu-based interface to the archive, and is an easy to use interface to archives of computer programs and information.

Table 4. Gopher servers related to chemistry

Address of server	Description
acsinfo.acs.org (134.243.230.66)	The American Chemical Society
atlas.chem.utah.edu.(128.110.196.10).	Material Safety Data Sheets
infx.infor.com (198.136.167.1.1)	BookCatalog
slvaxa.umsl.edu. (134.124.1.1)	Chemistry textbooks in print
jcp.uchicago.edu (128.135.44.113)	J.Chem.Phys.Preprints, JCP Express.
gopher.pdb.bnl.gov (130.199.144.1)	Brookhaven National Laboratory, the Protein Data Bank.
infomeister.osc.edu (128.146.36.5)	Computational Chemistry Mailing List (CCL) Archives (Port 73).
ftp.uci.edu. (128.200.80.20)	Material from the journal protein Science (Port 1071).
jcchemed.chem.wisc.edu. (92.90.150)	Journal of chemical Education
gopher.genethon.fr (192.70.45.2)	Back issues of journal table of contents.
gopher.incr.ac.uk (192.70.242.1)	The International Union of Crystallography.

Multimedia on the Network

The most recent and sophisticated information system available on the Internet is called the world-wide web or WWW or simply the web. In this system ftp, gopher and several other existing information systems are embedded such that existing archives can be utilized with this new technology. The web has capabilities for combining text, graphics, sound and video into a complete multimedia environment, and may be considered as one large database with information stored around the world. Among the many advantages of this system is the nice user interface which makes it easy for novices to the world of Internet. There exist both character based and graphics-based client software for the web and obviously the latter is preferred. As with gopher, web documents can be linked to each other so that a multi-page document may be stored on several servers around the world, and yet appear to the user as one document. When using graphics based

computer systems, the users simply point and click to obtain information. The information can be organised in clickable menus, clickable words in a text or clickable pictures. Different area of a picture (e.g. a geographic map) can be linked to different types of information.

One of the most popular client programs for the web (often called browsers) is called Mosaic and is available for a number of computer systems. If you consider using the web it is important to obtain the list of Frequently Asked Question (FAQ) to read the basic information on how to get started and explanation on technical details.

Each web document has its own 'address' called a Uniform Resource Locator (URL), which is similar to a symbolic address, but is appended by a directory and file name, and prepared by the name of the transfer method used by the server. The transfer method may be e.g. gopher or http.data. To direct the client to a certain document, the URL of the document maybe entered on the command line (or by another appropriate method depending on the client software).

Multimedia possibilities on the INTERNET open up many possibilities for enhanced exchange of information and data in chemistry, e.g. electronic publishing. It is possible to have a publication on the INTERNET where e.g. the molecular structure of a compound is drawn in a figure. By clicking on the figure, a helper program for viewing three-dimensional molecular structures is started on your computer and the co-ordinates of the molecules are sent to your computer and drawn by the helper program it is possible to rotate, render and view a three dimensional image of the molecule as you wish, which is not restricted to the projection and rendering chosen by the authores of a publication in a printed journal. Helper programs need to be obtained and installed separately from the Web client software.

Table 5 World Wide Web servers related to chemistry

Sr. No.	Description
1.	The official chemistry directory service on the Web
2.	Chemistry departements and services
3.	Another directory of chemistry Web sites and services
4.	Chemistry on the INTERNET. Chemistry resources
5.	The International Union of Crystallography

6. Crystallography Directory services
7. The Cambridge Crystallographic data centre
On line software manuals
8. Chemistry at Centre for scientific computing (CSC) in Finland
9. Web elements, Periodic table, isotope pattern Calculator and element percentage calculator
10. Computational chemistry mailing list (CCL) Archives
11. Molecular modelling information and resources A molecular modelling primer.
12. The Brookhaven National Laboratory Protein Databank (PDB)
13. Search for secondary structure elements in data from PDB
14. Full text search of data from PDB.
15. Three-dimensional structures of biochemical compounds
16. Chemical Abstracts Services Pproducts information.

Future Developments in online system

By the end of this decade, it is envisaged that most workplaces of scientists, administrators and decision-makers will be equipped with a computer terminal linked to a network which will allow the following possibilities.

- (a) Communication with anyother terminal on the network.
- (b) Access to numerical, statistical and bibliographic databases and databanks.
- (c) Access to major computational capabilities of the network.
- (d) Personalised mail, with text & graphics
- (e) Distance teaching and other educational services.
- (f) electronic shopping for goods and services.
- (g) News reporting and distribution
- (h) Teleconferencing.

Indeed the possibilities are limitless and these will fundamentally change the way people shop,bank,work and communicate, since they can do all of these things without leaving thier places.