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ABSTRACT

The first section of this precis summarizes the general nature of the present chemical information systems of the world. The discussion is presented in four parts: (1) the primary literature, (2) secondary sources and services, (3) libraries and information centers and (4) other elements categorized as informal communications. The second section presents material on advanced developments by discussing some facets of computer-assisted publication and presenting brief descriptions of four systems which use or will use computers in handling scientific information. Problems encountered by chemical information systems in trying to provide access to needed information to their users and some suggested solutions to these problems are discussed in the final section. (Author/NH)

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**AN OVERVIEW OF WORLDWIDE
CHEMICAL INFORMATION FACILITIES
AND RESOURCES
"A PRECIS"**

Prepared Under the Sponsorship of
**THE UNITED STATES OF AMERICA
NATIONAL SCIENCE FOUNDATION**

for the
Joint Study on the Communication of Scientific Information
and on the Feasibility of a Worldwide Science Information System
of the
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and the
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Summary of Characteristics, Resources and Flow

This first section summarizes the general nature of the present chemical information systems of the world. The discussion is presented in four parts which cover: (1) the primary literature, (2) secondary sources and services, (3) libraries and information centers and (4) other elements categorized as informal communications.

Primary Literature

The world's primary literature in chemistry, chemical engineering and borderline fields is very large and growing rapidly. It is estimated that about 300,000 papers, patents and reports were published in 1966.

Publication shows a growth of about 9% per year compounded, and will reach a rate of about 400,000 per year by 1970. The combined abstracting and indexing output of Chemisches Zentralblatt (since 1830) and Chemical Abstracts (since 1907) total about 4.5 million papers, patents and reports.

The "average" chemical paper is about five pages long, contains 3,000-5,000 words plus graphic and tabular material, is written by 2.2 authors and is published within 5-12 months of receipt by the journal although the publication delay may be as low as a few weeks or as high as three years.

The publication language of the original paper may be any one of about 56; however, English (54.9%), Russian (21.0%), German (7.1%), French (5.2%), Japanese (3.1%), Italian (2.1%) and Polish (1.8%) account for 95% of all papers published in 1966. The 1966 literature contained contributions from some 103 countries with the United States (30.0%), the U.S.S.R. (21.3%), the British Commonwealth (12.2%), Germany (6.8%), Japan (6.4%) and France (5.0%) accounting for 81.7% of all papers.

The number of journals which publish chemical information is presently about 12,000 and this figure is increasing at about 6-7% per year through establishment of new journals and through the addition of chemistry to their field of coverage by older journals. Approximately 300 journals have their entire contents oriented towards chemistry and chemical engineering and about 7,000 journals will publish one or more papers of chemical interest during a one-year period. Chemical Abstracts, for example, routinely covers about 12,000 journals; however, 75% of the abstracts come from about 1,000 journals and 90% come from only 3,000 journals.

Another important source of chemical information is the patent literature which accounts for about 30% of new information reported each year; however, considerable duplication is introduced by the practice of filing for patents on the same invention in a number of countries.

As the technologically developed countries expand their scientific activities and as the emerging countries begin to develop technology, there will be not only an expansion in the quantity of chemical information published but there also will be an expansion in the number of countries represented.

The increasingly interdisciplinary nature of science will tend to broaden the field considered to be "chemical information" as chemistry increasingly overlaps with fields such as biology, physics and medicine.

Secondary Literature and Secondary Services

These services exist to provide access to current and accumulated information contained in the primary literature. These services differ widely in their products and coverages according to the need which they attempt to fill and the selectivity with which they attempt to serve specific individuals or groups.

Secondary services as a group offer two general types of information support which may be used separately or in combination. Alerting services provide the user with a steady flow of current information in specified interest areas. Retrieval services provide the means for selecting information from the collected material of the past. These two types of services are frequently called "current awareness" and "retrospective search" to reflect the different orientations of the services. In recent years computer-based services have begun to offer services based upon the use of individual "interest profiles" for selection of pertinent material. These more individualized services have been called "selective dissemination of information" (SDI).

Secondary services, whether of the "awareness" or "search" type, operate on the general premise that the subscriber will use the material provided by the service only to decide whether or not he is interested in a particular original document. The subscriber to a secondary service is expected to refer to the original document for detailed information. Thus, secondary services will usually contain, at some level of detail, the following data elements:

1. Bibliographic Identification.
2. Author Name(s).
3. Document Title.
4. Abstract.
5. Index.

Bibliographic Identification -- This data is sufficient to allow complete identification of the source document and would include, as appropriate: title of periodical or report, issuing agency, volume or report number, issue number, page numbers, and possibly original language and cost.

Author Name(s) -- The name should be sufficient to identify a specific person; however, this is frequently not possible because of initial and/or name duplication. Considerable problems come about through use of initials instead of names, through variant transliterations (say, from Cyrillic) or translations (say, from Japanese) of names, through dropping of inflection marks and through use of computer printers which provide only upper case letters.

Document Title -- The title of a document serves to identify it and may serve to indicate the overall content of the document. A number of secondary publications exist which publish titles of papers for use in current awareness and alerting service. The titles may be arranged either according to the source journal or according to a selected set of subject category headings. Computer-based services may also offer a KWIC (Keyword-In-Context) index based upon the document title.

Abstract -- This is the commonest form for secondary services either in alerting or search services. It consists of a highly condensed version of the original document and is used to determine whether the original document should be consulted. Abstracts are usually categorized as either "indicative" or "informative" although there is a continuous shading between them which makes the distinction difficult to make in many cases. Generally speaking an "indicative abstract" is quite short and indicates the types and categories of information in the original. On the other hand an "informative abstract" tends to be longer and contains some or all of the information in the original. Abstracts used by secondary services may be an author-produced abstract from the original document or may have been specially prepared by the secondary service to meet its own standards and requirements.

Index -- Major products of secondary services are indexes of various types to assist the user in accessing the primary literature. While the primary literature usually contains indexes of some sort, the indexes prepared by secondary services are usually more useful because of the much greater coverage and depth. Usually-present and self-explanatory types of indexes are the Author and Subject indexes. Other types of indexes include:

- Report and Patent Indexes which index documents by the identifying numbers.
- Patent Concordances which cross reference patent numbers for inventions which have been patented in more than one country.

- Citation Indexes which index literature citations of papers. The premise is that the general content and focus of a paper is indicated by the literature references cited. The Citation Index brings together all papers which cite a specific paper and, thus, brings together papers having a certain content and focus.
- Molecular Formula Indexes index compounds cited in the literature according to their chemical composition.
- Ring Indexes are organized by the structural framework of cyclic compounds and are useful in deriving systematic names of compounds which can then be searched for in the Subject Indexes.
- Additional indexes which may be encountered include the Rotaform Index used by Index Chemicus and the Hetero-Atom-In-Context (HAIC) Index which has been announced for Chemical Abstracts.

Some representative existing secondary services in chemistry are discussed briefly in alphabetical order in the following six paragraphs.

Bulletin Signaletique -- This service is published by the Center of Documentations of the National Center of Scientific Research (C.N.R.S.) at Paris, France. It is published in French and covers all science and technology fields from a world-wide coverage of about 6,000 journals, French theses and European conferences and books. It is published monthly in 24 sections and presents short indicative abstracts, bibliographic entries, author index and detailed table of contents for each section. Cumulative annual subject and author indexes are provided for some sections. The service (and a predecessor service) date back to 1940. It published about 140,000 chemical abstracts in 1965 and about 138,000 in 1966. Related services include: microfilms of original articles, loan service of periodicals and translation service.

Chemical Abstracts -- This service is published by Chemical Abstracts Service at Columbus, Ohio, U.S.A. It is published in English and covers all chemical and chemical engineering information from a world-wide coverage of about 12,000 journals, books, monographs, reports, conferences, symposia, other secondary services and patents. It is published in 80 sections (each section appears biweekly) and presents informative abstracts, bibliographic entries, author index, keyword index, numerical patent index and patent concordance. Semi-annual and quinquennial cumulations are published for keyword, author, numerical patent and formula indexes. The service dates back to 1907. It published about 195,000 abstracts in 1965 and about 217,000 in 1966. Related services include: photocopies of original Russian articles, List of Periodicals which are covered (with annual supplements), microfilms of abstracts and the Ring Index.

Chemisches Zentralblatt -- This service is published by a group of German organizations active in chemistry. It is published in German and covers all theoretical and applied chemistry from a world-wide coverage of about 3,000 journals, books and patents from 22 countries. It is arranged in eight chapters and a number of subchapters and appears weekly. It presents bibliographic entries, informative abstracts, author index and patent number index. Annual and quinquennial cumulations are published for author, subject, patent and formula indexes. The service (and predecessor services) dates back to 1830. It published about 160,000 abstracts in 1965 and about 159,000 in 1966. Related services include: a list of periodicals (Periodica Chemica), micro cards of issues from 1830-1950, microcards of the 1922-1934 general index and a version printed on one side only.

Index Chemicus -- This service is published by the Institute for Scientific Information, Inc. at Philadelphia, Pennsylvania, U.S.A. It is published in English and covers synthesis, isolation and identification of new chemical compounds from 162 journals from 28 countries and from another publication by ISI, Current Contents. It is arranged by the title of the original journal and appears weekly. It presents bibliographic entries, graphical representations of material (where possible), molecular formulas, verbal material (not necessarily in English) where available, subject index, author index, journal index and molecular formula index. Semi-annual and annual cumulations are published for author, subject, molecular formula and journal indexes. The service dates back to 1960. It published about 12,000 abstracts in 1965 and about 14,000 in 1966. Related services include: an annually cumulated Index Chemicus with specialized indexes and a tear-sheet service for original articles abstracted.

Nuclear Science Abstracts -- This service is published by the United States Atomic Energy Commission. It is published in English and covers nuclear science and technology from a world-wide coverage of 2,000 journals, reports, patents, books, conferences, symposia and dissertations. It is arranged into 13 categories with subcategories and appears semi-monthly. It presents bibliographic entries, informative abstracts, author index (both personal and corporate), subject index, report number index and report depositories. Quarterly, semiannual and annual cumulative indexes are published. The service (and a predecessor) dates back to 1947. It published about 48,000 abstracts in 1965 and about 47,000 in 1966. Related services include: semiannual list of journals and addresses of agencies from which original articles may be obtained.

Referativnyi Zhurnal -- This service is published by the All-Union Institute of Scientific and Technical Information (VINITI) of the U.S.S.R. It is published in Russian and covers all science and technology from a world-wide coverage of 23,000 journals, conferences, books, dissertations and patents from 20 countries. It is arranged into 60 sections and 165

subsections and appears semi-monthly. It presents bibliographic entries and informative abstracts but no issue indexes. Annual indexes are published for formula, subject, Cyrillic author name, Latin author name, numerical patent and inventor-corporate patent indexes. The service dates back to 1953. It has published about 600,000 abstracts per year in recent years. Related services include: photostatic and microfilm copies of original articles and translations.

Libraries and Information Centers

Libraries and information centers serve as repositories for the primary and secondary literature to support the researcher. It is believed that at least 10,000 libraries in the world possess literature collections which support chemical information transfer. The libraries may be roughly classified into (1) those whose collections are comprehensive enough and broad enough to provide major support in many fields of science and technology and (2) those whose collections are specialized in nature to support primarily chemical and chemical engineering activities. Geographically these libraries are concentrated in industrial and academic centers with about 40% in Europe, 29% in North America and 22% in Asia. About one-third of libraries serving chemistry are associated with educational institutions while about 15% are supported by state and national governments and the remainder serve industry, research institutions, etc. The primary focus of libraries serving chemistry has been on the scientific journal. Major research libraries devote about 75% of their collections to periodical literature with the remainder divided among books, patents, dissertations and technical reports.

The store of chemical information is so large that libraries cannot individually afford to maintain complete collections and they have therefore set up various cooperative efforts to provide the best service possible. Any given library attempts to meet within its own resources the major needs of its own clientele and relies upon cooperating libraries to supplement its resources in other areas. Various types of cooperation between libraries are discussed in the following four paragraphs.

Shared Library Records -- This takes the form of such publications as the World List of Scientific Periodicals, List of Periodicals Abstracted by Chemical Abstracts, Union List of Serials and New Serials Titles. All of these publications, and others, provide guidance as to where collections of specific serial publications are held and serve as a guide to arranging access to these collections.

Cooperative Acquisition -- This takes the form of cooperative arrangements between libraries for accession of materials which are then available to all cooperating members. An example is the Farmington Plan in which a group of cooperating United States libraries attempt to acquire at least one copy of each new foreign publication which might reasonably be expected to be of interest to a researcher.

Depositories -- This takes the form of designating certain libraries as depositories and arranging that copies of all material in certain categories will be automatically forwarded to the depositories by the originator or publisher.

Interlibrary Lending -- Sharing of materials between cooperating libraries is carried out through the mechanism of the interlibrary loan. This has been a powerful and popular means of sharing library materials; however, the system sometimes results in substantial delays in availability of material. The delays may be long enough that the requestor no longer has a need for the material when he finally receives it.

Standardization of Library Methods -- Differing forms of bibliographic description and classification between various libraries tends to render cooperative use of materials more difficult. Efforts are being made to develop standards which can be universally used and which, when implemented, will ease cooperative use of materials.

Library operations are beginning to be affected by the recent advances in computer technology and the effect may well be profound in the near future. Projects are under way to provide machine-readable catalog data which will speed up cataloging and reduce effort as well as providing for eventual bibliographic search by computer. Computer-based indexes, some of which are currently in operation, will profoundly affect library operations both in terms of speed and in the depth of indexing which may be feasibly used. Computer-based indexes and searches, when supplemented by facsimile transmission and by microform documents, open the way to greatly improved library services.

Information centers have come into existence principally to supplement libraries through provision of specialized services which the libraries, for any of a number of reasons, cannot provide. Generally information centers provide services beyond those of libraries, have subject specialists on their staffs and usually publish the results of their work. The United States operates a number of specialized information centers under the Atomic Energy Commission and the Department of Defense. The National Bureau of Standards has established a number of centers in conjunction with the National Standard Reference Data System. The Medical Literature Analysis and Retrieval System (MEDLARS) operated by the National Library of Medicine services a number of information centers in various medical specialties. Information centers in other countries include: the Iron and Steel Institute and the British Iron and Steel Research Association

in Great Britain, the Gmelin Institute in Germany, the Indian National Scientific Documentation Center, the Centre of Scientific and Technical Information in Israel, and the Japan Information Center of Science and Technology.

Informal Communications

Informal communications are not part of the "official" information system but make up a real part of the overall system. Primary journals are the normal point of entry of material into the permanent scientific literature; however, the material may be circulated informally long before publication in a journal. The usual mode of informal information transfer is through personal discussions and exchange of letters and preprints within small groups of scientists working in specific areas of a field. Informal exchange of information is important but is outside the scope of the present report.

Advanced Developments

This section presents material on advanced developments by discussing some facets of computer-assisted publication and presenting brief descriptions of four systems which use or will use computers in handling scientific information.

Computer-Assisted Publication

The use of computers to assist publication is in its infancy at present; however, it is probable that there will be major impacts in the future. Some facets of this impact are discussed in the following three paragraphs.

Text Processing -- Traditional methods of publication require several stages of processing with careful handling and review at each stage to prevent ambiguity and to eliminate errors. Use of computers cannot assist in removal of ambiguity but it can eliminate transcription errors as the material passes through publication steps not only at the primary literature level but in the transferral of material from the primary literature into the various types of secondary literature. Transferral of material from one publication to another in machine-readable form also eliminates the major costs of re-keyboarding material at each stage of publication.

Index Compilation -- Processing text by computer leads naturally to use of the computer to assist compilation of indexes. The computer can be used with human assistance or, eventually, perhaps, by itself to select indexing terms from the text for subject indexes. Author indexes may be compiled automatically from the text and entry of names and/or structures of compounds can be processed to produce entries for subject indexes, formula indexes and ring indexes. Use of the computer can allow much greater depth in indexing, automatic generation of cross-references and reorganization of data for access along various routes. The computer is particularly useful for such mechanical tasks as sorting and merging indexes for issue indexes and cumulative indexes and for fast searching of indexes for compilation of bibliographic data leading to literature access.

Composition -- Computers are already in use for composition of scientific journals and, while problems still exist in such areas as tabular and graphical material, this use will become increasingly important in the next several years. Use of this technique avoids much of the time and cost of rigorous checking of material at the galley and pageproof stages of the present printing processes.

Computer-Assisted Storage and Retrieval

Several projects are presently active in using computers for assistance in storage and retrieval of chemical information. Four of these developments are briefly described in the following paragraphs.

The German System -- This development will use a computer to link several German information services into a system for handling compound-related data. The compound-related data handling system was developed by industry and then made available for use in the processing operations of Chemisches Zentralblatt, Beilstein's Handbuch der Organischen Chemie and Gmelin's Handbuch der Anorganischen Chemie. The system includes both a full record of compound structures and a fragmentation code which may be used for substructure search. The files and search programs are available to supporting organizations. The system started with synthetic organic chemistry and is being extended to the full range of coverage of Chemisches Zentralblatt. It will be extended later to include computer-stored subject indexes. This system has been discussed continuously with the developers of the system which is to be described next and the two systems are believed to be compatible.

Chemical Abstracts Service System -- This system is part of the overall system being developed to support publication of Chemical Abstracts. The system gathers information derived from processing Chemical Abstracts and processes it into a form for use in information storage and retrieval. The system has a computer-based technique for recognition and storage of typed structural diagrams and has associated files of bibliographic and nomenclature data on compounds. This system now contains about 600,000 substances, 1.3 million references and 800,000 chemical names. Chemical Abstracts is converting its whole operation to a computer-based system, including photo-composition of publications. This conversion is scheduled for completion by 1970. Other American Chemical Society activities in the field of computer-based information systems include: photo-composition of the Journal of Chemical Documentation, composition of several Chemical Abstracts Service publications by computer printout, coordinated computer-based development of primary journal and Chemical Abstracts issue indexes, and projects to use computer search systems for assistance in preparation of reviews.

MEDLARS System -- This system, operated by the U. S. National Library of Medicine has, since 1964, provided search capabilities and special bibliographies as well as publication of Index Medicus. A project is under way to link this system with the U. S. Food and Drug Administration system and the Chemical Abstracts system.

Nuclear Science Documentation Systems -- The European Nuclear Documentation System is a computer-based system for processing queries against a file of index terms for abstracts. Index terms are selected from the Euratom Thesaurus for input to the system and are computer-checked for conformance

to the thesaurus and limited correction of spelling and keypunch errors is performed automatically. The queries are presented in terms of thesaurus descriptors and the computer selects document references for copying from a central file. The U. S. Atomic Energy Commission and the U. K. Atomic Energy Authority also cooperate with Euratom which operates this system. The editorial staff of Nuclear Science Abstracts assigns Euratom descriptors to abstracts published in NSA. In a related project, the International Atomic Energy Agency has undertaken an ambitious development of an International Nuclear Information System. This project plans to have each country abstract and index its nuclear science literature, following which all the pieces will be merged, processed and made available for computer-based searches of the material.

Microforms of Documents

The availability of various forms of micro-documents will make an increasing impact on library and information center operations. The use of microfilm, microfiches, microcards, aperture cards, etc. make it possible to store information at much higher density than can be achieved with the traditional printed publications. Recent equipment provides: (1) direct readability, (2) rapid location of specific page images and (3) immediate production of photocopies of material. In the field of chemistry a number of publications are presently available in some type of microform, including: Chemical Abstracts (since Volume 1), Beilstein's Handbuch der Organischen Chemie and Chemisches Zentralblatt.

Problems and Suggested Solutions

Access to Primary Literature

The accepted base of all chemical information lies in the primary literature. The basic purpose of all secondary services is to make available the information of the primary literature either through repackaging the material or by providing routes to the material through abstracts, titles and various types of indexes. The increased use of automation which gives improved and deeper indexing, automatic searching of indexes, close attention to differentiation by indexes and partial storage of data in computers will help to solve the problem of finding references to the primary literature. Even after the chemist has determined his interest in a particular original document there is, however, the problem of physical access to the document. Various solutions, either singly or in combination, offer assistance in this areas such as: microform documents either on hand or transmitted on request, photocopies provided from central depositories, faster interlibrary loans facilitated by better information on holdings, and by computer searching and library interconnections by teletype and/or facsimile.

Avoidance of Redundant Keyboarding

During the processing of material through the primary literature and the various secondary publications, material is presently keyboarded many times at considerable cost for keyboarding, proofreading and correction at each stage of processing. The use of computers gives promise of providing the means to process material through all stages from a single, initial, keyboarding.

Nomenclature and Indexing

Chemical nomenclature serves as a major base for indexing of the literature. As chemistry develops the nomenclature becomes more complex and changes in some details. The systematic rules for naming are extremely lengthy and complex and are not really usable except by experts. A non-expert can normally derive a non-ambiguous name for a compound but this name may well not correspond to the systematic name which is desired for indexing purposes. The computer may well provide the means for derivation of systematic names from structural diagrams and may also provide non-systematic names for generation of cross references.

As the rules for systematic nomenclature change, there is created a problem of substantial magnitude relating to correlation between present systematic names and the outdated systematic names under which compounds have been indexed in the older literature. It is usually possible to follow the trail of a compound forward in time by means of cross reference to the new names; however, tracing a compound into the past may be very difficult due to lack of cross references from present names to obsolete names.

The development of so-called linear notations (such as the Wiswesser code) provides one possible solution to the problem by generating an unique "cipher" for each compound according to specific rules. This cipher then becomes, in effect, another systematic name and may then be used for indexing and search. None of the large abstracting and indexing services presently use this form of indexing, however, mechanization of assignment of ciphers would provide a valuable tool for future use.

Problems in Automation

Automation gives promise of providing solutions (or at least assistance) to many of the problems facing the publishers and users of chemical information. However, automation brings problems of its own for which solutions are neither easy nor fast nor cheap at the present stage of technology in automated information processing. Five major problems are discussed in the following paragraphs and suggested solutions, where available, are noted.

Financing -- Present costs for publication and use of the primary and secondary chemical literature are many millions of dollars annually. Development and implementation of new methods of information processing and handling will require the expenditure of many additional millions of dollars in the next decade or two for research, development, implementation, procurement of equipment and operation of improved systems.

Primary publications presently are financed in a variety of ways, including various combinations of: subsidy by sponsoring scientific societies; subscriptions; page charges; advertising; subsidies by governmental, industrial and philanthropic organizations; and through contributed or volunteer effort. Secondary publications utilize much the same sources except that page charges and advertising are of little importance.

Financing of future work can be expected to follow much the same pattern although the proportional contributions will undoubtedly change.

Design and Implementation -- Computer technology is in its early stages and really effective methods for design, development and implementation of large-scale information processing systems are not publically available, if they exist at all. The increasing store of "know-how" is not widely disseminated in such a form as to make it readily available.

Availability of personnel with the skills and experience to develop large-scale information processing systems is extremely tight at present. Educational institutions have given little recognition to the rapidly growing needs in this field and operating organizations are forced to develop and train their own staffs. A shortage exists in the area of development of human-computer interfaces and interactions, and results in fragmentation of systems and a consequent need to redesign and modify the systems as operating experience points up deficiencies.

Most systems which have been implemented and documented have been rather small in size. There exist no general techniques for scaling up these small systems. Also, small systems usually do not have a requirement to operate efficiently and a large-scale system which operates with comparable efficiency is totally unacceptable.

Related to the above problem is the present inability to make accurate predictions of system efficiency. For small or multi-use systems this may result in high costs but is seldom disastrous. In a large-scale single-use system the result may be catastrophic.

When a new or modified system is put into operation it is necessary to run both old and new systems in parallel until satisfactory operation of the new system is assured. This necessity is costly and must be repeated each time significant changes are made.

Standards and Compatibility -- Documentation standards and programming languages for processing scientific information are presently at a low state of development.

Equipment specifications are not standardized so that procurement of equipment from different manufacturers is difficult. Different computers may require different programs, different file structures and different techniques for effective operation. Even between different users of what is nominally the same equipment, the presence or absence of various equipment options may render programs and files incapable of use without major modifications.

User Education -- Even if all the problems of implementation of scientific information processing systems were solved and the systems were in operation today, they could not be used effectively, if at all. The prospective

users must be educated to a new and vastly different method of using information services. The new systems will be capable of vastly improved speed, completeness and selectivity; but, only when the user has been educated to use them properly. The educational process will be expensive and time-consuming but is absolutely essential. Furthermore, present practice will preclude undertaking this educational process by the information processors. User education may well be the rate-determining step in maturation of computer-based scientific and technical information services.