although it is truly new since it has only recently arrived on the addendum file.

Since 1976, the various developments in chemical information at DIALOG have led to a series of robust files available on-line with frequent updating and unique value-added features. Perhaps one of the more significant of these features developed in the last several years has been that of ring system information. CAS elected to remove this information from the most recent versions of the Registry Nomenclature File. Experience with the DIALOG Information Services' CHEMNAME and other chemical-substance files clearly indicated that this information provided a cost-effective, inexpensive way to group chemical substances on the basis of structural features. As a result, complete new algorithms were developed by chemical information staff at DIALOG to generate the ring information in accordance with the rules and definitions published in the CAS *Parent Compound Handbook*. These data have been the subject of several presentations and will be more fully described in a subsequent publication.

SUMMARY

Chemical information at DIALOG Information Services has developed through licensing of databases from Chemical Abstracts Service and providing the first on-line implementations of several of these. *Chemical Industry Notes* and *Patent Concordance* were first made available in 1976. Also, the CA CONDENSATES file for several collective index periods and the CASIA indexing file were first made available on-line in 1976 by DIALOG Information Services. In that same year, the CHEMNAME chemical-substance file was created from CASIA and the *CA Index Guide*. As a result of that work, the *Index Guide* was also used to enrich the combined CA CONDENSATES/CASIA file first offered on-line in 1977 by DIALOG Information Services.

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Evolution of Industrial Chemical Information Systems

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A modern industrial chemical information system is an integrated system that provides for the storage, retrieval, and manipulation of internal and external information to meet the needs of the organization. It incorporates some of the most modern tools and methods available in an effort to be cost effective. The various components of an industrial chemical information system are enumerated, and their evolution is described and anticipated.

INTRODUCTION

Unlike many other areas of chemistry, most of the initial work in chemical information was carried out in an industrial environment rather than at universities and research institutes. Chemical companies pioneered the development of indexing and retrieval techniques. Many of the early advancements in manipulation and handling of chemical structure information were also made in the information groups or laboratories of industrial firms. The introduction of computers into chemical information was also an area where the industrial information chemist led the way.

A detailed description of the many advances made in the chemical industry is beyond the scope of this paper. Instead, we will describe a typical information system as it is found in the industrial environment. In so doing, we will point out those areas that are unique to industry and will then recount the developments that have led to the present structure and function of an industrial chemical information system.

MISSION OF AN INDUSTRIAL CHEMICAL INFORMATION SYSTEM

The mission of an industrial chemical information system is not very different from any other information system. It is charged with providing a means of preserving information that may be of value in the future, maintaining a retrieval process that assures timely and accurate recovery of the stored information, and providing access to tools for manipulating that information. However, there are some very important distinctions between an industrial information system and a public or government system.

One of the main differences is that an industrial information system must include in its collection the technical information generated internally in the firm. Much of this information is proprietary in nature and must be protected from untimely or unauthorized disclosure. Another difference is that time is, in some instances, a much more important factor in the storage, indexing, and retrieval of information in the industrial environment. Failure to obtain the needed information in a timely manner could result in a substantial economic penalty to the organization.

An overriding constraint on the operation of an industrial information system is that it be cost effective. The determination of what is cost effective is a difficult one, but one that the manager of such a system must be ready to defend and expound frequently and regularly. This pressure to maintain cost effectiveness has made industrial information managers seek out services from many sources as they make every effort to avoid unnecessary duplication of effort in either operating or development efforts.

EXTERNAL INFORMATION

The greatest portion of the chemical information used by an industrial chemical firm comes from outside the organization. It typically comes from journals, books, government

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reports, and other reports. In order to serve the organization, the chemical information center must not only make the desired external information available, but it must also devise ways of making people aware of the appearance of pertinent external information. This effort is a combination of an acquisition policy and an alerting program to make individuals aware of information being added to the store or published.

The information system provides a store of external information that is particularly relevant to the mission of the organization as well as access to the entire chemical literature. The acquisition policy of the information center will determine the size and scope of the store of chemical information available in the system. The magnitude of the amount of external chemical information available and the escalating costs of journals and other publications have forced organizations to prioritize their acquisitions to a much greater extent than before. The use of microform as a storage medium has increased in popularity both because of its compactness and because of the cost savings that are available.[1,2] Most industrial information centers keep some external information in microform.

The information system manager relies on a number of methods for shaping the acquisition policy. Some use advisory panels that provide suggestions of what materials should be acquired and help to prioritize items when this has to be done. User suggestions are weighed heavily when making acquisition decisions. Another approach that is used to set acquisition policy is to maintain a record of the use of materials. This provides an indication of the relative use of those materials already in the store as well as the frequency of requests for items not available in the store. This usage information is utilized to determine how well the acquisition policy fits the changing needs for information in the organization.

An important function of an industrial chemical information system is to provide a way by which the members of the organization can be alerted to the appearance of pertinent information in a timely manner. The individual bears the major responsibility for being aware of new information. However, many information systems provide ways to assist the individual in keeping up with current developments. Some organizations provide alerting bulletins that abstract the published literature that is deemed to be of interest to those working in the organization. Such efforts are costly and very resource intensive. The availability of *Chemical Abstracts* section groupings and later the development of commercial alerting services based on topical profiles such as *ASCA-TOPICS* and *CA Selects* have made alerting services available at significant savings.[2a] If such a service can be used, it is usually more timely, more comprehensive, and cost effective. Some organizations have contracted with the producers of these services for custom-designed alerting bulletins that meet the specific needs of that organization. In many instances, alerting services are coupled to an acquisition service that will provide the desired document upon request.

One of the tasks of an information system is to provide a way of identifying pertinent information in response to specific queries. The sheer size of the store to be searched is overwhelming. Fortunately, the chemical industry has available to it a number of excellent tools for retrieving published information. The major services, *Chemical Abstracts*, *Science Citation Index*, a major product of the Institute for Scientific Information, and *Beilstein*, provide access in different ways to the world's chemical literature. These access tools are available in most industrial chemical information systems. In addition, the use of on-line services has become almost routine in the searching for external information.

Once a reference has been identified, the needed information must be found and made available to the requester. There are a number of approaches that have been used to meet these needs. Some commercial services such as The Genuine Article and Chemical Abstracts Service Document Delivery Service make papers available. Advances in copying technology have made photocopying a routine method for distributing information. Such widespread copying raises the issue of copyright, which is discussed elsewhere in this anniversary issue.[4] The industrial chemical information manager must be cognizant of the requirements of the copyright law and serves, in many instances, as the control point for the organization in copyright matters.

For many years, references have been assumed to be information. The focus of most information systems has been the retrieval of references that point to documents assumed to have the needed information. As the volume of published chemical information has grown, the number of documents that must be retrieved to obtain the needed information has greatly increased. This growth requires additional efforts to glean the pertinent information from the document retrieved. It is only recently that the technology has become available to allow for the retrieval of specific information rather than references to documents. In some fields, such as infrared spectroscopy, mass spectroscopy, crystallography, etc., large

amounts of data are available for direct retrieval. Efforts to develop databases of physical properties are also making such data readily available.

The industrial chemical information system must also provide access to information, such as handbooks, government reports, etc., that is not readily accessed through commercially available indexing and retrieval services. Standard cataloging procedures are used to provide access to this material, although in most cases the standard techniques must be modified to fit the needs of the particular organization. This is necessary because a typical collection in an industrial chemical organization is specialized in a relatively narrow area of technology and additional cataloging depth or detail must be used in order to provide meaningful retrieval.

PATENT INFORMATION

A significant portion of the external information pertinent to the needs of an industrial chemical organization is found in patent specifications. Although patent information is external information, its special character requires a separate discussion. Unlike journal articles, chemical patents do not provide a clear-cut exposition of chemical information. Patents are legal documents meant to disclose enough of the information to meet the requirements of the law, but at the same time they are general enough that a distinction between what actually was done and what is projected is often difficult. In addition, one of the purposes of the patent specification is to delineate the area of coverage that is reserved to the inventor. For obvious reasons, this area is made as broad as possible, thus further obscuring the actual scientific information being disclosed. The processing of patent information must be approached in a different manner than the journal literature.

Today's industrial chemical information systems rely primarily on two organizations to provide access to the chemical patent literature. They are Derwent Publications, Ltd., and IFI/Plenum. Each uses a different approach, but each is necessary to meet the needs of the industrial chemist. *Chemical Abstracts* includes coverage of patents, but it has been generally recognized that its treatment of patent information has not been as satisfactory as the other organizations. However, significant efforts have recently been made by Chemical Abstracts Service to improve its treatment of patents.

INTERNAL INFORMATION

A major portion of the resources of an industrial chemical information system must be directed to internally generated information. Since most of the information is of a proprietary nature, all efforts to store, index, and retrieve it must, of necessity, be done internally. This requires that internal indexing and retrieval systems be developed and made an integral part of the information system.[5] Unlike external information, there are no commercial services available to process internal information. The one exception is the Private Registry Service, offered by Chemical Abstracts Service, which provides for the registration of chemical substances on a contract basis. Use of this service makes all the chemical identification tools developed by Chemical Abstracts Service available to the subscriber for his own substances.

Over the years, chemical companies have developed their own approaches to the storage and retrieval of internal information.[6-9] As computer technology has evolved, the complexity and the capability of these systems have increased. However, an integral and essential part of any of these systems is the human intellectual effort that has to be expanded to characterize the information.[10,11]

Recently, a number of systems have been made available to the chemical industry on a turnkey basis. Such systems provide the computer hardware and software that will allow the input, storage, and retrieval of information. Most of these systems are based upon some form of manipulation of chemical structure and will be discussed later in this paper. However, they do not provide adequate tools for searching the text of an article, although they do provide facilities for searching bibliographic material. There are some computer software systems that provide for the storage and manipulation of text, but they do not have capabilities for handling chemical structures. An industrial chemical information system has to make use of both of these features. As a consequence, many industrial organizations have developed their own capabilities or use a mixture of the above-mentioned commercially available tools.

CHEMICAL STRUCTURE

An industrial chemical information system must provide a way for storing, reproducing, and manipulating information about chemical substances. Chemists have used two ways of identifying chemical substances, nomenclature and diagrams. Both approaches are designed to convey information about the chemical structure of the substance. Standardized chemical nomenclature has evolved to such a point that there are only a few people who are knowledgeable enough to be able to confidently name a substance properly. On the other hand, a structural diagram needs only a few standards in order to be understood by most chemists. The major focus of chemical information systems has been the manipulation of chemical substances.

The representation, storage, retrieval, and manipulation of chemical structure diagrams has been a significant portion of the efforts expended by the chemical industry in the development of their information systems. Intimately involved with and influencing these efforts has been the evolution of computer systems. As computer systems have become less expensive and more capable, a shift from earlier coding techniques to direct input and display of chemical structure diagrams has occurred. Today, most state-of-the-art chemical information systems allow for the input of structural diagrams as the representation of chemical substances. These diagrams are then stored in some fashion that allows for determination of uniqueness to the file and for future retrieval. Queries involving chemical structures, either as complete substances or as substructures, can now be framed by simply drawing a structural diagram. There is no need for extensive coding of queries by a set of rigid and unique rules.

TYPICAL INDUSTRIAL CHEMICAL INFORMATION SYSTEM

An industrial chemical information system is an integrated system that has evolved to meet the unique requirements of a variety of chemists in the industrial environment. A typical industrial system contains the following elements: a core of journals and periodicals in the areas of specialization of the organization; a core of books, monographs, handbooks and encyclopedias; a variety of indices and abstracts to access external literature; a store of internally generated information, usually proprietary; an indexing, storage, and retrieval system for use with internal information; a system for storage and manipulation of chemical structure diagrams; a system for the storage and retrieval of data on specific substances; a system for tracking and accessing patents in the areas of specialization; a system for retrieving external information, usually by use of available on-line services; a system for alerting individuals and groups in the organization to new information.

EVOLUTION OF COMPONENTS

The last 25 years has seen phenomenal changes in some of the components of information systems, whereas there has been

little change in others. The remainder of this paper will describe some of the salient developments in the evolution of these components. Most of these advances have been related to the developments of computer technology.

ACCESS TO BIBLIOGRAPHIC REFERENCES AND ABSTRACTS

As the volume of chemical information increased, publishers turned to computers to maintain currency and cost effectiveness. Computer typesetting and composition and other such applications greatly reduced the manual efforts required to move a manuscript to the printed page. Similarly, computer technology played a major role in the transformation of the processing of abstracts and indices at Chemical Abstracts Service. All of these developments resulted in the transformation of the information into a form that could be easily manipulated without further major human effort.

As information became available in computer-readable form, a number of experiments were conducted in industry to explore the possibilities for novel approaches to information dissemination. One of the first sizable collections of computer-readable information available was *Chemical Titles* published by Chemical Abstracts Service. This publication listed the basic bibliographic information (titles, authors, references, etc.) for articles selected from about 600 core journals in chemistry and chemical engineering. All these articles were also included later in *Chemical Abstracts*. The printed publication provides a permuted listing of the titles as well as an author index. Magnetic tape versions of the publication were made available on a biweekly basis, and a number of chemical companies acquired the tapes. Extracts of these tapes were used to provide alerting notices to employees.[12,13] A variety of approaches were tried, ranging from printed lists of references to individually printed cards for each reference with facilities for ordering the original articles.

These experiments were successful and a number of internal systems were implemented.[14-16] As additional information became available in computer-readable form, it was also included in such services. Chemical Abstracts Service developed two specialized publications that served as prototypes for the complete computerization of their process. These publications, *CBAC* and *POST*, provided, in computer-readable format, the complete text of the abstracts in addition to the full bibliographic record. *CBAC* dealt with chemical–biological–oriented articles, and *POST* covered polymer-oriented articles and patents.

Attempts were made to search the entire text in these documents.[17] However, the computer technology had not advanced to the point where such searching could be done economically and efficiently. It was only until more advanced technology became available that searching of full text became a practical reality.[18] Some experiments have been run accessing the full text of the journals of the American Chemical Society However, the economics are still marginal, and widespread use of full-text searching of the technical literature has not yet become a common occurrence. There are some commercial services that provide text searching of access to legal documents (LEXIS) and news articles (NEXIS).

As computer searching for alerting purposes became widespread, the impetus for retrospective searching became greater and greater. Three events had to transpire before such searching became possible. The first and most important event was the development of a searching language that would allow for an easy way to frame queries. The second was the development of high-density on-line computer storage devices at reasonable cost. The third was the passage of time, which allowed for the accumulation of enough information into a database to make searching efforts worthwhile. In order to make such a database available for searching, considerable preprocessing had to be done. This required the expenditure of significant resources and made it prohibitive for a single company to operate such a system solely for its own internal use. A logical evolution was the emergence of a number of commercial services that made these databases available for on-line searching to a large number of users, thus spreading the development and initial processing costs over a wide base of users.

Originally, it was thought that individual scientists would be able to use such on-line search services on a routine basis. Training efforts to teach individuals how to use such systems were undertaken in a variety of ways.[19] However, experience has shown that a person must be very familiar with the searching language and the data base in order to conduct effective searches. The occasional user of such a system was unable, in most cases, to obtain satisfactory results without an inordinate amount of effort in relearning the characteristics of the system. Information managers have found that it is more effective to allow individual scientists to employ searching specialists when accessing the vast chemical literature that is now available on-line.[20] A number of studies have been made to compare the effectiveness of on-line searching with conventional manual searches.[21,22] In general, a proficient searcher can produce excellent search results with the currently available commercial on-line services. On-line searching has become an integral part of modern industrial chemical information systems.

ACCESS TO CHEMICAL DATA

Although on-line searching systems have facilitated the retrieval of chemical information, they still only provide pointers to articles where the desired data may be. The need for systems that would provide access to data directly has been recognized for a long time. Handbooks such as the *Handbook of Chemistry and Physics* or more extensive compilations like *Beilstein* have provided the user data without having to go to the original source of the information. Individual chemical companies have developed computer-based systems to provide access to collections of proprietary data, particularly where there were large amounts of the same type of data, as with results of biological screening of chemical substances.[23,24]

Physical and chemical property data have also been the subject of attention for on-line retrieval, although most of these advances have occurred in government laboratories.[25,26] Much of this work led to the development of the Chemical Information System[27] within the National Institutes of Health and the Environmental Protection Agency, which is described elsewhere in this issue. Industry has made use of this system to retrieve data on chemical substances. Such systems present different challenges[28] and have not achieved the level of maturity of on-line bibliographic systems. However, an industrial chemical information system must provide access to data, and on-line systems of this type will continue to be explored. Internally developed systems that provide access to proprietary data are in common use.

MANIPULATION OF CHEMICAL STRUCTURE INFORMATION

One of the unique characteristics of chemical information is the ability to represent chemical substances by structural diagrams. This allows for the precise description of a substance and provides a way to classify chemical information. Most queries about chemical information can be framed around the identity of a chemical structure or substructure. A chemical information system must incorporate a means for storing and manipulating chemical structures and substructures. Much of the effort associated with the development of chemical

information systems has been devoted to the handling of chemical structure information. Another paper in this issue addresses these developments in depth, and only a few will be mentioned here.

The extensive and rigorous discipline required to comply with up-to-date nomenclature rules has precluded any significant applications of systematic nomenclature in industrial chemical information systems. Instead, efforts have been focused around the storage and manipulation of structure diagrams. Again, computer technology has played an important role in the evolution of this information system component.

Early efforts centered around development of coding systems that described, primarily, structural fragments.[29] This allowed for the identification of groups of substances with similar structural characteristics. Typically, these systems were operated manually or with the aid of a punched card sorter. As file sizes grew, the precision of such searches deteriorated, flooding the user with false drops. Most of these early systems provided an indication of the absence or presence of a particular structural moiety, but they did not provide any information as to the spacial relationship between the structural fragments.

In an effort to overcome these shortcomings, a number of chemical notation systems were devised.[30-33] These notations provided a complete, unique, and unambiguous description of structural diagrams. These were, in a sense, substitutes for systematic nomenclature and shorthand descriptions of chemical structures. The symbols used were chosen so they could be manipulated by existing computer technology. Early application of Wiswesser line notation in an industrial chemical information system[34] led to extensive modification of the notation system by a group of users[35] and resulted in widespread use of this system within the industrial environment.[36,37] However, all these notation systems suffered from the same drawback as systematic nomenclature. In each case, a structure diagram has to be translated to a series of symbols by a set of rules, which, although not as complex as nomenclature rules, require significant training and intellectual effort.

Another approach, which was taken to circumvent the need for the application of rules and expenditure of limited human resources, was to encode the structure into some form of a computer-readable list of all the atoms (excepting hydrogen) and their connections to other atoms in the structure. A series of computer manipulations sorted through the lists to provide an internal computer representation, which was unique for each structure diagram. This approach was adopted by Chemical Abstracts Service for their registry system and is the basis for a number of systems that provide access and manipulation of chemical structures. Commercial services are now available, which allow searching of the published chemical literature by structurally defined queries.[38,39] The inquirer need only draw a diagram of the structure or substructures desired, and the query is translated into the proper form for matching against the seven million substances now in the Chemical Abstracts Service Registry System.

Industrial information systems use similar approaches for accessing internal information. In some cases they use internally developed systems or make use of commercially available systems such as Private Registry[40] or MACCS.[41-43] Answers to these types of queries can be presented in graphical form, making chemical structure diagrams the common denominator in the communication and dissemination of chemical information.

ACCESS TO PATENTS

Access to the patent literature has always presented a challenge to designers of industrial chemical information systems. In many instances, the information disclosed in chemical patents is much more pertinent to industrial firms than the journal literature.[44] The nature of chemical patents requires a different approach than the one used for nonpatent information. Chemical substances are usually not clearly defined but are presented as broad categories of similar compounds, making clear-cut indexing difficult. Initially, Chemical Abstracts Service indexed only very specific compounds and information that was clearly and explicitly stated in the patent specification, making it difficult to gain access to the information that was only inferred. In many instances, it was this latter type of information that was needed from the patent literature.

Two commercial services were developed in response to this need. One concentrated on U.S. chemical patents, and the other undertook coverage of the major patent-generating countries. These services were and remain relatively expensive and were frought with many problems in their early days. Some companies responded by developing internal systems.[45,46] However, the volume of the patent literature and the amount of effort required to maintain a comprehensive patent information system proved to be beyond the financial capacity of any one organization. Some of the systems developed for internal use in the chemical industry were made available to the commercial organizations. This influx of technology along with concerted development efforts by the commercial services has resulted in significant improvement in the tools available for accessing the chemical patent literature. Chemical Abstracts Service has also taken significant steps to improve its techniques and coverage. Today, an industrial chemical information system can make use of three sources to obtain patent information.[47-49]

A LOOK TO THE FUTURE

The last 25 years have brought profound changes to information systems. As the initiator of many of these changes, the chemical industry has seen the transformation of its information systems. Many of these changes were the result of and paralleled the rapid growth of computer technology. There is no expectation that this rapid rate of transition will change in the next quarter of a century, but we can expect a different approach to the evolution of industrial chemical information systems. Most of the developments and innovations will not come out of the information departments of the chemical industry. Instead, the emphasis will be on the adaptation and procurement of new technology from the now well-established information industry. The use of vendor-supplied systems and services will take precedence over development of proprietary systems.

As computer technology continues to make more powerful computers available at lower and lower cost, the trend toward direct on-line access to information will continue. Personal computers will not only become more versatile and capable, but their use will become widespread. Query languages will become easier to use, making the individual's direct access to the desired information more attractive. Information specialists and managers will function less frequently as intermediaries and will assume the role of coordinators and assemblers of information systems as well as trainers of users.

There will be a much greater emphasis on the storage and retrieval of data as opposed to references to the sources of the data. As more and more on-line data systems become available, the facility for manipulating the data retrieved will become an integral part of the information system, facilitating data analysis, prediction, and estimation. The development of chemical data systems will present a major challenge to the system developer and user. As data are extracted from various sources and aggregated in data systems, the link between the

data and the source is lost. Currently, as a scientist extracts data from a report or paper, an assessment can be made as to the reliability of the data. The scientist can examine the techniques used for obtaining the data as the data are extracted. This user evaluation of the data is impossible with a data system, since the data are no longer associated with the remainder of the information. It will be imperative that a methodology be developed for tagging data with an indication of its limitations and quality. Efforts in this direction have begun, but the issue of data quality will become one of the major concerns of information users.[50,51]

SUMMARY AND CONCLUSIONS

Industrial chemical information systems have changed to meet the ever-increasing influx of new chemical information. A number of significant developments in information science occurred in the industrial environment as industrial systems were developed. However, the broad recognition of the need for timely access to chemical information has spawned a number of commercially available services, which are replacing the need for the development of proprietary systems. Advances have been made and will continue to be made in the application of computer technology, making the widespread desk-top access to data and information a reality.

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