

## End-Users and Chemical Information

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End-users have been classically defined as processors of information (generators of knowledge) who use information sources directly. A more recent definition includes the direct use of computerized information sources, specifically online. End-user searching is described, past and present, and the present context is largely limited to chemists and chemical engineers. Training of end-users to search chemistry files online is described primarily by using our experience at Amoco as an example. A successful program was found to involve self-motivated scientists and engineers and to include training for information awareness as well as online computer skills. Local support is also important, both from information specialists and from management.

In this paper, we discuss education and training of end-users to do their own searching of the chemical literature. We are not involved in education as a career; our experience involves providing continuing education. However, we believe that education is a lifelong process that does not cease when one leaves school. We have been inspired as we are sure many others have been by the following ancient Chinese saying:

If you give a man a fish,  
He will have a single meal.  
If you teach a man to fish,  
He will eat all his life.

Kuan-tzu

### DEFINITION

Is there such an entity as an end-user? Is it just another example of computer hype? Have scientist/end-users existed all along? If the current definition requiring use of computers is applied, end-users are a recent phenomenon but not necessarily hype. If a classic definition is used, scientists, especially chemists, have always been big users and consumers of information. Therefore, end-users have always existed, and contrary to the views of some in the industry, they have never disappeared.

A recent definition of end-user searching is "...literature searching by the eventual recipient of the information, namely the customer, client, the expert (or the would-be expert), or decision maker. This 'end-user', if an expert in a technical subject, is usually in research. Computer-based searching, specifically online, is implied."<sup>1</sup> The chemist performing his own information services or even doing his own searching never really disappeared. Granted, many scientists and chemists have used information intermediaries to an increasing extent over the last 2 decades. Near exponential growth of chemical information produced ever increasing complexity, and the necessary computerization aggravated the complexity even more for the typical chemist. However, recent advances in, and availability of, hardware (mini- and microcomputers), software (word processing and database management programs), and systems (time-shared operating systems, communications, database management systems) have extended the motivated chemist's information "arms reach" to include direct use of computer-based information systems.

The arms-reach concept is hardly new or original. Typical scientists, when faced with a need for information, data, solution to a problem or direction that is not readily derived from their own project or research, will first consult files and books in their own office, then proceed down the hall to query

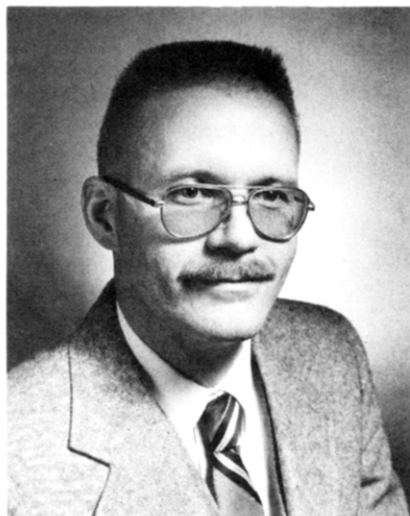
colleagues, and finally arrive at the library or information center (either physically, by phone, or electronically). Once "there", the search has been performed directly by the scientist, or aided by or performed by information personnel. Now, however, suitably trained and equipped scientists can extend their arms reach by proceeding to the nearest terminal or microcomputer equipped with outside communications and perform a good deal of their own searching.

Should all scientists do their own searching? All their own searching? Is the information specialist/intermediary obsolete? Certainly not, but the phenomenon (species?) is here to stay, at least to some extent. Some information professionals and information managers have spoken against end-user searching. They claim that it would not be cost effective for the organization as a whole and could lead to inadequate or "bad" searches. However, appropriately motivated and trained chemists and chemical engineers are capable of doing good, cost-effective, arms-reach searches. Many organizations, after much debate, have decided that some potential end-users will do their own searching anyway and have decided that information groups and professionals should assist end-user training because it reinforces and is an extension of their own service, and can be cost effective. The following philosophy has been expressed: "End-user searching is inevitable. Participate in the training of end-users or, either by inaction, or, worse yet, by active resistance, participate in your own demise."<sup>1</sup>

### BACKGROUND

Not only has the chemical literature grown in sheer volume, it has grown in complexity, including content, number of sources, and media of access. If the required search result is an isolated fact or datum, the source where it is found is by definition the best source. However, many searches are broader in scope and need to be more comprehensive so the days of "one stop shopping" are over. As a result, more sources, files, and systems must be learned, and that involves time and money. The job is even more onerous for the end-user because the end-user is, by definition, a part-time searcher.

Subject content is undeniably more complex. Chemical information is unique in that the definition of chemical structure and the special mathematics of chemical reactions are essential. New methods of analysis and ever growing human creativity have allowed the description of more and more complicated structures, and the documentation system has been struggling to keep up. This has produced problems both for the producers of chemical information systems and products and for users, either intermediaries or end-user. For



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example, in 1972 Chemical Abstracts Service incorporated a drastically revamped systematic nomenclature, the *Ninth*

*Collective Index* nomenclature, into the registry system implemented in 1965. Many information professionals were preparing for big changes when the first semiannual volume issue of the *Chemical Substance Index* appeared in early 1973, but not the end-user. It was only a matter of time before the plaintive wail was heard around the library: "What have they done with styrene?!" We all survived and prospered, and although it was not advertised, some information professionals saw the capability of substructure searching by systematic nomenclature. Implementation of this capability required computerization of the appropriate files, which did not occur until 1976-1977.

Computerization not only has allowed for the proliferation of information sources but has been necessary for the survival and effectiveness of most of them. However, only recently has the use of computers become a typical tool used by chemists in the performance of their work. By decade, the following milestones appear on the path to computerization of chemical information: the 1960s were the decade of batch systems running on large computers in large data processing installations, including database construction, batch searches, and SDI (selective dissemination of information, better known as computerized current awareness); the 1970s were the online decade; and the 1980s are apparently the decade of microcomputers, word processing, and networks. Lack of training, accessibility, and money kept most chemists from directly accessing computerized information sources until the "democratization" of computer access began to accelerate in the late 1970s by means of proliferating terminals, word processors, and microcomputers.

The relative inaccessibility of the computer to most chemists promoted the growth of computer-based information services run by intermediaries. The proportion of direct searching by chemists certainly decreased, and the absolute amount probably decreased as well. Even the 1970s bred end-user entrepreneurs, however. The editor of this Journal, for example, reported<sup>2</sup> on a "do-it-yourself" SDI search system that ran all night once every 2 weeks processing *Chemical Condensates* tapes on a minicomputer ordinarily used only during the day.

Although it has not always been realized, the chemist has, or should have, a large appetite for information. Formerly, life was much easier. A few key journals covering one's field could be read, and one or two secondary services covered the rest of the current literature to a high level of satisfaction. One of the key reasons for belonging to a professional society was discounted journal subscription rates, and until the 1950s, American Chemical Society (ACS) members even received a personal copy of *Chemical Abstracts* (CA) as a membership benefit. In addition, CA could be scanned directly as a current-awareness tool. If one was lucky, a monograph or review was available that described the field of interest well and contained enough seeds of wisdom and omission to generate endless man years of research projects. By the 1960s, many things had changed. Journal subscriptions were still heavily discounted, and graduate students could still think about subscribing to one or two, but secondary sources and abstracts were both expensive (only affordable by libraries) and getting so large as to be not directly usable as a current-awareness tool (unless the field of interest was very narrow, well-defined, and always appeared only in the same place). Monographs had begun to escalate in price, and things were moving so fast that really interesting work was not covered anyway. Additional secondary services began to appear that competed for limited resources of time and money. By the 1970s, libraries began cutting back on resources of all kinds, including *Chemical Abstracts*.

How did a chemist learn to use chemical information? Some courses existed on chemical information usage but were

evidently not very well attended because many in the industrial sector feel their chemists and engineers do not have sufficient training in information use. Apparently, most training was informal (specific task oriented tips from advisors and colleagues) or chemists were self-taught. Three surveys have been made recently of education for chemical information.<sup>3-5</sup> Some formal training is offered in the majority of chemistry departments polled,<sup>5</sup> either through dedicated courses or by the integration of chemical information training into other courses. This is especially true of laboratory courses. However, in only a minority of cases does the material appear in required courses. Hopefully, training is on the increase. The need for chemical information training is now expressed in the CPT (ACS Committee on Professional Training) guidelines.<sup>6</sup> The ACS Division of Chemical Information (CINF) now has an Education Committee that is beginning to accumulate and evaluate materials for instruction in chemical information.

Computerization became necessary to produce secondary services, including abstracts, and also began to be used to prepare the indexes to the abstracts. In addition, computerization spawned new forms of established services or even whole new services and concepts. For established services, it would seem that the computer version of the index, on a suitable search system, could be a good teaching tool. In the case of *Chemical Abstracts*, that was not the case in the early days of availability. Although some end-users learned the effective use of the keyword string index at the rear of each weekly issue of *Chemical Abstracts*, a more effective means was subscription to an information service that provided output by using a customer-initiated profile of interest. Perhaps even fewer chemists used the service, and virtually none of them used it directly. The machine-readable index used was *Chemical Condensates*. Because it was the computer version of the weekly CA index (plus titles and other bibliographic items now searchable for the first time), it became the only effective way to use this index retrospectively when it was provided on two excellent online services in the mid 1970s. However, it became apparent that many searches still required the additional use of the CA volume and cumulative indexes,<sup>7</sup> and the call was made for computer-searchable versions of the latter. Because of the deficiencies of *Chemical Condensates*, its use could not be recommended for instruction on the background and use of *Chemical Abstracts*. Shortly after the detailed index (CASIA) became available online, one of the authors was demonstrating its use to a visiting chemistry professor who then asked the fateful question: "Could this be used to teach the use of *Chemical Abstracts*?" The answer has come to be increasingly "yes" in the years that have followed.

From a chemical information specialist's point of view, readily available online searching dates from July 1973, and by 1975-1976, many information centers were supplying results from online searches on a regular basis. Even in the early years, a few end-users attended online searching training sessions. As time went on and the files and systems improved, two trends in customer attitude appeared. Because of the rapid rate of change in both chemistry and information technology, many users were less and less aware of what impact the advances could have on their information needs. Simultaneously, more and more scientists became curious about the new technology and wondered if they could be directly involved to any extent. The latter group could usually typify the "ideal user"—well aware of the demands of his research, able to formulate problems, and able to help to define what would be acceptable answers and realistic means of acquiring them. Also, in many cases the chemist or chemical engineer was in the process of automating some experiments or pilot units. Many of them could foresee their microcomputers doing double duty.

## THE AMOCO EXPERIENCE

At Amoco we perceived these trends and noted, through professional society meetings and conversation with colleagues, that ours was not an isolated situation. Although we felt we had a good Information Group and provided value-added service, we also perceived that appropriately motivated and dedicated users of our services would eventually teach themselves how to search or acquire the training somewhere. Therefore, we decided to be involved in the process and share our years of experience gained in answering their questions and helping to solve their problems.

Others had also noted the potential for end-user searching. Charles Meadow, in 1977, published the pivotal paper for justification of end-user searching.<sup>8</sup> Computer programming was compared to searching, and both programmers and searchers were described as having "...the keys to the kingdom..." and behaving accordingly. The implicit words to the wise (searcher) were get involved.

"There are at least three approaches to training end-users to search: user-friendly systems, user-friendly interfaces, and user-friendly intermediaries."<sup>1</sup> User-friendly systems,<sup>9</sup> typically programs that run on local hardware that simulate remote, time-shared search systems, are quite expensive to develop. Until recently, the same could be said for user-friendly interfaces, but several have been commercially available since 1983. Such programs, now called "gateway software"<sup>10</sup> for microcomputers, lead searchers along step-by-step through search strategies (menu driven) and often allow for recording and cataloging search results. At Amoco, we have only one end-user who regularly uses a gateway program on his microcomputer. It satisfies his immediate information needs, and he still patronizes the Information Group for more detailed searches.

In 1981, we at Amoco decided to use the third approach, user-friendly intermediaries. We already had intermediaries who were interested, and we had neither the time nor the money to develop or acquire the other two approaches. Very few results of other programs were known so we developed our program from scratch. We predicted that some end-users would wish only heightened awareness of literature sources and searching methods and some would want to do their own online searching. Therefore, we set up a program of classroom courses with both lecture and demonstration describing sources, databases, and searching methods. Upon completion of the course, attendees were given the opportunity to sign up for individualized, hands-on training for online searching. Interestingly, only one-third of the class attendees have elected to proceed to learning online searching. The remainder are satisfied with enhanced awareness of technical information and appear to be better users of information.

The courses were arbitrarily split into two series. Course I covers *Chemical Abstracts*, and course II covers several other topics including patents (in general), Derwent WPI (World Patent Index) files and products, IFI U.S. Patent files, API (American Petroleum Institute) files and bulletins, *Engineering Index*, *Physics Abstracts*, *Science Citation Index*, PROMT (*Predicats Marketing Abstracts*), CIN (*Chemical Industry Notes*), etc. Credit is given for a technical continuing education course, and we ask for a supervisor's signature. The courses were divided into three 1-h sessions. The first covered printed sources and search methods; the second featured demonstration of online searching of the appropriate files. For the third session, sample questions were solicited from the attendees, and searches of most of the questions were demonstrated in class. Course I has been given 10 times and course II twice. Proposed changes include lengthening each session to 1.5 h and reorganizing course II. Instead of being organized by computer vs. printer versions of the sources, we propose

to give at least four modules covering reference and physical properties, patents, API (American Petroleum Institute) files and publications, and business and marketing files.

Neither course is a prerequisite for the other, but we usually require attendance at either of the courses as a prerequisite for individualized training. No charge is made for the classes. Password request forms are sent to those attendees who request them, and we require a supervisor's signature and a project number. We provide a searching quick guide for the vendor and a brief handout prepared in-house, but all other expenses are charged back to the end-user. All passwords are maintained under a group account. End users receive a copy of the bill after it is paid but avoid the hassle of paperwork. We also ask that they provide their own terminal. Although early trainees mostly used terminals, personal computers are the most common hardware used by recent trainees. One veteran end-user searches exclusively from his personal microcomputer at home and recently acquired a BRS/After Dark password because he was interested in full-text files like the ACS Journals file and Kirk Othmer online. (BRS/After Dark is a service offered by BRS Search Systems that features menu-assisted searching and reduced rates.)

Although few follow-up training sessions are requested, most trainees continue to consult with their trainer (all Information Group staff) on an individual search basis. In addition to our training, we have made vendor training available on-site and encourage off-site vendor training for more background on the system or for specific databases. On-site training sessions include SDC Basic, business files overview (Dialog), searching for chemists (SDC, DIALOG, and API), and CAS ONLINE and Derwent Dictionary searching (for both intermediaries and end-users).

For a number of reasons,<sup>1</sup> including historical availability of three of the files of most interest to us (*Chemical Abstracts*), API, and Derwent), SDC was used for course demonstrations and most of the basic training. However, six scientists were trained on DIALOG, and several of the SDC trainees have subsequently received DIALOG passwords and training. Of the 158 course attendees, 57 (36%) requested passwords, but nine dropped out before they could be trained. Of the remainder, only three have dropped out.

Several other industrial end-user training programs have been described recently<sup>11-15</sup> as well as one vendor program.<sup>16</sup> Results described varied, but all authors felt they were responding to local needs of customers, and everyone involved seemed to derive benefits from the process. End-users were perceived to require a realistic view of their own information needs and self-motivation both to be trained initially and to continue to search after training. Retention rates of trained end-users varied for a number of reasons, the most common of which appeared to be a lack of time or suitable questions. All seem to assume that not all available candidates will request training and not all trainees will continue to search, but none regretted participating in the process and hope to continue with constructive changes in their methods.

## CONCLUSIONS

Several conclusions can be drawn:

- (1) The best chance for success seems to occur where the trainees make their own decision to acquire the skills (assuming that management support for both the trainers and trainees is essential). Self-motivation and individual perception of need are very important.
- (2) There is an even larger market for increasing the information awareness of end-users than that of training online end-users.
- (3) It can be a win-win situation for all participants. The trainers learn more about their craft by teaching it, and

trainees become better users of information by going through the experience.

(4) Trained end-users do not stop requesting searches of information groups. Most make about the same amount of requests after being trained or somewhat less, but the requests that are made seem to be more complex and better thought through.

(5) Local support is important. For example, at Amoco we feel that at the minimum we should provide some introduction to online searching before the trainee receives vendor training. The vendors know the situation, and DIALOG knows that their courses must serve three types of end-users: those at sites with trained intermediaries, those at sites with intermediaries not trained in chemistry, and those at sites with no intermediaries or libraries. Course presentation and follow-up is geared accordingly.

(6) Continued interest in online searching will be maintained through integration of office automation technologies. As office automation functions become available throughout organizations, end-users will begin to request online searching capabilities not only of internal database but of external information sources as well. We see those types of requests already within our own company from clients who have not formally been users of any outside service. Interest is being generated within users' groups that have been outside the circle of direct use of chemical information. We have seen interest from the staff of technology planning, marketing, and forecasting groups.

Online searching is not for everyone, but those who persevere will be rewarded. We think the material discussed above should be sufficient motivation for information professionals and research management to establish and participate in end-user training programs.

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## Information Chemistry in Japan

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A brief history of the abstracting services for journal articles in Japan, starting with *Kagaku Soran* in 1927 and leading to the recent development of the nationwide on-line information service system of TOOL-IR, is given. Current activities in information chemistry in Japan are also reviewed. The importance of the basic terms in science and technology is stressed in relation to the promotion of better exchange of chemical information. It is also observed that the old Asian documents may be considered as a kind of database of chemical substances. Although Western chemical science grew as an analytical science, presently it relies on the databases of chemical information. The latter fact may be considered as the merging of the standpoints of chemistry in the East and the West.

### INTRODUCTION

**Historical Sketch.** In the past few decades, enormous developments have been achieved for chemistry through the use of computers. They have occurred in the fields of computational chemistry, chemical information, and physicochemical measurements. The latter include access to data, control of samples, instrument interfaces, and data handling such as accumulation, fast Fourier-transform analysis, and other sophisticated data manipulations. More recently, computers have been widely used for the generation of bibliographic databases and for the retrieval of information.

Those active in the fields cited above organized meetings that dealt with topics of computational chemistry and chemical information. The former were oriented more to the software problems of chemical information and the latter more to the studies of the database management system (DBMS) or to the problems of retrieval of chemical information.

Apparently both phases of activity cited above are equally concerned with chemical information, although each has a somewhat different purpose. Recently, it has been recognized that activities in computational chemistry and in chemical information could be merged into one, because both overlap with and rely on each other. Thus, the division of information chemistry was formed within the Chemical Society of Japan in 1983 with Prof. S. Sasaki as the chairman. Its annual meeting in 1984 was considered the seventh. That took into account the number of previously held meetings on chemical information.

The abstracting service for the journal articles was first started in 1927 by Prof. Toshiyuki Majima at Tohoku University. He built *Kagaku Kenkyukai*, which published *Kagaku Soran* (*Complete Abstracts of Japanese Chemical Literature*).<sup>1</sup> Prof. Shinichiro Fujise continued the work of Prof. Majima until 1963. *Kagaku Kenkyukai* was succeeded by the Japan Information Center of Science and Technology (JICST) in 1963. The latter is an organization fully supported by the Japanese government. *Kagaku Kenkyukai* is still active in the promotion of information chemistry, such as granting fellowships or research funds to young scientists.



Shizuo Fujiwara graduated from the Department of Chemistry, Faculty of Science, University of Tokyo, in 1944 and obtained his Dr.Sc. degree in 1949. He was appointed assistant professor at the University of Electro-Communications in 1949 and full professor in 1956 and moved to the University of Tokyo as professor of analytical chemistry in 1960. He served there as director of the Research Center for Spectrochemistry (1977-1979), the Research Center for Information and Library Sciences (1978-1981), and the Central Library (1978-1981). He retired from the University of Tokyo and moved to the Chiba University as chemistry professor in 1981. He served as a titular member of the Interdivisional Committee on Machine Documentation in the Chemical Field (1969-1976) and of the Commission on Atomic Weights (1969-1976) of IUPAC and as a council member (1979-1981) and vice-president (1981-present) of FID. He is now president of the Japan Society for Analytical Chemistry and editor of *Analytical Sciences*.

The Science Council of Japan (SCJ), started in 1949, maintains a national committee on information. That committee had two divisions before the reorganization of SCJ in 1984, one on information of documentation and the other on numerical data. The first division has been concerned with the problems of journal publication, standardization of articles, management of libraries, and codings. It also acts as the