excellent public relations vehicle.

Why, after their initial enthusiasm and eagerness to learn, do the end user-searchers not make greater use of these systems? It is obvious from the literature[2,3] that there are a variety of approaches to training end users, but there are certain factors that must be present as far as the end user is concerned, in order for the training to "take"—that is, to keep the user-trainee searching.

First of all there must be a *need* for information—with most researchers, this need is not sufficiently constant to allow them to use online systems as often as is necessary to keep search skills sharp. There are certain stages in a research project that are information-intensive. There is a great deal of information activity at the beginning of a project, and then, as research progresses, more limited periods of activity mark problems or changes in direction. Ongoing information needs are met by scanning current journals or by a selective dissemination of information service that automatically generates new references to update a previously stored search strategy. Thus, without the opportunity for constant practice, especially for new users, every search becomes a relearning situation—very frustrating and time consuming. There must also be *motivation* to continue to use the newly learned skills. Our users feel that the complexity of the systems and database structure, together with the availability of excellent service from the search staff, reduces the motivation of "do-it-yourself". Where there are no library services readily available, as with the Canadian group, motivation is higher. Lastly, *interest* in doing one's own searching is important. Most researchers simply find their own work more interesting and demanding. Online searching can be productive, but if it cannot be done easily and well, researchers lose interest and will not take the time from their regular work to pursue searching. Most of our continuing users have no illusions about their skills—they use the systems for general information, to find a few references to "tide them over" till a searcher can fill in more detail, or for an overview to give them some idea of what is going on in a particular area of technology.

It is heartening to learn that the Cyanamid experience is not so different from that reported in other companies. The information needs of the end user are generally not sufficiently constant or pressing to warrant taking time away from primary responsibilities to become and remain reasonably adept at online searching. No matter how the training is structured, end-user usage quickly falls off, leaving a small number of users that search with some sort of regularity.

Having said all that, will end-user training at Cyanamid continue? Definitely! As long as there are users in our organization that feel they could profit by self-searching, instruction geared to their needs will be provided!

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Meeting the Needs of the End User

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Performing a computer literature search has traditionally required an information specialist or librarian to perform the search. As the demand for more information increases, the person requesting the information, an "end user", is becoming more involved in the search process. The experiences and guidelines DIALOG uses in training the end user in searching computerized chemical information are discussed.

How can we best meet the needs of the end user? Unfortunately, neither the question nor the answer is straightforward. The underlying difficulty with this question is that the term "end user" covers a broad spectrum of information seekers with diverse needs. In order to attempt to meet their needs and assess the value of doing so, three things should be established about end users.

(1) Who are they? Where do they come from?

(2) What do they need? Do they want what they need and do they need what they think they want?

(3) Where will they go from here?

Answering questions two and three seems to return us continually to question number one. Who are the end users, how do they differ, and how are they alike?

In the discussion that follows, the term end user has been defined as someone who is not an information professional but desires to do his or her own information searching. For the purpose of this paper, a further qualification has been placed on the end user in that we will be discussing scientific end users who must have a chemical or physical science background. This is because end users from other disciplines (medicine, law, business, etc.) have also been learning to do their own

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searching. The needs of these groups are typically quite different from those of a scientist, and the databases taught are not so complex in subject nature as chemistry or engineering.

END USERS—WHERE DO THEY COME FROM?

DIALOG Information Services has participated in many projects that have trained a number of end users. Most of these projects have been conducted under the auspices of information centers and qualified information professionals at various organizations. The results of some of these projects have been published earlier. In addition to these custom-tailored on-site sessions, we have been training scientific end users in our System, Science and Technology, and Chemical Information Seminars for several years. These seminars were originally developed to teach librarians and information intermediaries what they needed to know to perform their jobs effectively. In the past 5-year period, those attending DIALOG seminars have changed from being almost entirely information professionals (e.g., librarians) to being 90–95% end users from every discipline.

It was the experience gained from having end users in these sessions that led to the conclusion that end users have needs quite different from information professionals and that it was necessary to revise our training approach to satisfy those needs. This was especially true for the chemical and engineering end users who did not appreciate, or have a use for, search examples dealing with the humanities and social science databases on DIALOG.

On the basis of our past experience, we have identified three categories of scientific end users: (1) those aware that computer-searching services are available from a qualified technical information specialist; (2) those aware of information retrieval but feel there is something beyond what their nontechnical librarian is providing; (3) those coming from organizations that lack a library or information department.

Those end users who belong in the first category typically have one of three motives driving them to do their own searching. One reason may be that they may want to avoid the delay in receiving search results from a backlogged information center. Second, the first category of end users contains the group of scientists motivated by the fear that the "information explosion" will get the better of them. They want to learn how to do their own computerized information retrieval so they will not be left behind when the dust settles. This particular motivation is reinforced by intensive marketing of personal computers, as well as an occasional attitude that "if the information specialist can learn to do it, so can I...it must not be that difficult". Finally, the third motive within category one is the desire to seek information for information's sake. These end users are anxious to learn about any tool that will help them keep up with the volume of information being generated in their specialty, as well as the related literature in their technical field.

DIALOG has conducted at least one (usually multiple) on-site training session at over 50 different company locations since 1979, the majority of which were hosted by large industrial organizations. The end users attending these sessions have had the motivations described in category one. The majority of the sessions were arranged by the Information Centers at the respective companies. The large number of sessions indicates that the information professionals as well as company management recognize the potential value in allowing scientists to do their own searching.

At many companies chemical managers are encouraging research staff to become more familiar with the many new products and technologies. Online searching should help accomplish this goal. In addition to on-site sessions, there have been an increasing number of chemist end users attending our regular training sessions who fit into category one.

The second category of chemists and scientists who desire to learn online information searching came to our attention via the customer service toll-free lines. There have been numerous conference calls comprised of a DIALOG representative, frustrated chemists, and librarians with "chemical-file phobia". Our experience in the booth at the National American Chemical Society (ACS) Meetings and other conferences reaffirmed the suspicion that there are a large number of chemists who do not have the benefit of a qualified technical information professional to fill their information needs. Many chemists would stop by the booth and ask us to try a search that their librarian had found to be impossible.

In an attempt to reach these end users as well as those in the third category, DIALOG decided to offer an end-user workshop in conjunction with the National ACS Meetings. The intent was not to take business away from the organizational libraries but to educate the chemist in the basics of searching so that he/she could formulate chemical queries in a manner that would be beneficial to both parties.

The third category consists of those scientists who belong to companies or colleges that do not have a large library collection or access to online information retrieval within the organization. Of the three categories of end users encountered, this group is perceived as having the greatest need to do their own searching.

END USERS—DO THEY WANT WHAT THEY NEED AND DO THEY NEED WHAT THEY THINK THEY WANT?

The goal in the development of training materials, as well as the scheduling of classes, was to address the needs of the end user regardless of his category. Obviously, the needs of the group, the success of the course, and the continued use of the system would vary depending on their environment, user aids available, and the search assistance available.

In order to begin searching, one must learn and understand the basics of using an online system: using the terminal, the system commands, Boolean logic, and database organization within the computer.

Most chemists are interested in searching the chemical databases. To conduct a satisfactory search, they should first learn something about the organization of chemical information in the hardcopy publications. This is one area of training that is often overlooked by the beginning searcher but necessary in that there is a direct correspondence between the indexes created for publication and the online version of the database.

Finally, a requirement unique to the end users is that the training take as little of their time as possible. Since doing an online search is not normally their primary function within an organization, their management might frown upon them devoting more than 1 day to learning the basic techniques. In discussing what the most ideal time period would be, most said that 1 day from their laboratories would not be considered excessive, while a day and a half might be considered too much.

Between 1981 and early 1983, DIALOG responded to requests for end-user seminars by merging topics from our introductory course (the System Seminar, which was designed to be given in 1.5 days) with the Chemical Information Seminar (which is 1 full day). Using these materials, we attempted to teach end users ALL the commands covered in the System Seminar, as well as introduce them to the organization and retrieval of chemical information. This was attempted in a 1.5-day session, occasionally cut down to a single day! During the hands-on practice time held at these sessions, it was found

that, (1) although end users had quickly grasped Boolean logic and the basic commands, they were using only a fraction of all the techniques covered and that (2) they were completely confused by the organization of the files. Some even left the class thinking they could search only the Chemical Abstracts Service (CAS) derived files. They did not understand that, using the commands they had learned, they would be able to make use of the wealth of scientific information in the other databases on DIALOG.

Careful consideration was given to these observations; and it was decided to develop a new end user oriented training seminar, which was titled "Searching Chemistry on DIALOG", otherwise referred to as the "SYSCHEM" Seminar because it is a combination of the System Seminar and the Chemical Information Seminar. The goal was to teach the end users selected principles of searching DIALOG and the applications of the principles to databases of interest to chemists without overwhelming them. End users who might later feel restricted by their limited knowledge could either take additional training courses or read the documentation. It was decided that it was better to get a few important points across to many rather than try to get all topics across to a few.

The following outline reflects our most recent conclusions as to topics and the order in which they should be presented to a group of end users.

I. Searching DIALOG
   A. Basic Commands
II. DIALOG Chemical Information System
   A. Introduction
   B. Information Organization (hardcopy vs. online)
III. General Search Features
   A. Literature Files
   B. Substance Files
IV. Search Techniques
V. Sample Searches (demonstrating a cross section of scientific databases available on DIALOG)
VI. Appendix

This new seminar was originally offered with the first two sections reversed. The comprehensive overview of chemical information organization was presented first, followed by an introduction of the basic commands with hands-on-practice after lunch. With that sequence, the group concentrated so much on the basic commands that they could not relate the search options to the organization of chemical information. Reversing the order of the sections had a very beneficial effect on the groups' understanding. The key seems to be the "hands-on" time after learning the basic commands, which is done in the first hour of the course. Once end users realize how simple it is to conduct a basic search, they return to the lecture confident and eager to learn more. In attempting to teach so much in so little time, it becomes important to retain the enthusiasm and attention of the class at all times.

The new SYSCHEM seminar teaches the searchable fields end users are likely to use most often. The only prefix terms discussed are AU=, CS=, and RN= in the literature files and MF=, RC=, RN=, and SY= in the substance files. The use of DIALINDEX, MAPRN, and other search techniques is introduced only once and used in examples that follow. It is assumed throughout the course that scientists have been trained in inductive reasoning and can therefore apply what they see to their own search topics. This approach differs in degree from other DIALOG training curriculums.

The last significant difference in the SYSCHEM seminar is the size of, and topics included in, the Appendix. All database blue sheets (summary searching guides) that are considered related to chemistry are included in the seminar materials. Complimentary chapters (detailed searching guides) for searching CHEMNAME and CA SEARCH are made available to seminar attendees. This is done to ensure that the end users have everything they need to conduct a search. The less time they have to spend tracking materials, the more likely they are to apply what they have learned before it is forgotten. Having a password available at the conclusion of the seminar is another factor that tends to influence use of the newly learned skills. Training and practice passwords are provided by DIALOG at the end of the class. The practice passwords access a group of databases that are of limited size to allow the attendees to practice using the commands and developing search strategies. It usually does not take much time after practicing at DIALOG's expense for the users to feel confident in searching DIALOG.

The SYSCHEM seminar was first given at the Seattle National ACS Meeting in the Spring of 1983. On the basis of the questionnaires returned at the end of the session as well as the searches that were performed at the end of the class, we felt that our goals had been accomplished.

END USERS—WHERE WILL THEY GO FROM HERE?

One thing we do not want end users to do once they complete our course is think that they are information specialists. This would be an unrealistic assumption for even the brightest end user. Most end users who have an on-site information professional gain respect for their skill and knowledge following this introduction to chemical information science. Others, who do not have access to an information specialist, are cautioned to consult DIALOG Customer Service for assistance with a difficult search. Throughout the end-user seminar, it is stressed that what is being taught is only an introduction to chemical information retrieval and is by no means meant to be comprehensive. The following situations are mentioned as guidelines for seeking the skill and knowledge of a technical information professional: (1) if the search is comprehensive or involves using search techniques not discussed in the end-user seminar; (2) if there is a dollar value or project decision dependent on the results of the search; (3) if the search fails to locate information that is thought to exist; (4) if the need arises for a search to be performed in databases outside the expertise of the end user.

As stated earlier, the final version of the end-user seminar accomplished teaching the attendee enough to perform a basic DIALOG search. Whether or not end users will continue to perform some of their own searches several years down the road remains to be seen. The answers will depend on their needs and what sort of information-retrieval alternatives are available.

End users who attended the first ACS End User Workshop were contacted to see how many continued to perform searches. Out of the 14 people who attended the session, 9 were reached by phone. One year after attending the workshop, seven people were doing their own searching. One attendee was not doing his own searches but incorporated what he had learned into the curriculum of one of his classes. One other person who was not doing his own searching said that his company management would not support any sort of technical information retrieval (the company did not have a library), but he found the class enlightening and would probably eventually obtain a password for personal use.

We have not attempted to collect statistics from all of the on-site end-user seminars to determine how many of the end users have continued to perform their own searches. It was felt that the statistics themselves would not measure the value of meeting the needs of the end user, nor would they indicate whether we should continue end-user training. More significant are the comments we have been hearing from many of the information centers that have coordinated in-house seminars, as well as the increased demand for additional end-user

seminars, within the same organizations.

Following end-user training, within an organization, many information specialists are reporting that they are actually busier than before and that the searches brought in are more challenging and better thought out by the scientist. The comments we receive from scientists are those of enthusiasm, appreciation, and awe of their newly learned power. Without question, these scientists should not be denied the training needed to access online scientific information.

As information grows in volume, it becomes more difficult to assimulate; but as it grows in volume, technology has made it easier to store, manipulte, and disseminate. The technology that exists and the knowledge that online searching provides must be extended to all people that need it...the end users.

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TOSCA: A Topological Synthesis Design by Computer Application†

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TOSCA is a deductive method for the design of syntheses both in the forward and in the backward retrosynthetic direction. The use of strategic selection criteria makes it possible to use the system in particular in heterocyclic chemistry. It is shown by means of examples how empirical selection criteria lead to an intelligent reduction in the number of proposals. Structural features identified in precursors and the target of the synthesis form the basis for a further, subjective selection.

INTRODUCTION

Chemistry is an essentially experimentally and, hence, phenomenologically oriented science. Not surprisingly, the first synthesis design methods involving the use of computers were likewise empirically oriented, since they simulated the thought processes of the chemist by directly applying literature knowledge to an actual problem of synthesis.[1]

This reasoning by analogy is effected in empirical synthesis design methods with the aid of a library of transformation instructions that has been derived from chemical reactions. The amount of work that is necessary to cover specific areas of chemistry in this way naturally increases with their complexity. The variety of heterocyclic chemistry makes it very time consuming to put together a suitable library of transforms. For this reason, we were interested in examining to what extent a mechanistic-[2] or logic-oriented method[3] might be suitable to cover the industrially important heterocyclic area.

The starting point for the development of such a method was an algebraic model of constitutional chemistry[4] where synthesis proposals are generated by combinatorial changes to the bonds and bond orders between the atoms of given molecules. The number of transforms, i.e., transformation instructions, with this logic-oriented synthesis design method is much lower than that with the empirical method, since the electrons are manipulated purely combinatorially, that is, without consideration of the structure of the molecule and independently of the nature of the atoms.

However, a purely combinatorial procedure that only takes account of electron pairings produces not only proposals that can be interpreted in a chemically meaningful way but also so much more that is just garbage.

It is therefore necessary to resort to the computer-based application of selection criteria. For this purpose, we have differentiated the atoms according to potential donor or acceptor reactivities.

† Dedicated to Professor Rolf Sammet on the occasion of his 65th birthday.

This differentiation makes it possible to select charge-controlled reactions. This strategic option is also associated with division into reactions which involve umpolung and those which do not.[5] This concept, which is important in particular in the field of heterocyclic chemistry, is also important in extended areas of aliphatic chemistry.

In this way, the idea of combining a nonempirical method with selection criteria of universal validity is realized in TOSCA. Additional empirical selection criteria and interactive selection options then lead to a further reduction in the number of synthesis proposals.

IDEAS BEHIND TOSCA

Simulation of Reactions. The number of computer-generated precursors in a deductive synthesis design method is critically affected by (1) the decision about which of all the bonds present in the target of the synthesis are breakable, i.e., reactive, (2) the number of combinations of bonds to be broken in any one step that can be made from the set of all breakable bonds, and (3) the number of ways of recombining the reactive centers thus formed.

About 75% of all known chemical reactions involve the breaking and simultaneous forming of two or three bonds as depicted schematically in Figure 1.[6]

Such a method did not appear sufficient to be of wide applicability. For this reason, TOSCA incorporates an algorithm that permits up to 11 bond cleavages and 11 bond formations per reaction step. These numbers include the breaking and forming of multiple bonds. As in the majority of cases only two or three bonds are reoriented in a reaction, this method increasingly simulates reaction sequences in one step from four participating bonds onward.

Fundamental molecular changes are frequently difficult to keep track of. For this reason, TOSCA calculates the chemical distance between the individual precursors, which can then be arranged to form manageable reaction sequences. Identical precursors are automatically rejected in favor of the proposal involving the smallest shift of bonding electrons.[7]

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