BASIC INFORMATION SCIENCE TRAINING FOR CHEMICAL ENGINEERS*

O. M. KUT[1], R. QUERALT[2],
AND L. M. ROSE[1]

[1]*Swiss Federal Institute of Technology (E.T.H.) Zürich, Switzerland.*
[2]*Instituto Quimico de Sarria, Barcelona, Spain.*

The objective of this paper is to indicate the possible contents of such a course and to relate some experiences already gained in teaching the subject to chemical engineering students.

WITH THE INCREASING amount of published information and improved methods of assessing this information, there is a new awareness within chemical engineering that systematic information retrieval from the literature is an important starting point for any type of project. To match this awareness (already prevalent in industry), chemical engineering courses should include some instruction in the subject of information science.

There is more to information retrieval than simply knowing where the library is and knowing how to use an index. It is possible to give students a more thorough background in information science in a comparatively short course—if it is well organised. The objective of this paper is to indicate the possible contents of such a course and to relate some experiences already gained in teaching the subject to chemical engineering students.

COURSE OUTLINE

A modern information and documentation course for chemical engineers should cover printed bibliographic information, numerical data, and methods of computer retrieval, both of numerical and bibliographic data.

Available Printed Information

Traditional literature searching has always concerned itself with searching the scientific journals—*the primary publications.* Since chemical engineering is a mixed discipline, it is often worthwhile to look in other specialized areas for relevant material—statistics, operations research, chemistry, mechanical engineering, computing, and electrical engineering all overlap with various chemical engineering subjects, particularly at the research level.

Primary literature goes beyond the published journals; conference pre-prints, dissertations, and patents all belong to the primary literature, but are more difficult to obtain than the international journals. The difficulty in obtaining these very important publications is overcome by the development of the secondary publications.

The *secondary publications* are abstracts of the primary literature, the most famous of which is *Chemical Abstracts. Chemical Abstracts* is so important to the chemical engineer that he should be able to use it without difficulty, understanding the concepts of its indexing and registry numbers for components. Chemical engineering has some lesser known abstracts of its own: *Theoretical Chemical Engineering Abstracts* (POB 146, Liverpool, England), *Chemical Engineering Abstracts,* (University, Nottingham, England), and *DECHEMA,* (PF 970 146, D-6 Frankfurt-97, W. Germany). Abstracts in overlapping fields (*INSPEC* for mathematics and control, *Engineering Index* for heat exchange) can also be useful.

Under secondary publications one can also list the *Science Citation Index* (SCI) which enables forward searches to be made, and the ISI weekly publication of contents pages of the scientific journal, *Current Contents,* enabling the contents of most of the recent journal issues to be effective-

*This paper was commissioned by the European Federation of Chemical Engineering, Working Party on Information and Documentation.

ly followed.

Finally there is the tertiary literature. This is an organised summary of the literature in each particular field: handbooks, monographs, data collections, and textbooks. Perry is, of course, the most important. Then there are the encyclopedias of chemical technology of Kirk-Othmer and Ullmann.

Numerical data are very important to the chemical engineer, and these are generally found in the tertiary publications. General data concerning chemicals are best covered by *Beilstein* (organic) and *Gmelin* (inorganic). Though both these works were in German, new editions are now in English. Other publications concentrate on particular properties.

Finally there are the monographs and textbooks. They often provide an excellent starting point for any search by summarizing the particular technology up to a certain point in time—which is often adequate for the needs of many problems.

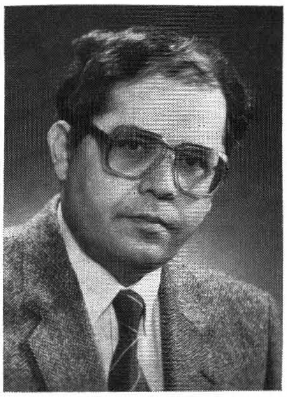
The graduating chemical engineering student should be aware of these facilities in his library. He should be able to carry out searches in *Chemical Abstracts,* know where to obtain numerical data, know how to use the subject and author catalogues in the library, and know that the librarian is a trained professional, there to help him when he has difficulties.

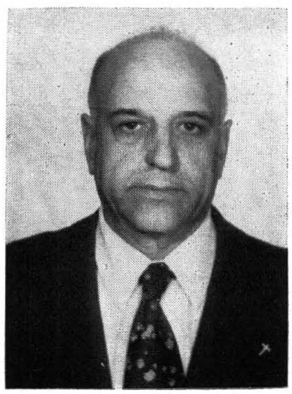
Computer-Stored Information

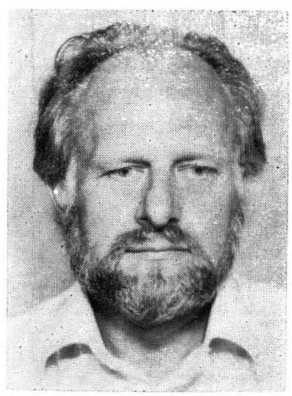
Bibliographic Data Bases: The history of the development of computer readable bibliographic data bases is a fascinating opening to the subject of the production of SDI (Selective Dissemination of Information) tapes. To rationalize the production of the printed abstracts, the total abstracts were coded onto magnetic tape. It was then a small step to the distribution of these tapes to institutions wishing to perform their own searches electronically rather than waiting for the printed versions to be posted and going through them manually!

It is interesting for most chemical engineers to know the principles on which the computer searching is done. The availability of the abstracts on tape, the need to have a thesaurus and to invert the SDI tapes to be able to recover which abstracts refer to each particular keyword are important points to explain in the course.

There is a growing feeling among information scientists that the engineer himself should understand how computer searches are done. The need to choose the individual keywords carefully and to define a suitable search strategy, to know the pitfalls of not including enough alternative descriptions, and to know how to improve the relevance by including further keywords. It is particularly important that the chemical engineer know which data bases are likely to be of most use to him. Surveys in Europe have shown *Chemical Abstracts* to be the most useful (although it is far from ideal for most chemical engineering problems). *Chemical Abstracts* needs backing up with *COMPENDEX* or *INSPEC,* where appropriate. Besides these three there are many other data bases covering particular areas of use to chemical engineers—part of the NIH-EPA Chemical Information System for safety







Oemer Muhan Kut received his M.Sc. and Ph.D. degrees in chemical engineering from the Swiss Federal Institute of Technology (ETH) in Zurich. Since 1972 he has been a research associate at ETH. His major research interests are in the areas of applied catalysis, catalytic reaction engineering, and modelling of multiphase reactors. **(L)**

Rafael Queralt received his diploma in chemical engineering from IQS and since 1963 has been an assistant professor at the Instituto Quimico de Sarria. He is also head of the Library and Documentation Services at IQS, which is a pioneer centre of automized chemical information in Spain. **(C)**

L. Murray Rose has a B.Sc. and a Ph.D. in chemical engineering from Birmingham University. Before joining the Systems Engineering Group of the Technical Chemistry Laboratory of the Swiss Federal Institute of Technology (ETH) in 1971, he spent twelve years in industry. His efforts are toward instigating the sensible use of computers in all branches of chemical engineering. **(R)**

and chemical properties, DERWENT for patents, PREDICAST for commercial information, DECHEMA for equipment design and corrosion problems, etc. The undergraduates should be made aware of the scope and limitations of the various fields.

It is also good for the undergraduates to be informed on the component parts of the computer literature searching system—the abstractors, the files and inverted files, the hosts, the communications networks—that all need paying for every character retrieved. And then, the multitude of languages!

Numerical Data Banks: Parallel to computer retrieval of bibliographic data, banks of physical properties for use by chemical engineers have been developing and are now generally accessible by any terminal connected to the telephone network. Most normal chemicals in commerce ($\cong$800) are now available on these banks which store numerical physical property data, or use predictive methods to give estimated values for those not available. PPDS, EPIC and DECHEMA systems are available in Europe, and PPDS in the US.

The subject would be given more status if it were a short course in its own right, and not simply squeezed into odd hours.

For teaching purposes, a number of small demonstration banks exist. CHEMCO is probably the most widespread. There is no better way of making a student realize that these modern tools are available to him than to let him use them during a design project.

Such data banks could be handled in an information and documentation course or in a thermodynamics course, since they are excellent for demonstrating enthalpies, chemical equilibrium, vapour-liquid equilibria (VLE), and equations of state. For them to be handled in both courses would have the advantage of helping integrate the whole curriculum.

SEARCH PROCEDURES

There are two fundamental types of literature searching

- **Retrospective searching, where a comprehensive list of relevant literature published on a special topic is sought**
- **Current awareness searching (SDI = Selective Dissemination of Information), where the interest concerns the current publications on the topic under study.**

The selection of information sources and the mode of information retrieval will depend on the type of search. For starting a systematic literature search, the problem and its limitations should be clearly defined. In manual as well as in on-line searches, the effectiveness of the study depends on how well-prepared the search strategy is. To get some experience in strategy preparation and optimization, the library users should practice manual searching techniques before starting on-line searches.

A very useful start for undergraduate students in chemical literature are small search exercises in *Chemical Abstracts* using the printed indexes. The user should become familiar with the Index Guide and the Chemical Substance Index using the *Chemical Abstracts* nomenclature. He should also learn the concept and the limitations of the Registry Numbers. These numbers, characterizing a single, well-defined chemical compound, build a link between different bibliographic and numerical data banks. The user should also practice how to select relevant keywords with all their synonyms and truncations. He should also be familiar with the linking concepts (and, or, not) creating combinations of sets selected by the keywords. For narrowing the search strategy the user should also be aware of other possible limitations such as language, document type, country, or publication year.

Even with all these preparations, electronic information retrieval continues to be a difficult task for the average user without the assistance of information specialists. For example, the *Chemical Abstracts* (CA) SEARCH files are accessible from many host systems such as Lockheed, SDC, or Data Star. However, every host system has its own software and its specific advantages and disadvantages, making different set combinations and search strategies possible. The fine structure of the programs are developing. An average end-user making only a limited number of on-line searches cannot be aware of all the progress made to reduce the search costs. Although development in the direction of "user-friendly systems" is progressing, at the moment the optimal combination seems to be co-operation between the information specialist who knows the information systems and the end-user who knows the extent of his information requirements, so that the on-line systems can be used efficiently as an interactive system adapting the search strategy to the given information. This need for teamwork between the information specialist and the engineer is ground enough for the undergraduate engineer to be made aware of the principles of information retrieval.

TEACHING EXPERIENCE

Experience in the Swiss Federal Institute of Technology (E.T.H.)

In common with many other universities, the time-table structure at E.T.H. makes it virtually impossible to introduce new courses, so modern methods of information and documentation have to be squeezed into two hours borrowed from another course, with practical exercises carried out as part of a semester project. The introduction to the semester project enables an additional two-lecture-hours on manual searching to be given. Because the particular semester project is concerned with literature retrieval (four days), the students get ample practical experience on manual searching. The total of four lecture hours (which includes a computer search demonstration) is not really adequate to properly cover the material—six to eight hours would be better. The four-day manual search project is more than necessary for the normal chemical engineering student. However, in the Technical Chemistry Department at E.T.H. there is a strong emphasis on chemistry, which is consistent with extended information retrieval exercises.

The subject would be given more status if it were a short course in its own right, and not simply squeezed into odd hours. This could conveniently be taught together with odd hours given on communication (report writing, specification writing, drawing standards, speaking and lecturing) to provide sufficient material for an independent course on communication.

Undergraduates do not carry out computer searches, but postgraduates are allowed to carry out some of the searches by computer in collaboration with an information specialist.

Experience at the Instituto Quimico de Sarria

Since 1979 the Higher Technical Education Centre for the formation of engineers has provided a course on Scientific and Technical Documentation for the fifth-year students (the last year of the chemical engineering curriculum). It is compulsory for those students who opt for the research course, at the end of which a *Trabajo de Fin de Carrera* (final report on conclusion of studies) has to be submitted before the degree (in chemical engineering) can be awarded. It is, however, optional for those students who do not go for this research course and who will consequently not complete their studies with this degree.

The course is run for one week with two hours every day, giving a total of ten hours for the presentation of the various topics. The exercises are done on an individual basis outside the regular course time, which means an average extra time requirement of three hours for the practical exercises. In the presentation of the material, emphasis is put on practical application, the importance of one-line systems demonstrated, and extensive use of visual material like slides and transparencies is made. The course contents are remarkably similar to Table 1, which is the proposed curriculum we are recommending.

The experience with this course during the last five years has been highly positive. The students have learned or improved their ability to handle basic documentary sources (like *Chemical Abstracts, Beilstein, Science Citation Index*). They know the possible ways of using information media in their search for information, how to access them, and finally, and this is very important, they realize the complexity of the process for searching for information and are aware of the assistance available from the specialist in information and documentation.

COURSE CONTENTS

The European Federation of Chemical Engineering has had a Working Party on Information

Continued on page 142.

TABLE 1
Average basal metabolic rate for males and females of various ages [2]

AGE	Kcal/hr•m² MALE	FEMALE
10	45.0	43.0
20	39.0	35.0
30	37.0	35.0
40	36.5	35.0
50	35.5	34.0

ture because of 'no air pocket' assumption.

It can be easily shown that the required thickness does not change with various age groups as the heat production rate is not significantly different (Table 1). In cases where the ground temperature is cooler than the atmospheric temperature, we can make a conservative estimate of the bag thickness by taking both the ground temperature itself as the surrounding temperature and the thermal conductivity of the compressed packing material.

It was found that the assumption of cylindrical shape for the body does not alter the result significantly. □

ACKNOWLEDGMENT

Contributions of Umesh K. Jayaswal, Atul Bansal, and V. L. N. Murthy are gratefully acknowledged.

REFERENCES

1. Ravichandran, V., "Chemically Processed Mathematics," to be published.
2. Bell, George H., J. N. Davidson and D. E. Smith, *Textbook of Physiology and Biochemistry*, 8th Ed., 1972.
3. Foust, A., L. A. Wenzel, C. W. Clump, L. Maus, and L. B. Anderson, *Principles of Unit Operations*, 2nd Ed., 1980.

INFORMATION TRAINING

Continued from page 131.

and Documentation in existence for a number of years, with the objective of assisting the introduction of new methods into the chemical engineering profession. As part of this work they have developed a suggested curriculum for a course in information and documentation for chemical engineers. This is given as Table 1. This table could be taken as the basis for any new course developed for chemical engineers.

CONCLUSIONS

The aim of this paper has not been to give a quick course on information and documentation, but simply to mention the trends in this quickly moving area and to indicate that there is sufficient material relevant to a chemical engineer to form a short course on the subject. If the reader is left confused, but impressed, then we have achieved our aim and suggest he get together with his own information scientist (librarian) to develop a course for his undergraduates.

We believe a course of about nine to twelve hours would be ideal. This would enable about three hours of exercises in the library to be made and a computer retrieval demonstration to be attended. If this amount of time is not available, then two hours of lectures could survey the material and practical experience could be gained in association with laboratory work and project work. At least, practical experience should be planned and guided—not simply left as a random search for the student to undertake when all else has failed. □

TABLE 1
Proposed Curriculum for Basic Information Science Training

SOURCES OF INFORMATION

Printed
- a) Primary Sources: Journals and reports, conference reprints, patents, dissertations.
- b) Secondary Sources: Chemical, Chemical Engineering and Engineering Abstracts; SCI.
- c) Tertiary Sources: Handbooks, encyclopedia, books. Advances in . . . List important ones.

Computer Data Bases
- a) Bibliographic data bases.
- b) Numerical data banks.

SEARCH PROCEDURES

- a) Manual: Indexing, Search Techniques; Bibliographic, Data.
- b) Computer Searching:
  - Bibliographic: files, networks, host computer; data base selection; searching techniques; costs
  - Numeric Data Banks: available banks; procedure, cost
- c) The role of libraries and information scientists

ACKNOWLEDGMENTS

The authors wish to express their thanks to those members of the E.F.C.E. Working Party on Information and Documentation who commented on the draft outlines of this paper. Their comments were gratefully received and incorporated

into the final text.

REFERENCES

Baltatu, M. E., "On-Line Information," *Chem. Eng.* (NY), p. 69 (1984).

Fidel, R., D. Sörgel, "Factors Affecting On-Line Bibliographic Retrieval: A Conceptual Framework for Research," *J. Am. Soc. Inform. Sci. 34* (3), pp. 163-180 (1983).

Fries, J. R., "Data Base Searching in Chemical Engineering," *Chem. Eng.* (NY) *88* (26) p. 71 (1981).

Graham, M. H., A. B. Lamy, B. Lawrence, and L. Y. Stroumtsos, "Information Retrieval," in *Kirk-Othmer*, 3rd. ed., *13*, pp. 278-336, (1981).

Hall, J. L., M. J. Brown, "On-Line Bibliographic Data Bases." *An International Directory*, 2nd. ed., Aslib, London (1981).

Henry, W. M., J. A. Leigh, L. A. Tedd, and P. W. Williams, *On-Line Searching: An Introduction*, Butterworths, London (1980).

Kaback, S. M., "On-Line Patent Searching: The Realities," *Online 7* (4), pp. 22-31 (1983).

Rasmussen, P., "Data Banks for Chemical Engineers," Danmarks Tekniske Højskole, Lyngby, Denmark (1980).

Rose, L. M., "Uebersicht über die gegenwärtig verfügbaren Datenbanken für physikalische Eigenschaften," *CHIMIA 33*, p. 256 (1979).

Stanley, W. G., "Unique Information Resources for the Chemical Engineer," *Chem. Eng. Prog. 77* (6), pp. 80-82 (1981).

RECYCLE WITH HEATING

Continued from page 139.

the apparatus, plotted against 1/Q. The energy input of the pump is found from the gradient to be about 210 watts. The intercept (about 0.3°C) probably represents the scale reading difference between the two thermometers.

A further refinement that is possible with the apparatus is to run the dynamic experiment in the limiting case of recycle with no through-flow. With no through-flow the apparatus is analogous to a well-mixed batch reactor, whereas it is analogous to a CSTR when through-flow is present. Fig. 8 shows results for this case for three different recycle rates. The three lines do not coincide because different starting temperatures were used. The results show that after 30 seconds or so there is, as expected, a linear temperature rise with time. The temperature rises with no limit at least until the safety cut-out of the shower heater operates. The gradients of the lines on Fig. 8 are all the same and by using the combined heater and pump energy input of 3.21 kW it is possible to estimate the effective recycle volume. This is 3.95 litres for the results shown, about 5% less than the value obtained using the through-flow method. The most likely cause is the time taken to heat up parts of the metalwork of the pump; this experiment lasts only four minutes, compared to ten for the through-flow method.

Students always say that the apparatus could be improved by lagging the pipework to reduce heat losses, but simple measurements on a cooling curve indicate that the heat losses are very small. Also, for some of the temperature response

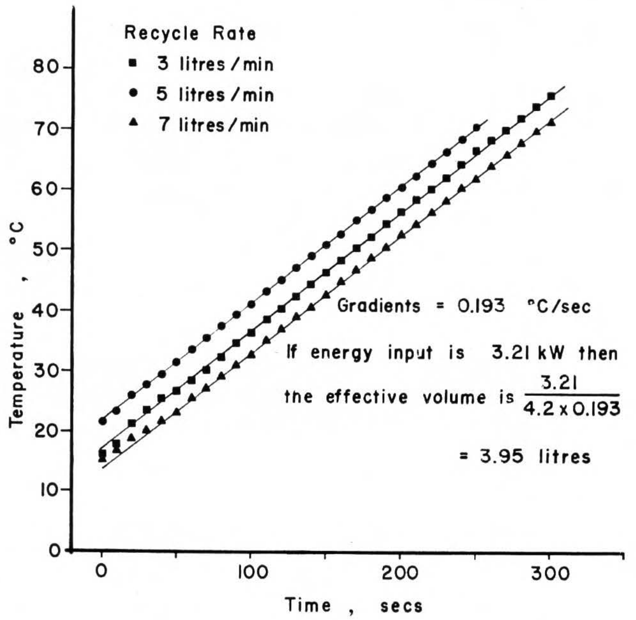


FIGURE 8. With no through flow the recycle loop temperature rises without limit as can be seen above. Using the combined energy input of the heater and pump (determined on Fig. 3) the effective volume of the recycle loop can be determined using the gradient of the lines. This volume can be compared with the value determined on Fig. 6 (4.17 litres equivalent). The lines are for different recycle rates which, as expected, have no effect. Different initial temperatures were used. Up to the first minute it can be seen that the system is not well-mixed.

curves the water temperature is below the ambient air temperature and so the system is gaining heat rather than losing it.

CONCLUSION

Our apparatus has been in service for several years without giving trouble, perhaps a consequence of using well proven domestic components. The recycle experiments performed with it can range from simple mass and heat balances right through to the dynamics. Its main purpose, however, is to provide a vivid demonstration of basic mass and heat balances in a system with recycle. □