ChE curriculum

A NEW APPROACH TO TEACHING ChE USING COMPUTERS

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THIS PAPER WILL DISCUSS a continuing project which has been in progress in Hungary during the past few years. Within the framework of this project, universities and specialized colleges concerned with the teaching of chemical engineering science have undertaken to develop and compile, according to a coordinated plan, chemical engineering computer programs for a new approach in chemical engineering education. In Hungary this unified system, consisting of the computer programs and the series of textbooks which explain the theoretical basis and practical application of the programs, has been assigned the task of laying the foundations for the training of chemical engineers who will be able to apply computers creatively.

The rapid development of the computer as an aid to engineers has opened up new potentials for the automation of technical activities, permitting a number of possibilities defined in part by size, performance and peripheral features of the computer and in part by the level of application. Programs aiding the engineers' work in industry may be further developed and economically utilized only if universities train experts with that aim in view.

HIERARCHY OF THE FIELDS OF CHE

On the basis of accumulated experience, the acquired knowledge of a chemical engineer falls into a hierarchy of three levels [1]:

On the first level we find disciplines related to the properties and transformation of materials, e.g.

- **physical properties**
- **thermodynamic properties**
- **transport properties**
- **reaction kinetics**

On the second level we find disciplines dealing with the industrial scale implementation of physical and/or chemical transformation of materials, such as

- **unit operations and reactors**

On the third level there are disciplines related to large-scale industrial production, e.g.

- **theory of chemical technological networks**
- **theory of process control**

This analysis provides sufficient guidance for the revision of the whole chemical engineering curriculum based on the universal availability of computers.

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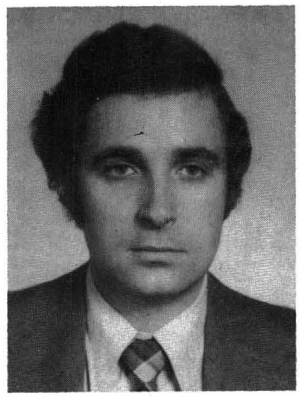

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Breaking chemical engineering into these levels is regarded as a historical process and is a consequence of differentiation in science. In chemical engineering education, each step toward differentiation was followed by another step of methodological nature toward integration. Between levels 1 and 2, integration led to mathematical modelling, while integration between levels 2 and 3 led to a systems approach with a methodological nature.

This analysis provides sufficient guidance for the revision of the whole chemical engineering curriculum based on the universal availability of computers.

COMPUTER PROGRAMS IN CHE

Slightly overstating the above conclusions, this notion means that the complete curriculum of chemical engineering consists of a single large data base and a library of programs, or rather, sub-routines [2, 3]. Within each subject this philosophy denies automation with relation to unmastered problems posed by the particular subject, but for problems pertaining to each previously mastered subject, it makes automatic response necessary and sufficient.

The individual chapters of chemical engineering science, broken up into hierarchical levels, were assigned to participating departments and institutes according to their special field.

The establishment of the above mentioned data base and subroutine library is a task which surpasses the capabilities of any single research institute or university department. An effective solution can only be attained through the cooperation of several units of research and education.

THE CHEMISYS PROJECT

Since 1979, several Hungarian universities which train chemists and chemical engineers have been involved in implementing the above objectives in the CHEMISYS project. While organizing the project, the researchers and teachers took into account the possibilities and foreseeable developments in the field of computers in Hungarian universities. The work began with the assumption that the easiest way to provide every student with a computer would be through the development of computing centers with a network of terminals. Therefore, those taking part in the CHEMISYS project decided to create a data base and a subroutine library as mentioned earlier.

The so-called CHEMISYS System is, on one hand, a computer program itself, and on the other hand it is a system of rules and prescriptions which should be taken into account when writing or adding subroutines to the system.

The basic advantage of CHEMISYS is the considerable simplification in handling data files. The inexperienced user is spared the need to learn and apply a difficult collection of statements for creating and handling data files. Of course, subroutines can be run under the control of a deliberate main program written by the user, or can be used as stand-alone routines independent of the CHEMISYS system.

ORGANIZATION OF THE PROJECT AND EDITING OF TEXTBOOKS

The individual chapters of chemical engineering science, broken up into hierarchical levels, were assigned to participating departments and institutes according to their special field. In this context we may consider any of the previously outlined thematic fields as a chapter, e.g. thermodynamics or chemical networks. By combining both teaching and research aspects, a curriculum supported by computer methods on every possible point has been compiled. Part of the curriculum consists of the chapters of seven textbooks, one for each thematic field. The programs prepared for those fields have been written, according to identical principles, in a high-level programming language.

This activity has been organized by the Institute for Science Management and Informatics, which is the institution of the Hungarian Ministry of Education and Culture.

The application of the results of this work is not compulsory, but the departments taking part in the project have introduced the new method in their own programs and textbooks. The next step is for these departments to adopt the results of the other participants. In the near future we hope the results of this project will be generally used in the curriculum of chemists and chemical engineers in Hungary. According to the general opinion, this will require five to ten years to accomplish. Of course, such a centralized organization of a project like this would be impossible in a country having many universities and departments of chemical engineering, but it can be carried out in Hungary where the number of uni-

versities and departments teaching this field of science is relatively low and the number of students is limited and planned according to the needs of industry and research.

In the present experiment the different fields of chemical engineering sciences are shown in Table 1. From the point of view of this project, the different fields are considered as independent subjects and are revised by taking into account the new possibilities provided by the computer.

Each book consists of three parts: the first part treats exhaustively the theory of the given thematic field; the second part provides know-how needed for the discussion of the theory and the computer programs suitable for the solution of the given problems; the third part gives illustrative examples of problems raised in part I and solved by programs outlined in part II.

The main sections of the series of textbooks follow the logical concept introduced herein: the first section discusses the lowest hierarchical level of chemical engineering science, the second section discusses the middle level, and the third section is devoted to the highest level.

Besides providing a survey of principles, the sections contain appropriate flowcharts on which actual computer programs have been implemented within the CHEMISYS system. A number of problems included in each section have been solved using those computer programs.

The CHEMISYS system has been established on the appropriate size computers in Hungarian university centers so that the system is available, through terminals, to educational staff and students. With the present dramatic development of computers and related devices, the participants in the project are making use of subroutines on different micro- and personal computers in a conversational form.

INTERNATIONAL RELATIONS

The introduction of computer methods in chemical engineering education was started more than twenty years ago by the CACHE (Computer Aids for Chemical Engineering Education) Committee in the U.S.A. [4] and by EURECHA (Euro-

TABLE 1

Titles of Seven Volumes with Some Problems Solved with the Published Computer Programs*

1. CHEMICAL THERMODYNAMICS OF LIQUIDS AND GASES
   - **Subroutines, calculating the substance-specific constants of the pseudo-mono-component**
   - **Subroutines for the calculation of fundamental physical-chemical properties of pure components**
   - **Procedures to calculate vapour-liquid equilibria**
   - **Subroutine for the calculation of isothermal and isobaric chemical equilibrium**
   - **Adiabatic compression**
2. TRANSPORT OF FLUIDS AND TRANSPORT PHENOMENA
   - **Friction factor**
   - **Reynolds number**
   - **Pressure drop in tube section**
   - **Flooding velocity of liquid-liquid systems in packed towers**
   - **Heat transfer coefficient by KARMAN's analogy**
   - **Mass transfer coefficient for evaporating droplets**
   - **Design of air cooler with fine gills for isothermal condensation by direct method**
3. SEPARATION PROCESSES
   - **Steady-state simulation of distillation plate columns**
   - **Determination of the number of theoretical plates of distillation columns using short-cut methods**
   - **Calculation of equilibrium constants of hydrocarbon mixtures using the McWilliams equation**
   - **Modelling and design of countercurrant extraction using the stagewise/stirred cell/model.**
4. CHEMICAL TECHNOLOGICAL NETWORKS
   - **Identification of maximal recycle loops by power raising of the adjacency matrix**
   - **Recycle loop identification by tracking the graph**
   - **Determination of the calculation sequence**
   - **Convergence acceleration by the Wegstein method**
5. DYNAMICS AND CONTROL OF CHEMICAL PROCESSES
   - **Responses of a first order process to unit step, pulse and ramp functions**
   - **First-order process under P-controller action**
   - **First-order process under PI-controller action**
   - **Capacitive plus first-order processes under P-controller action**
   - **Setting of controller parameter by the continuous cycling method**
6. COMPUTER TECHNIQUE IN ANALYTICAL CHEMISTRY
   - **Simulation of density function like signals**
   - **Credibility test of measurement data values**
   - **Fast Fourier transformation**
   - **Calculation of discrete convolution**
   - **Fitting and statistical characterization of calibration lines**
   - **Analysis of multilcomponent linear systems**
   - **Cluster analysis by Forgy method**
7. METHODS OF OPERATIONAL RESEARCH

*In December 1983 the CHEMISYS System contained about 350 subroutines.

pean Committee for the Use of Computers in Chemical Engineering Education) in Europe [5, 6].

We are in very close contact with EURECHA, which makes possible a continuous interchange of experiences and computer programs and visits by experts. Together, we have worked out a standard of writing chemical engineering computer programs which is widely used both in Hungary and in other countries joined by EURECHA. We believe that the realization of the CHEMISYS system represents a significant advance since it represents a unified system; the projects organized earlier by CACHE and EURECHA are characterized by the lack of any common system. In order to promote the foreign applications of the CHEMISYS subroutines, an agreement has been signed between the ETH (Eidgenössische Technische Hochschule, Zurich, Switzerland) which is the Secretariat of EURECHA, and the Institute for Science Management and Informatics.

AVAILABILITY

The CHEMISYS algorithm is available as a collection of computer programs. They have been written in FORTRAN and run on RJAD-22, 32, and 40 series computers in Hungary. Of course, the programs can also run on larger computers without any difficulty as well as on IBM 360 or other computer in the same size range.

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HYDRAULIC ANALOG METHOD

Continued from page 65.

that reaction orders smaller, equal or greater than unity are obtained with various shaped containers, as shown in Fig. 6. Large cone angles give large deviations from first order kinetics, and as cone angles approach zero the reaction order approaches unity.

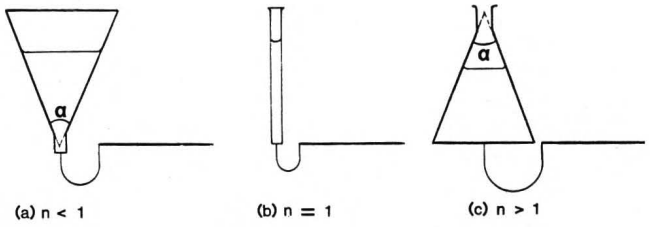

FIGURE 6. The relationship between shape of the container and reaction order.

2. Capillary length does not affect the reaction order. However, for ease in running the experiment it is suggested that the length be chosen such that the half life of the reaction is between 2 and 3 minutes.

3. In order to get accurate data it is better to measure ΔV from the outlet of the capillary with a burette (as shown in Fig. 1) instead of reading water levels on the funnel directly.

4. One can combine the set up here with additional burettes and funnels to give multiple reactions of various types as outlined in our previous paper [1], such as

$$A \rightleftharpoons R,\ A \rightarrow R \rightarrow S, \text{ etc}$$

Interpretation of such systems with non-linear kinetics is not easy and provides a challenge to the brighter students and practice on the computer.

5. The large variety of combinations of setups and capillary lengths will allow each student in the laboratory to run his own experiment, even in China with its huge student population.

ACKNOWLEDGMENTS

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