INTRODUCTION TO COMPUTER TECHNIQUE IN STOICHIOMETRY

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Needs for Computers

Many educators have seen the need for computer technique by the undergraduate chemical engineering student. This need arises from a number of sources. We have observed in recent years the extensive use of computers in such fields as research and development, where they are used for design of experiments to give the best statistical choice, and in many other applications. Computers have also come into wide use in plant design, where they are used for making tedious calculations as required for multicomponent distillations, rating of heat exchangers, optimization of design parameters, numerical solution of differential equations, and various other computations of this sort. We have also seen computers being used in such new engineering disciplines as systems engineering and operations research. Also, wide application is now being made in engineering economic studies.

There are very few engineering offices today which do not make use of computers. Some of the most conservative engineering offices are now acquiring computers, because they see that they are at a competitive disadvantage with those organizations which do use computers.

This has been due to the fact that computation jobs which were unthinkable in engineering a few years ago now have become practical. In minutes or hours, it is often possible with the aid of computers to accomplish calculations which used to take a man several months or years to complete.

Intimate Knowledge Necessary

As regards the knowledge of computers required of the chemical engineering graduate, it is the author's belief that a reasonably intimate knowledge of computers is necessary, if he is to be considered a professional engineer. Many have argued that intimate knowledge of computers is not required because the engineer can depend on professional computer operators and mathematicians to translate his engineering problem to a computer program. At first glance this sounds good. However, many times in actual practice the professional computer operators and mathematicians are too busy to give full attention to a given individual's problems. Then too, communications often break down and the engineer has difficulty in explaining what he is trying to accomplish. If he has an intimate knowledge of the computer, the engineer is much better able to communicate and to visualize his problem.

Moreover, a more intimate knowledge of the machine will give him a much better appreciation of its potentialities. Inexperienced persons are often awed by a computer and will blindly accept the machine answer as absolutely correct. Personal experience wmth a computer, however, will soon impress the operator with the general limitations of these machines. They cannot, for instance, rise to an occasion not provided for in their program. If, in the course of a computation, the machine must subtract two functions which have unexpectedly similar values, most of the significant figures will be lost, and an answer with no physical meaning will be furnished. Only an intimate knowledge of the physical parameters, as well as the machine's limitations, will give the necessary confidence to question a computer result.

Why Stoichiometry ?

Perhaps the first question that may enter our minds would be why pick stoichiometry as a means of introducing the chemical engineering student to computer technique. As a matter of fact many educators propose special early training courses devoted solely to the topic of computers and not interwoven necessarily with other specific academic courses(1). Stoichiometry does lend itself as a medium by which the student can be introduced to computer technique. But it certainly does not rule out other courses for the same purpose.

First of all, stoichiometry is usually one of the first chemical engineering courses a student takes. This is generally given in the second or third year. The conventional stoichiometry course is characterized by incessant drilling in the performance of heat and material balances around chemical plants. The essence of the problem is always the same, but as the course proceeds, the computations become more complicated, tedious, and time consuming. The student may start with the simple conversion from mol composition of a gas to weight composition. Then he may take problems in heat and material balances around a natural gas or coal-fired furnace. Finally, the complexity of the problem may be increased until he is making a balance around something as complicated as a pig iron blast furnace.

In all these exercises the pattern of computation is the same. The only thing that changes is the degree of complexity. A general formula which might be used for all of these problems is:

$$\text{(energy in)} = \text{(energy out)} + \text{(accumulation)}$$

and

$$\text{(mass in)} = \text{(mass out)} + \text{(accumulation)}$$

With the current modern trend in engineering education to include more and more principles in the curriculum at the expense of practice and factual information, it becomes necessary for us to review the treatment of such subjects as stoichiometry, which has been strictly a drill-course. In essence, the only principles which the student has learned in this course is energy and material balance.

It was with this view in mind that the author decided to attempt introduction to computer technique in the stoichiometry course. The problems are of such a tedious and repetitious nature that they lend themselves to demonstrating the value of computers.

Tried in the Classroom

The author has had the opportunity on two different occassions to introduce computer technique in a stoichiometry class. A class term consists of ten weeks, in which there are eight contact hours during any one week. Two hours are set aside for lectures, and the other six are set aside as recitation-laboratory periods, wherein the students are allowed to work their problems under teacher supervision. This schedule was very amenable to the introduction to computers, because this extra laboratory time made it possible to teach the basic knowledge of the machine rapidly.

The IBM 650 was chosen as the computer for this course, chiefly because this was the computer with which the author was most familiar. Also, the basic machine language of the IBM 650 is relatively simple, and this type of computer is widely used.

An outline of how this material was presented to the class may be of interest. First of all, the author took the students through the conventional stoichiometry drills for about four of the ten weeks. In this time the degree of complexity was gradually increased up to cases such as oil and coal-fired furnaces. By this time the students also had such problems as equilibrium flash calculations.

At this point the students were given a furnace problem in which they were required to calculate the material balance using purely algebraic symbols and no numbers. This was a break with tradition since engineers are usually discouraged from doing problems by algebraic formulation. Rather, we were taught to go through logical numerical steps so that we could visualize the problem as we went. This also minimized the possibility of ridiculously great numerical errors. It can be understood that this algebraic approach was meant to condition the students for setting up the algorithims by way of computer programming. It was explained to them that the algebraic solution of one of these problems was one extreme, whereas the conventional numerical solution of these problems was another extreme, and that programming them on a computer would be somewhere between.

The students were then allowed one to two weeks for familiarization with an IBM 650. They were given the usual diagram explaining the input, output, the storage drum or memory, the arithmetic unit or accumulator, and all the various other essential components. Their interrelation and functioning were explained. The students were given an explanation of the operation code of the machine. Then they got simple problems in arithmetic with whole numbers, just to demonstrate the functioning of the equipment. This was followed by an introduction to floating decimals, and with this they were able to program simple material balances in which there was no chemical reaction. After this, they were able to make multiple additions and subtractions according to the directions of the streams in and out of the systems studied.

Iteration processes were introduced together with the use of index registers. This allowed the students to calculate, say, temperatures from vapor pressures by trial and error solution of algebraic relationships. Then they were given exercises in coding furnace-type problems with basic machine language. With the basic idea of programming somewhat mastered, the students were then required to use their knowledge of programming vapor pressure-temperature relationships in coding equilibrium flash calculations. These were complicated enough to demonstrate the utility of a computer in this realm. The students could well appreciate this because previously they had done an equilibrium flash calculation by hand and spent considerable time in trial and error calculations.

There was just enough time left in the course to mention such topics as compilers, but the author felt that the students had acquired quite a bit of know-how, appreciation,and competence in the application of computers to chemical engineering calculation.

Students Enthusiastic

The reaction of the students to this program has been one of enthusiasm. Our general feeling is that they take this as something new, exciting, scientific, and to their liking. This program in the stoichiometry course came as a surprise to them and they feel it is going to help them solve problems in the future. Also, the author has noticed that students feel that they have benefited from the course as regards training. They believe that they need this subject, that it is going to be useful to them, and that it is going to give them a more mature viewpoint toward the solving of problems.

This situation is further intensified by the fact that our students are on co-operative education and spend alternate 10-week periods working in industry and working in the classroom. Many of these co-operative students have been exposed to computers in their industrial work and have a mature appreciation of the need for computers. In a couple of cases the author has found students who try to teach him about the computer. These students had been actually working on programming or in some capacity related to the utilization of computers. In the case of many of these co-op students they know what they need in their engineering training. They cannot be fooled. They have been out in the world; they have seen what are being used as the basic tools of the engineers around them.

Teaching with Compilers Alone

Intimately involved in this discussion is the question as to whether machine language should be taught to the students or simply compilers, such as MAD, GAT, or FORTRAN. The author's opinion is in favor of teaching basic machine language to the student if time permits. It is felt that in this instance, time is not a problem. In the case of the IBM 650, the machine language is relatively simple. It does not take more than a week or two to familiarize the student with it. But compilers would have been covered more thoroughly had there been enough time. However, it was felt that machine language was more important for the student to learn, because it is more basic. Once the machine language is understood, and the student has a working knowledge of it, he can easily pick up the use of a compiler, but the converse is not true.

Also it is felt that the student should be as close to the machine as practicable, and learning the basic machine language first is one way of attaining this objective. This more intimate knowledge of the machine, as mentioned before, helps in the liaison between the engineer and computer personnel. If the practicing engineer's program written with a compiler does not work, he may then need an intimate knowledge of machine language for the debugging step.

Also it is believed that a knowledge of the basic machine language gives the student a better appreciation of the machine's possibilities in purely logical programs rather than algebraic computation programs.

Need for Experimental Knowledge

Tied in with this topic is the question of the need by the student for experimental knowledge of the computer. Is it sufficient that he be taught how to write programs in the classroom, or should he actually be able to get near the machine, and actually feed input information to the machine by pushing the proper buttons and sitting at the console, and actually operating the machine? Does he need to do all this? Well, it is the difference between experimental knowledge and abstract knowledge. When the student actually puts numbers in and gets numbers out of the computer, his knowledge and appreciation take on a new dimension. He gets a greater feel for the machine. To learn to write programs without getting familiar with the physical operation of the machine would be like a man studying the rules of football without ever having played the game or seen it played. Even though the student may never expect to become a professional computer operator. it is felt that he should get some minimum familiarization with the machine.

With this attitude it became necessary for the author to seek some means by which the student could gain this experimental knowledge. There was a Burroughs computer available on the premises of this institution not similar enough to the IBM 650 to use for experi-demonstration. Therefore, the author arranged for the local IBM sales office to give lecture demonstrations of the IBM 650 at local computation offices. During one term the facilities of the Chrysler Corporation were made available to us, whereby an IBM lecturer would use one of Chrysler's IBM 650's to give a lecture demonstration in the use of the machine. In the other term, the facilities of the Michigan Bell Telephone Company were used. The author believes that this is not the ideal way of doing it. However, this inter-cooperation with local industry has a beneficial effect on the students, on the educational institutions, and on the industrial concerns themselves. The author is very much in favor of inter-cooperation between industry and educational institutions in enterprises of this kind.

Value of Mental Training

It is believed the students not only benefit from this training because of the increasing widespread use of computers in industry, but also there is a certain inherent mental training that goes along with the indoctrination which the student receives. It introduces the student to a whole new philosophy of approach to problems. Most of us have been accustomed to attacking numerical computations by a kind of pragmatic, feel-as-you-go approach. When most people make complicated calculations, they find it hard to keep track of where they came from and where they are going. We tend to "muddle through" in our calculations. Now, with the introduction of the concept of writing flow sheets to represent a computation we have to think out the problem attack with logical exactitude. This opens up a whole new horizon in the general philosophy of problem solving. This particular contribution of computer technique to the education of engineers is of itself well worthwhile.

Future Work Planned

In future stoichiometry classes the author hopes to continue this work, which is necessarily of an experimental nature. One significant difference in the coming year is that we hope to switch from the IBM 650 to the IBM 1620, chiefly because the 1620 replaces the 650, but also, this institution has acquired an IBM 1620 which will be available for use. Whether the increased complexity of the IBM 1620 will force an abandoment of basic machine language is yet to be determined. We hope to assign a limited number of problems, which the student can actually solve on the machine. The IBM 1620 is part of the equipment in our newly formed computer center. This will guarantee that competent computer personnel will be available to assist various teachers who wish to introduce the use of computers into their course work.

Serious study is also under way by various segments of the faculty to provide introduction to computers at the freshman or sophomore level. One possibility is to give the students a course under a computer center mathematician, but because of the squeeze on the engineering curriculum this would probably have to be a one-semester-hour course. Also, the Engineering Graphics department is making an effort to introduce freshman and sophomores to computers during their regularly scheduled engineering graphics courses. They are covering the use of the analog, as well as digital, computers. Such steps as these, it is hoped, will eliminate the need for basic computer instruction in stoichiometry and allow time for study of more advanced problems.

Other Courses

We hope that we will be able to integrate the use of computers, analog, as well as digital, in all courses where applicable computations are involved. It is a tool which can be applied to other diciplines and more difficult calculations that will come along in the later courses. This is in keeping with the findings of Dr. Katz and co-workers in the computer project at the University of Michigan(1).

(1) Katz, D. L. , Organick, E. I., "Use of Computers in Engineering Undergraduate Teaching," Journal of Engineering Education, Vol. 51, no. 3, pp. 183-205, December 1960.