A JUNIOR COURSE IN CHEMICAL ENGINEERING COMPUTATIONS

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IN THE SPRING of 1973 the author was asked to develop a three unit course in chemical engineering computations based on the text "Material and Energy Balance Computations" by E. J. Henley and E. M. Rosen.[1] This was to be the second semester course in the two semester Elements of Chemical Engineering sequence for third year chemical engineering students at Washington University, St. Louis. It was a listed prerequisite for the senior Systems Analysis and Design course.

Typically at this stage, students have had a course in thermodynamics, and a course in the use of mathematics and the methods of engineering in the analysis of chemical and physical processes. In addition, they have had a course in basic chemical process principles including stoichiometry, ideal gas law and gas mixtures, vapor pressure, solubilities and energy balances. Only those interested (about 1/3 to 1/2 of the students) had taken the optional one unit digital computer programming course. In general, the student had not used the computer as an integral part of his previous course work. The traditional unit operations courses covering such topics as distillation, absorption and heat transfer were no longer offered, though a two semester junior sequence in transport phenomena was a listed requirement.

The basic approach to the material in the text has been described previously.[2] Major emphasis was given to the machine methods chapters in the text, chapters 5, 8 and 9. Table 1 gives the general outline of the course and the number of sessions devoted to each topic. Each session was scheduled for 75 minutes twice a week in the evening hours. Almost one third of the course was devoted to graphical methods in distillation and absorption. This was done in part to fill the lack of exposure to the unit operations. Outside reading[3,4] was used in support of this portion of the course in addition to the use of a secondary text.[5]

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CONDUCT OF THE COURSE

THE COURSE WAS A traditional lecture type with homework (which was not graded) assigned from the text or specially designed and handed out. In addition the class was divided into teams of three persons each for the purpose of doing the five computer problems that were assigned and which formed 20% of the course grade. The reason for the teams was two-fold:

- **Some members of the class did not know FφRTRAN programming.**
- **It was desired to hold the computing bill down.**

Eight one hour exams, of which only the highest six were counted, (60% of grade) were given, plus a final (20% of grade). The comparatively large number of exams was designed to prevent members of the class from falling behind and to provide them a means of gaining new insights to the topic areas. The number of exams received little class criticism though not grading the homework (though it was always discussed) apparently gave the students little motivation for doing it.

THE COMPUTER PROBLEMS

THOUGH THE COMPUTER problems were intended to be a major portion of the course they were weighted comparatively lightly since knowledge of FφRTRAN was not a course prerequisite. It was intended that every member of each team would participate equally in the computer problem analysis and that those members knowledgeable in coding would teach the unknowledgeable ones. This, it was felt, closely paralleled the environment found in industrial organizations. Each member of the team was required to hand in a problem analysis though only one computer output per team was required. However, this did not turn out satisfactorily, since the knowledgeable FφRTRAN students spent a disproportionate amount of time coding and debugging the computer problems while the others spent comparatively little time.

TABLE 1—COURSE OUTLINE

Session Numbers	Topics
Part A. Chemical Process Calculations	
1-2	Course Conduct
	Review of General Energy and Material Balance Equations
3	Matrices and Vectors
4-5	Independence, Orthogonalization and Rank. Solution of Linear Equations and Material Balances
6-7	The One Dimensional Nonlinear Equation and Flash Calculations
8-9	Chemical Reactions and Their Independence. The Extent of Reaction.
10	Chemical Equilibrium
11-12	Energy Balances: Adiabatic Flash and Adiabatic Flame Temperatures.
Part B. Distillation and Absorption	
13-14	Binary Distillation—The McCabe-Thiele Method.
15-16	Minimum Stages and Minimum Reflux. Analytical Shortcut Methods.
17	Multicomponent Methods—Tridiagonal Equations
18-19	Absorption—Graphical and Analytical Methods
Part C. Plant Simulation	
20	Streams and Building Blocks
21	The Split Fraction Concept
22-23	Partitioning and Tearing Equations. The Convergence Block Concept
24	Direct Substitution and Wegstein's Method
25	Information Feedback
26	Comprehensive Flow Sheet Calculations

The intent was for the student to formulate the problem, code the main program but let the subroutine do the tedious work of computation.

At the start of the course source decks for the four FφRTRAN subroutines listed in the rear of the text[1] were handed out to each team. (This was necessary since only the WAT IV compiler which required all source coding could supply adequate turnaround). The four subroutines supplied to each team were:

GSMT	**Gram Schmidt Orthogonalization**
GELG	**Simultaneous Linear Equation Solver**
ROOT	**One dimensional Root Finder**
BSφLVE	**Simultaneous Nonlinear Equation Solver**

The intent was for the student to formulate the problem, code the main program but let the subroutine do the tedious routine work of computation. The five problems were either formulated by the author or adapted from the recently released CACHE committee volume of computer programs on Stoichiometry.[6] Table 2 lists the titles of the problems for the course and the subroutines which were to be used.

COURSE EVALUATION

A TOTAL OF ELEVEN students enrolled in the course and were asked to fill out a questionnaire at the conclusion of the course. The questionnaire asked the student to rate each of the computer problems for instructive value and interest. Other questions relating to the usefulness of the computer problems and course organization were then asked. Finally the student's response to specific topics was queried. Table 3 lists the raw responses of the class to the questionnaire. Overall the course elicited a broad range of rather strong responses. Students with an adequate computer background appeared to respond favorably while those without the background appeared to be much less satisfied. There appears little question that a prerequisite for the course should be coding proficiency in FϕRTRAN by all participants.

TABLE 2—COMPUTER PROBLEMS

Problem	Description	Use of Subroutine
1. A.	Inconsistent and Incomplete Material Balances[1]	GSMT
B.	Linear Material Balances[1]	GELG
2.	Flash Vaporization	ROOT
3.	Simultaneous Gas Phase Equilibrium Reactions	BSϕLVE
4.	Theoretical Maximum Flame Temperature[2]	ROOT
5.	Recycle Calculations Using Split Fractions	GELG

1. Taken from Reference (6), p. 85, 147.
2. Adapted from (6), p. 198.
3. Copies of the problems may be obtained from the author on request.

The use of teams seems to be little justified. Students complained that only one person on the team did all the work and were not sufficiently credited for their effort. There seemed little basic difficulty with the level of the course material in the text though some complaints were recorded about its clarity in places.

Efforts were made continuously to relate the numerical methods portion of the course to direct applications though it should be noted that the text separates these functions for ease of reference and development. This meant considerable jumping around in the text and required carefully planned reading assignments.

Rather strong interest was displayed in the unit operations section of the course as evidenced by the desire for more time to be spent in this area. No time was spent on heat transfer calculations and this would certainly be an area for course expansion. Whether or not the course was best separated into its three distinct parts or could better be integrated into a single topic called process simulation is unclear at this time. □

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REFERENCES

1. Henley, E. J. and Rosen, E. M. MATERIAL AND ENERGY BALANCE COMPUTATIONS John Wiley (New York), 1969.
2. Rosen, E. M. and Henley, E. J. "The New Stoichiometry" Chem. Eng. Ed., Summer 1968.
3. Smith, B. D. DESIGN OF EQUILIBRIUM STAGE PROCESSES McGraw Hill, 1963.
4. Van Winkle, M. DISTILLATION McGraw Hill, 1967.
5. Henley, E. J. and Staffin, H. K. STAGEWISE PROCESS DESIGN John Wiley, 1963.
6. Henley, E. J., Editor, COMPUTER PROGRAMS FOR CHEMICAL ENGINEERING EDUCATION—STOICHIOMETRY Sept. 1972.

TABLE 3—RESPONSE TO QUESTIONNAIRE

Questions 1-5: Computer Problems

	Material Balance	Flash	Equilibrium	Max. Temp.	Split Fraction
Very Instructive	1	3	2	1	
Instructive	8	5	6	5	3
Adequately Instructive	2	3	2	1	4
Not Instructive					1
Very Interesting			3	1	1
Interesting	5	6	1	3	4
Fairly Interesting	3	2	4	6	3
Dull, Dull	1	1	1		

6. The computer problems

Added substantially to the course.	4
Added to the course	4
Added marginally to the course	3
Detracted from the course	—

7. Supplying the subprograms

Was very useful and did not detract from the problems	10
Was useful but made the problems less instructive	—
Marginally useful	1
Was a poor idea	—

8. **The course was**

Well organized	5
Fairly well organized	5
Adequately organized	1
Poorly organized	—

9. **Topic**

	Should be Ex-panded	Re-duced	About Right	Dropped
A. Phase equilibrium	3		8	
B. Inconsistent material balances	2	1	7	1
C. Chemical reactions	7		4	
D. Distillation	5		6	
E. Absorption	7		4	
F. One dimensional equation solving	2	2	7	
G. Multi-dimensional equation solving	4		7	
H. Plant simulation	5	1	4	1
I. Matrices and vectors		1	10	
J. Energy balances	6	1	4	
K. Independence and orthogonalization		5	6	

CHEMICAL ENGINEERING DIVISION ACTIVITIES

3M COMPANY INCREASES LECTURESHIP AWARD GRANT

The 3M Company has increased its annual grant in support of the Chemical Engineering Division Lectureship Award from $1500 to $2500. The additional $100 will cover an honorium and expenses to allow the awardee to present his lecture and visit on the campus of three institutions to be selected by the Chemical Engineering Division. The increased funding is effective beginning with the 1974 award.

The suggestion for the new visitation program was made by Prof. L. E. Scriven of the University of Minnesota, a former award winner and transmitted to 3M by Prof. Leonard Baker when he served as Division Chairman. Announcement of the increased support was made by W. W. Burton of 3M to Dr. George Burnet of Iowa State University, who participated in the discussion with 3M and was instrumental in obtaining the original grant from that company.