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ABSTRACT

To improve the instructional process, time shared computer-assisted instructional methods were developed to teach upper division undergraduate chemical engineering students the concepts of process simulation and analysis. The interactive computer simulation aimed at enabling the student to learn the difficult concepts of process dynamics by allowing him to assess and explore the dynamic behavior of simulated processes, assisted by the provision to him of immediate responses to the user-initiated changes of model parameters or inputs. A CDC-6600/6400 computer was used, along with FORTRAN and the DYFLO dynamic simulation routine, A simulation subrouting was prepared for pieces of process equipment, and homework modules containing information and procedures to be learned were assigned. Objectives of the modules were the transmission of facts and the development of operating experience including concepts such as start-up, shut-down, control, and process parameter sensitivity. Students were favorably oriented toward the material taught and to the computer as an instructional adjunct, and they absorbed factual matter well. However, successful operating experience was not achieved to the desired degree. (Author/PB)

INTERACTIVE COMPUTER ASSISTED INSTRUCTION IN TEACHING OF PROCESS ANALYSIS AND SIMULATION

by

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COMPUTER-BASED SCIENCE
AND
ENGINEERING EDUCATION

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ABSTRACT

Described are methods that were used to teach upper division students the concepts of process simulation and analysis through computer-based instruction. A simulation subroutine was prepared for individual pieces of process equipment, such as the dynamic continuous-stirred-tank reactor. For each subroutine, several homework modules containing the information to be learned and procedures were prepared and used by the students. Typical objectives of the modules were the transmission of facts and the development of operating experience including such concepts as start-up, shut-down, control, and process parameter sensitivity.

Those features of the hardware and software that may be of use to others are discussed, and a detailed example is given demonstrating the application of a typical module.

The effectiveness of the method with respect to instructional objectives and students' attitudes were measured, and the significant conclusions are reported here.

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INTRODUCTION

Time-share computing in the last five years has evolved into a powerful tool to assist in teaching a wide variety of technical concepts. Combined with appropriate graphical displays, time-share facilities make possible the illusion of operating a real physical process. This paper describes some of the work carried out as part of a four-year project under Project C-BE at The University of Texas at Austin, a project funded by the National Science Foundation under Grant GY-9340, that has the objectives of developing and evaluating innovative computer-based undergraduate curriculum materials to improve the instructional process.

Two somewhat different approaches seemed to have evolved with respect to computer instruction models. On one hand, one observes that courses are taught entirely by the computer which provides text instruction, tests, and feedback to additional text material depending on the student's test results. On the other hand, instructors use the computer as an important adjunct in a course in order to provide instruction and learning experiences that cannot be derived from textbooks, lectures, visual aids, or any of the standard teaching methods. We are concerned with this latter approach as applied to the instruction of process simulation in chemical engineering.

The purpose of this paper is to report on the development and application of interactive process simulation as an instructional method at the University of Texas. Those features of the hardware and software that may be of use to others are discussed, and a detailed example is given demonstrating the application of a typical module. The effectiveness of the method with respect to instructional objectives and students' attitudes were measured, and the significant conclusions are reported here.

COMPUTER AND SUPPORTING FACILITIES THAT WERE USED

Central computer facilities at The University of Texas at Austin are based on a CDC-6600/6400 system providing 64 time-share ports and several high speed remote job entry stations. Within Project C-BE numerous CRT, teletype, and graphic terminals are available for student use. The combination of a teletypewriter Model ASR-33 (with E.I.A. RS 232/C interface) and an X-Y plotter (timeshare Model TSP-212) was selected as the most satisfactory system for our specific application of teaching process dynamics for several reasons. First, the equipment is reliable, easy to use, durable and can provide complex graphic output as well as numbers. Second, it provides the student with hard copies of both the numerical output as well as the graphical results, so that he can use the information collected for homework calculations and review. Third, the teletype-plotter combination is one of the least expensive types of hardware that can provide graphic output. One disadvantage of the teletype is that its speed is usually limited to ten characters per second. However, higher speed (30 characters per second) operation is available at somewhat higher cost, or non-impact printers can be used with even greater speed at some additional cost.

The teletype-plotter system works sequentially with numerical data appearing at the teletype followed by the graphical output on the plotter. From the student's viewpoint, this combination provides the necessary numerical data and a convenient display of the important variables. Delays during the graphical output are not wasted time--they permit the student to reflect on what is happening and to reach a decision as to what to do next.

INSTRUCTION MODULES

Many important concepts in process dynamics are very difficult to teach via standard instructional methods, and often are only absorbed by engineers after extensive laboratory or industrial experience. Mathematical models used to represent processes and their solutions often remain nebulous concepts in the student's mind, even if reinforced by visual aids and lecture demonstrations, because the student is only taking a passive part in the learning process. With the aid of interactive computer simulation, however, most aspects of process dynamics become relevant and are then better understood by the student. Computer-based instruction using an interactive time-share system allows the student to assess and explore the dynamic behavior of simulated processes by providing immediate responses to user-initiated changes of model parameters or inputs. More specifically, the student immediately sees the graphical output, and can easily compare several processes by examining tracings on the same sheet of paper.

Several process models are being used to instruct students in the analysis of the dynamic behavior of chemical processes. The first of these models, the continuous well-stirred reactor model, will be described in detail to illustrate our work in general. This model was developed and tested first because of its direct application to existing chemical engineering processes and because of the abundance of textbook descriptions of the model. The equations representing a dynamic CSTR (continuous-stirred-tank reactor) are understood by chemical engineering students, but in general are too complex for them to obtain analytical solutions.

The continuous-stirred-tank reactor model is described in APPENDIX A. Students use the description in conjunction with instructional modules and the computer program. Each instructional module requires approximately one hour of student-computer interaction to treat a concept. The topics covered by the modules are reactor start-up, response to inlet parameter perturbations, reactor cyclic stability, feedback control, and reactor shut-down. The continuous-stirred-tank reactor model may also be used in studying more advanced areas such as stochastic modeling, control theory, and reaction kinetics.

The teaching modules have been structured to promote easy transferability for use by instructors at other universities. Our approach in developing the process simulation modules was to use the standard programming language FORTRAN IV, and the dynamic simulation routines, DYFLO, recently published by R. Franks[1]. The extensive documentation of the DYFLO computer code enables instructors to readily adapt the models to their computer system, and makes it easy for them to modify or add to the programs whatever material fits their particular courses. Other transferability considerations such as cost per student can be related to the computing time and price structure of the facilities at The University of Texas at Austin. Typical costs for using the continuous-stirred-tank reactor module are as follows:

BASIS: ONE HOUR OF STUDENT USE

Line Cost	Execution cost	Total cost
$0.40	$1.00	$1.40

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1. Roger Franks, "Modeling and Simulation in Chemical Engineering," Wiley-Interscience, New York (1972)

ADDITIONAL PROGRAM COST CONSIDERATIONS

Storage	
Permanent file	During execution
3264 words	14,848 words

TESTING AND EVALUATION OF THE MODULES

Two modules for the continuous well-stirred tank reactor program were tested by students in the upper division process simulation and analysis course. One of these modules, entitled Simulation of Reactor Start-Up, is shown in APPENDIX B. Implementation of the computer program and the instructional modules proceeded as outlined below:

1. The overall concept and definitions of continuous-well-stirred tank reactors was presented in lectures followed by homework assignments designed to introduce the mathematical formulation and corresponding nomenclature.

2. One class period was used to demonstrate the equipment for the time-share system and explain the software.

Equipment	Software
Time-share terminal	Log-on procedure
X-Y plotter	Program calling procedure
	Entering data in the model
	Log-off procedure

Prior to the demonstration, students were given instructional information describing in detail the time-share software and user instructions for the reactor model. The user instructions, shown in APPENDIX A, give a brief description of the computer program, a schematic diagram of the simulated equipment, a list of fixed and user-adjustable parameters, and a sample output from the teletypewriter.

3. Each instructional module was assigned as a homework problem requiring approximately one hour of student-computer interaction and an equal amount of time to answer questions related to the observed results.

4. During each session on the terminal, the student's reactions were evaluated by a proctor who was present to assist the students with operational problems related to the hardware.

Both before and after the homework assignments, several attitude and other tests developed by the Measurement and Evaluation Center of The University of Texas at Austin were completed by the students. After the completion of the teaching modules, a test was given to evaluate student progress in meeting the behavioral objectives of the module.

Two different attitude measurement tests were administered in order to ascertain the reaction of students to the computer-based instructional modules. A proctor checklist was also used to rate each student as he interacted with the computer and to isolate problem areas with respect to the instructional module. Information on student interest, anxiety, and probiems with the module provided feedback to assist in modifying the modules and writing future modules.

Orientation inventory tests were administered to classify students as to task-, self-, and interaction-orientation in order to determine if these personality characteristics affected the student's performance. Essentially all of the engineers tested were very strongly task oriented. Also, the students were given a questionnaire on orientation toward college. This test indicated that the students were occupationally oriented as opposed to scholarly, social, or individualistic aspects of college life.

To ascertain the students' attitudes toward the computer-based simulations, over sixty multiple choice (five answers) questions were completed by each student in class. Although we do not have space here to describe all the results, five typical questions, and the responses (13 in total) were as follows:

1. Concerning the course material I covered, my feeling toward the material before I started the lessons was

2. My feeling after I had completed the lessons was

Student Responses

	1	2
Very favorable	1	1
Favorable	9	12
Indifferent	3	0
Unfavorable	0	0
Very unfavorable	0	0

3. I felt frustrated by the computer-based simulation procedure.

4. In view of the amount I learned, I would say computer-based simulation is superior to traditional instruction.

5. While engaged in computer-based simulation I felt challenged to do my best work.

Student Responses

	3	4	5
Strongly disagree	0	0	0
Disagree	10	3	6
Uncertain	2	8	1
Agree	1	2	5
Strongly agree	0	0	1

Students were favorably oriented toward the instructional material before the simulations were carried out, and ended up perhaps slightly more favorably oriented after they were completed. Question 4 indicates that the students believed the computer-based instruction to be no better than the lecture-question sessions, but in another essay type question which asked whether or not they would recommend the computer lessons be used again the next time the class was taught, eleven students said yes, and two did not answer the question. Apparently, the students felt the computer sessions were best used as a supplement to the usual class presentation, but should not supplant them. We are now engaged in an analysis of the student responses as related to their grade point averages, SAT scores, class grade, etc.

Student gain of factual subject matter was tested by multiple choice questions and calculational problems. Concrete facts were readily absorbed, but a test of the extension of the students' knowledge to interpret the effect of a new type of simulation (not covered in the computer sessions) was missed by one-half of the students, so that the objective of providing operating experience for the students was not achieved to the desired degree.

This paper will be presented at the 4th Conference of Computers in the Undergraduate Curriculum, Claremont, California, June 18-20, 1973.

APPENDIX A

INSTRUCTIONS FOR THE CSTR PROGRAM

Program CSTR is a FORTRAN routine designed to simulate a continuous stirred-tank reactor with cooling and proportional-integral temperature control. The program provides many options and conveniences such as random data input, parameter updating while the simulation is in progress, a choice of print intervals for viewing the results. and both numerical and graphical output.

Figure 1 is a schematic diagram of the CSTR system showing the reactor, control loop, and some of the user adjustable parameters. Parameters given in Figure 1 relate directly to the mathematical model and may be changed by the user during a simulation run. These parameters correspond to physically adjustable conditions within an actual operating CSTR. The program will set default values for all parameters. Thus the user can operate the program without entering any data. The user may change or update parameter values by typing the appropriate two character symbol, an equal sign, and the new value as illustrated in Figure 2. If a mistake is made in entering a parameter, simply retype the desired change. A complete list of parameter symbols and definitions for the CSTR program are shown below in Table 1:

Table 1

Symbol	Definition	Default Values
F1	Inlet reactor flow rate, ft^3/min	18.0
F3	Inlet coolant flow rate, ft^3/min	8.0
T1	Inlet temperature, °F	190.0
T3	Inlet coolant temperature, °F	60.0
CA	Inlet concentration of reactant A, lb. moles/ft^3	1.0
SC	Assigns sinusoidal values to CA, 0.0, 1.0; off or on, respectively	
RX	Assigns random values to CA, 0.0, 1.0; off or on, respectively	
IR	Reaction order, 0.0, 1.0, or 2.0	2.0
CN	Controller off or on, 0.0 or 1.0, respectively	0.0
SP	Controller set-point, °F	180.0
PB	Controller proportional band	20.0
CR	Controller reset	30.0
PX	Plotter off or on, 0.0 or 1.0, respectively	1.0
SA →	Suppress drawing of axis	
TU	Upper bound on graph of T vs. t, °F	250.0
TL	Lower bound on graph of T vs. t, °F	50.0
CU	Upper bound on graph of CA vs. t, lb. mole/ft^3	1.0

Symbol	Definition	Default Values
CL	Lower bound on graph of CA vs. t, lb. mole/ft^3	0.0
PP	Printer off or on, 0.0 or 1.0, respectively	1.0
PR	Print interval, min.	10.0
TI	Simulation time, min.	50.0
RS →	Restart simulation at time zero	
GO →	Continue	
ST →	Stop	

Symbols may be entered in random order, and only those values of the parameters that are to be updated should be entered. Note: Symbols followed by an arrow operate directly, and thus do not require an equal sign or a numerical value.

The following parameters are embedded in the program and cannot be changed during the simulation:

Reactor Volume, 100 ft^3

Heat Capacities, 18 $\frac{Btu}{(lb\ mole)\ (°F)}$

Density, 3.48 $\frac{lb\ mole}{ft^3}$

Heat Transfer Coefficient, 1.667 $\frac{Btu}{(ft^2)\ (min)\ (°F)}$

Heat Transfer Area, 500.0 ft^2

Heat of Reaction, Btu/lb mole

Reaction Rate, $\left(\frac{lb\ mole}{(ft^3)\ (min)}\right)$, (min^{-1}), or $\left(\frac{ft^3}{(lb\ mole)\ (min)}\right)$

for zero, first and second order kinetics, respectively.

Integration Step Size, 0.1 sec

The user has a choice of zero, first, or second order reaction kinetics, and the corresponding reactions are:

Reaction	Kinetic Order
$A \rightarrow B$	0
$A \rightarrow B$	1
$2A \rightarrow 2B$	2

The user can select the kinetic order by entering an appropriate numerical value for the symbol IR. The default value of IR is 2.

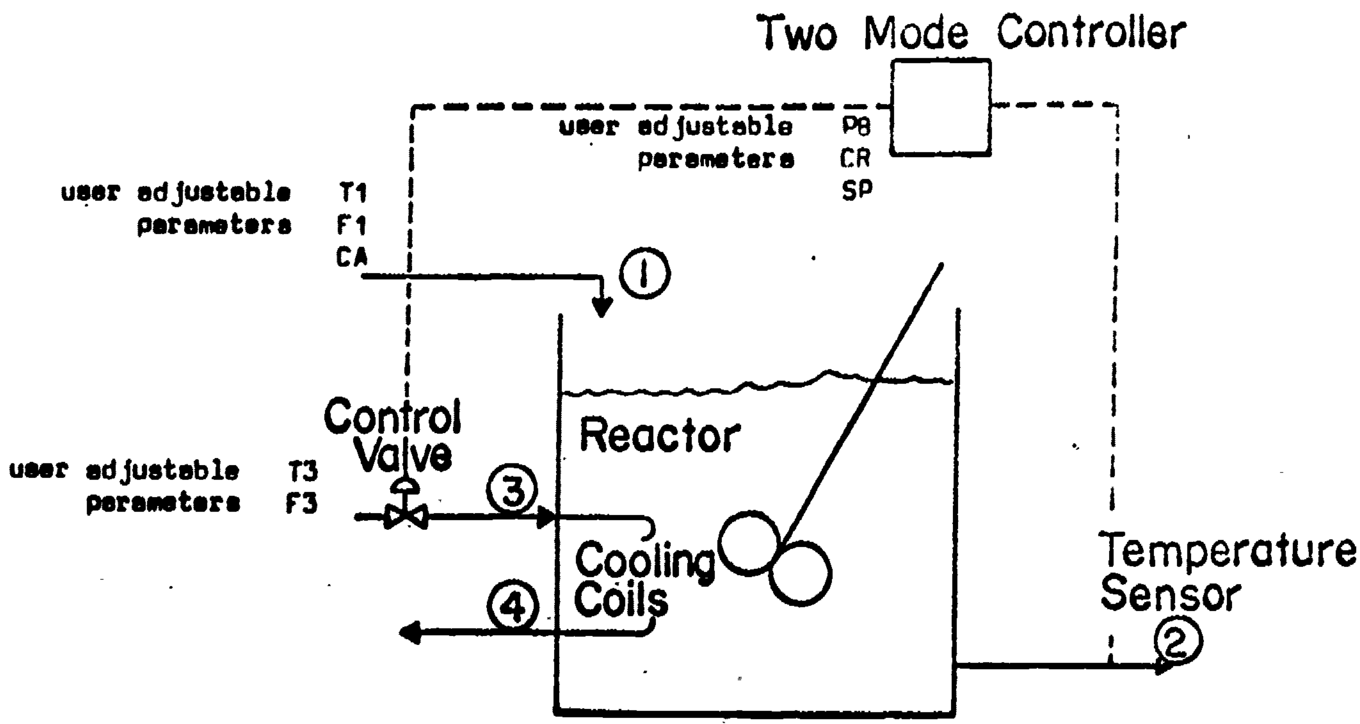

Figure 1

SCHEMATIC DIAGRAM OF THE CSTR SYSTEM.

Design Data

Reactor: 1) Constant Volume, 100 ft^3.

2) Well Mixed.

Cooling Coils: 1) Heat Transfer Area, 500 ft^2

2) Heat Transfer Coefficient is independent of coo[illegible] flow rate and temperature.

Controller: 1) Measures temperature and controls the coolant flow rate.

2) Temperature range for the controller is 60° F to 210° F.

3) Linear valve on the cooling system, range 0.1 to 60.1 ft^3/min.

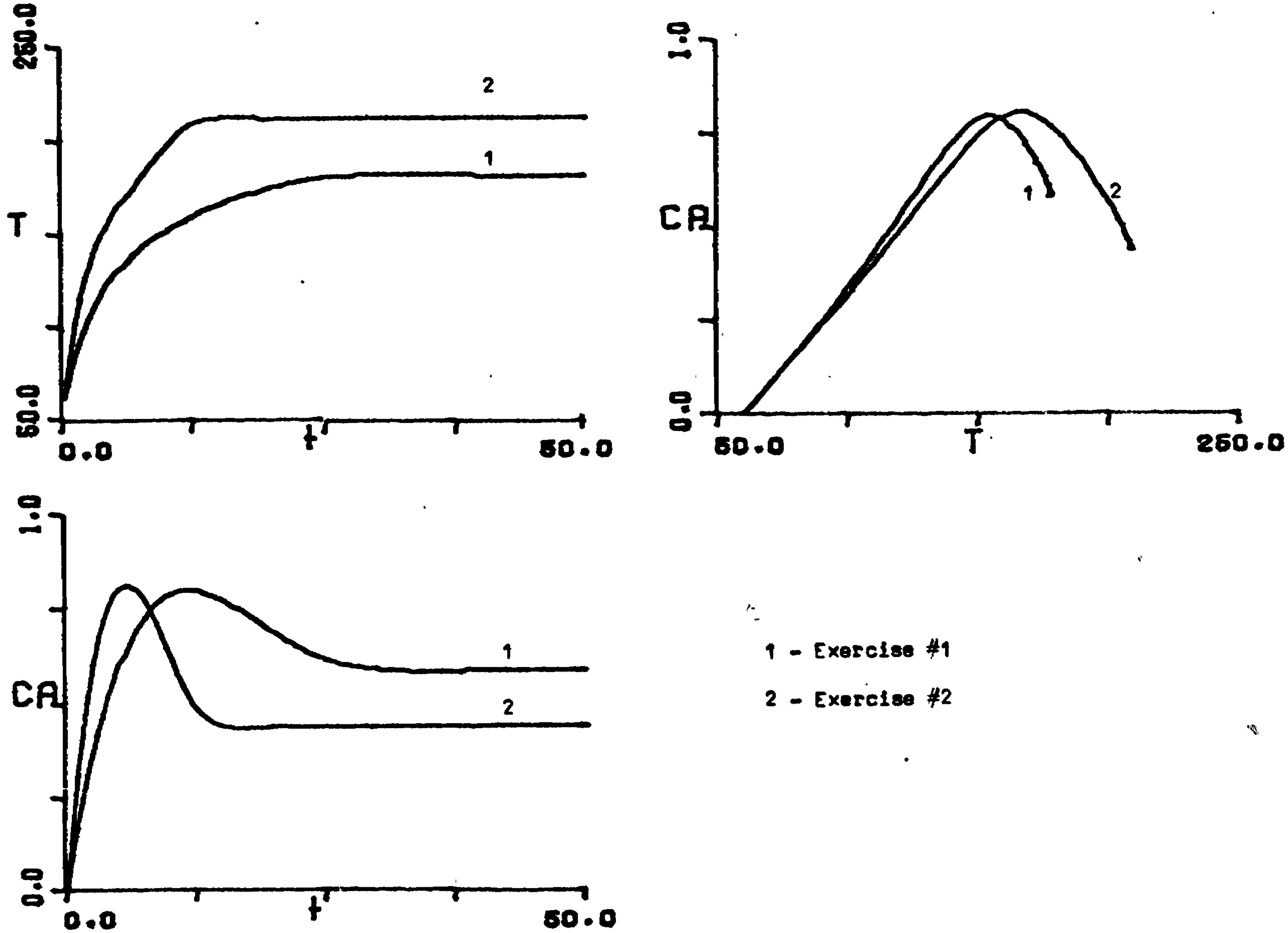

Fig. 2. Graphical output from Reactor Start-up Module.

CSTR Model

Figure 2

SAMPLE OUTPUT FROM CSTR PROGRAM

CSTR SIMULATION MODEL

ENTER DATA

GO

TIME =0

STRM NO	1	2	3	4
FLOW	1.800E+01	1.800E+01	8.000E+00	8.000E+00
TEMP	1.900E+02	6.000E+01	6.000E+01	6.000E+01
ENTHAL	1.190E+04	3.758E+03	3.758E+03	3.758E+03
COMP B	2.480E+00	3.480E+00	3.480E+00	3.480E+00
COMP A	1.000E+00	0.	0.	0.

ENTER DATA

GO

TIME =1.0000E+01

STRM NO	1	2	3	4
FLOW	1.800E+01	1.800E+01	8.000E+00	8.000E+00
TEMP	1.900E+02	1.492E+02	6.000E+01	1.410E+02
ENTHAL	1.190E+04	9.341E+03	3.758E+03	8.835E+03
COMP B	2.480E+00	2.698E+00	3.480E+00	3.480E+00
COMP A	1.000E+00	7.796E-01	0.	0.

ENTER DATA

T1=250.0
F1=20.0   USER CHANGES IN SYSTEM PARAMETERS
CN=1.0
PR=2.0
GO

DEFINITIONS

TIME = Simulation time, min
STRM NO = Stream numbers as illustrated in Fig. 1
FLOW = Flow rate, ft^3/min
TEMP = Temperature, °F
ENTHAL = Enthalpy, Btu/lb-mole
COMP B = Composition of species B, lb-moles/ft^3
COMP A = Composition of species A, lb-moles/ft^3

APPENDIX B

SIMULATION OF REACTOR START-UP

The object of this phase of the simulation is to investigate the dynamic response of a CSTR during the start-up period. Model CSTR simulates an operating well stirred reactor with heat exchange similar to equipment you would expect to find in a unit operations laboratory. You are able to control or change the flow rate of the inlet stream and the flow rate of the coolant. Assume for the purposes of start-up that these are the only two variables that can be changed.

You start with the reactor initially full of species B at a temperature of 60° F. All the other initial values of the variables and coefficients are as listed in the CSTR Model Instructions. Note the reactor volume remains constant in the simulation.

After the teletype types ENTER DATA you may introduce initial conditions or accept the default values listed in the user's instructions. Execute program CSTR and begin the simulation by using the default values, i.e., simply type GO. Repeat GO a sufficient number of times to reach the steady state. Compare the teletype print out with the graphs and follow the course of the response. After reaching the steady state, restart the reactor by entering RS and SA each followed by a carriage return.

Repeat the simulation, but increase the reactor flow rate, F1, by a factor of 2.

Again restart the simulation at time zero. This time, however, devise and implement an operating strategy by adjusting the coolant flow rate that will result in a shorter time to reach the same steady state as in the first run. Test your ideas.

QUESTIONS AND CALCULATIONS TO BE COMPLETED DURING OR AFTER THE SIMULATION

(1) Calculate the residence time for runs 1 & 2.

(2) What is the effect of increased reactor flow rate on the start-up time?

(3) Describe your best start-up strategy in less than 200 words.