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The Use of Computer Simulations in Engineering Capstone Courses: A Chemical Engineering Example—The Mobil Catalytic Reforming Process Simulation*

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While the power of computer technology has been successfully utilized in advancing research, it has been exploited less rapidly in the educational arena. Here we present the concept of using computer simulations of real industrial processes in the chemical engineering laboratory with the catalytic reforming process as an example. Students are introduced to the kinds of problems they might be expected to solve in industry. The assignment begins with students viewing the actual process (bench scale, pilot plant, construction, operation) on video. Realism is also introduced by incorporating statistical fluctuations, budget and time constraints. Schools report success in using the Purdue–Industry modules, not only in laboratory courses but also in kinetics, reactor design and process control courses.

INTRODUCTION AND MOTIVATION

ENGINEERING curricula may be described as a set of mathematics, basic science and engineering courses covering specific required areas, followed (usually in the senior year) by one or more capstone courses in which students are required to apply the various topics learned in the previous years. The problems assigned in such courses often have the following characteristics:

1. They simulate the type of assignment that the student might be expected to handle in industry.
2. They are open-ended, requiring decision-making, analysis and engineering design on the part of the student.
3. They are often assigned to groups of students who solve them as a team.

The premise of this paper is that computer simulations of real industrial situations lend themselves well to inclusion in such capstone courses. Before we list some of the advantages, we begin with a non-engineering example—learning to fly an airplane. Flight simulators are used to train flight crews to operate today's sophisticated jet aircraft. Some of the advantages of flight simulators include:

1. They are much cheaper to operate than real aircraft.
2. They are much safer to operate.
3. The flight crews—pilot, navigator, engineers—can be given simulated flight problems which they must solve together.
4. The flight instructor can introduce all sorts of emergency situations without actually endangering anyone—crew or public. Factors such as turbulence, equipment malfunctions and inclement weather conditions can be programmed by the instructor.
5. The simulation can be temporarily interrupted whenever necessary, so that the instructor can comment on the crew's performance or analyze future actions. The atmosphere in the simulator is much more conducive to a significant educational experience than the noisy and hectic cockpit of a real airplane.
6. The experience of the crew is made quite realistic—the aircraft controls, the instruments, and the external view.
7. Efficient use is made of everyone's time. For example, many practice landings at airports all over the country can be simulated in the same time as one or two real landings, since the takeoff, circling, cross-country flying and holding components of a real flight are not necessary in the landing simulations.

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The readers could probably think of additional advantages. We would like to end this discussion by pointing out that none of us would trust a flight crew whose entire training consisted of simulations. We are proposing, therefore, that engineering simulations, as valuable as we feel they are, should be used to complement and not to replace experience with real equipment in laboratories and plants.

Although the remainder of this paper describes the use of computer simulation in a capstone chemical engineering course, we believe that the basic concept has utility in all engineering curricula. Indeed, the use of computer simulations in engineering is increasing, as evidenced by work reported in education journals in various engineering disciplines and in the *Proceedings of the American Society of Engineering Education*.

PURDUE–INDUSTRY CHEMICAL ENGINEERING COMPUTER SIMULATION MODULES

Since 1986, a series of computer modules of state-of-the-art chemical engineering industrial processes have been, and are being developed at Purdue University [1–3]. Each module has an industrial sponsor, who furnishes data on a process on which the simulation is based, and also produces a 20 min. videotaped 'tour' of the process. To date, modules have been completed for the following processes:

1. Amoco resid hydrodesulfurization process [2].
2. Eastman Chemical methyl acetate reactive distillation process [3].
3. Mobil Research and Development Corporation catalytic reforming process simulation (this paper).
4. Dow Chemical Company styrene–butadiene polymerization process (publication in progress).

In addition, the Air Products hydrogen reactive cooling process is nearing completion and work has begun on the Ethyl Corporation ethylene oligomerization process. The computer modules are used as part of the chemical engineering measurements laboratory course, as described below. Emphasis has thus been given to planning of experiments and analysis of experimental data rather than detailed process design.

Each module is written as an industrial problem caused by a change of conditions in an existing process, requiring an experimental study to re-evaluate the characteristic constants of the process. These might include, for example, reaction rate constants, equilibrium constants, heat transfer and mass transfer coefficients, and phase equilibrium constants. The student teams are expected to design experiments which will enable them to evaluate the needed constants. This is referred to as the *measurements* section of the problem.

After the constants have been determined, the students must validate these by using them in an existing computer model of the process, and comparing the simulated and experimental results. When they are convinced that their constants are reliable, the students must use these constants to predict some other specific process performance characteristics. We refer to this as the *applications* section.

Each process is made to seem realistic not just by videotaped 'tour' but also by the assigned financial budget and time constraints. The problems are open-ended in that the experimental conditions, such as temperature, pressure, flow rates and compositions, are under the students' control. The cost and the associated duration of running experiments vary with the type of experiment and are also functions of operating conditions. Instructor-controlled statistical fluctuations are built into the simulations so that the results of duplicate experiments are not identical. The students must plan their experiments to obtain data from which, with proper analysis, the required constants may be determined without exceeding their budgetary and time constraints.

In the Purdue course, students work in teams of three and have eight 3-h classes to complete the assignment. After an introductory 2-h lecture, they are on their own. If they have queries, they are free to ask the consultant (the instructor, of course), but are charged a fee which must be deducted from their budget. Written reports and a 20-min oral presentation (which is videorecorded for later analysis by the instructor and the student) are required.

All of the previously mentioned advantages of the flight simulator example also apply to the Purdue–University chemical engineering simulation modules.

1. It is certainly cheaper and safer to run a simulator than a real plant.
2. Simulated experiments take up no laboratory space and are able to serve large numbers of students at the same time.
3. An experiment that can take hours or days in real life can be done in minutes on the simulator. Frustrations associated with otherwise malfunctioning equipment can be greatly minimized.
4. Realism, emergency situations and open-ended problem characteristics can be built into the module. If more than one student group is assigned to work on the same project, different data can be given to each (this is set by the instructor).
5. The emphasis of the experiments can be shifted from equipment operational details to experimental design and data analysis.

In the remainder of this paper, a specific chemical engineering example will be presented. It is to be understood that all of the 'experiments' designed, planned or run by the students in this project are, of course, actually performed on the computer.

THE MOBIL CATALYTIC REFORMING PROCESS SIMULATION [5]

Reforming is a process in which hydrocarbons in the gasoline range are 'reconstructed' without significantly changing their carbon number, to improve the quality of gasoline fuel. The predominant reactions can be characterized as dehydrogenation, dehydro-cyclization and isomerization. Naphtha feeds (n-paraffins and cycloparaffins with 5–12 carbon atoms and octane numbers in the 40–60 range) are upgraded to a product (reformate) containing aromatics and branched paraffins (octane numbers 90–120), the principal gasoline components. Low carbon-number paraffins (C_{5-}), outside the gasoline boiling range and therefore of lower value, are also produced through cracking side-reactions. These transformations take place through a complex set of chemical reactions involving more than 300 chemical species [5]. The schematic of a typical semi-regenerative catalytic reformer is shown in Fig. 1. Modeling such systems in a simpler way is accomplished by 'lumping' components as shown below.

$$C_{5-} \leftarrow P \underset{k_{2r}}{\overset{k_{1f}\quad k_{2f}}{\rightleftharpoons}} CP \underset{k_{3r}}{\overset{k_{3f}}{\rightleftharpoons}} CH \underset{k_{4r}}{\overset{k_{4f}}{\rightleftharpoons}} A \qquad (1)$$

where the lumped components are:

C_{5-}	pentanes and lighter	CH	cyclohexanes
P	paraffins	A	aromatics
CP	cyclopentanes		

All of the reactions are catalytic. While the catalyst deactivates with time, deactivation does not affect all of the reactions equally. This causes a change in product distribution as well as lowered reaction rates. As the catalyst deactivates during reformer operation, higher reaction temperatures will be required to keep the octane number (aromatics formation) at desired levels. Eventually, the reactor temperature will approach a maximum limit, at which time the reformer must be shut down, and the catalyst regenerated. The time elapsed between fresh catalyst startup and shut down due to attainment of the temperature limit is called the *cycle length*. The study of catalytic deactivation is the focus of this project.

An important factor affecting catalyst deactivation is the ratio of the partial pressures of hydrogen and hydrocarbons (P_H/P_{HC}). The catalyst deactivates due primarily to coke formation, which can be minimized by maintaining high hydrogen pressures. Consider a reformer run in which the temperature is increased during the cycle in order to maintain a fixed aromatics content in the product. If P_H/P_{HC} is kept low during the run, C_{5-} formation is minimized—since forward reactions in (1) are dehydrogenation reactions—and gasoline yield is therefore high (gasoline yield = wt reformate/wt feed = (wt feed − wt C_{5-})/wt feed). However, these same conditions also increase catalyst deactivation rate, thereby decreasing cycle length. This overall qualitative trend is shown in Fig. 2. An optimum P_H/P_{HC} ratio will often result from these competing trends, which will maximize plant profits.

REFORMING MODEL

We divide the description of the lumped reforming model into kinetics of the conversion reactions and catalyst deactivation.

Reaction kinetics

The reforming kinetics are based on a few assumptions.

1. The non-linear rate expressions of the lumped-component reactions are assumed to follow Langmuir–Hinshelwood kinetics and *n*th-order dependency with respect to hydrogen. The hydrogen dependencies of the rate are incorporated into the rate constants.
2. The same Langmuir–Hinshelwood type adsorption term is applicable to each reaction step.
3. Since commercial-sized catalysts are used in the

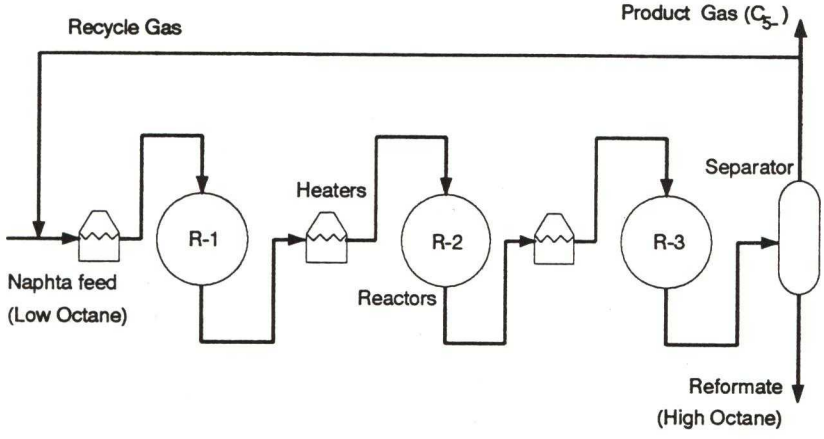

Fig. 1. Typical catalytic reformer (from [5], © 1987, Academic Press, Inc.).

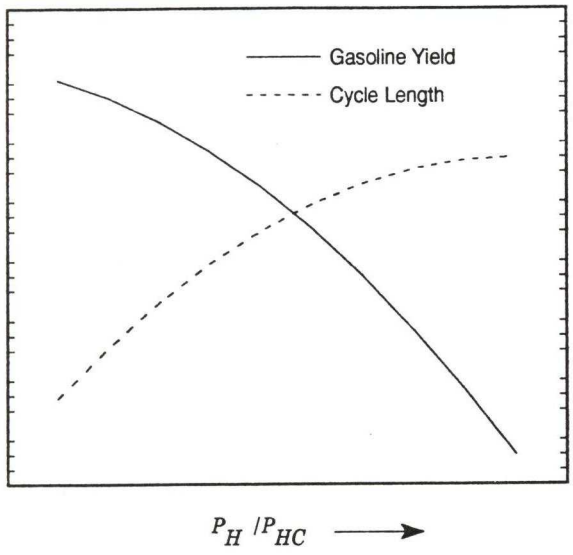

Fig. 2. Effect of P_H/P_{HC} on cycle length and gasoline yield.

kinetic experiments, diffusional effects are combined into the rate constants.

Based on these assumptions, the contribution to the overall rate of reaction of a component j (say, reactant) of reaction i is given by

$$\frac{dw_j}{dv} = \frac{\left[\frac{PV}{FRT}\right] k_{if} w_j \alpha_i}{1 + K_H P_H + \frac{PF_{HC}}{F} \sum_{j=1}^{5} K_j w_j} \quad (2)$$

where v is the fractional catalyst volume, w is the weight fraction, α_i corresponds to the effect of catalyst deactivation on reaction i, and the denominator consists of absorption-related terms (see the nomenclature section for details on the other symbols). The rate constants of the reactions follow the Arrhenius form and include the nth-order dependencies of the hydrogen partial pressures. For the forward reactions,

$$k_{if} = k_{if}^{o} (P_H)^{n_{if}} \exp(-E_{if}/RT) \quad (3)$$

The total effect on the weight fraction of the jth species is the sum of the effects of all the reactions in which species j is either a reactant or a product. For example, if j = CH, then

$$\frac{dw_{CH}}{dv} = \left[\frac{PV}{FRT}\right] \frac{[k_{3f} w_{CP} \alpha_3 - k_{3r} w_{CH} \alpha_3 - k_{4f} w_{CH} \alpha_4 + k_{4r} w_A \alpha_4]}{1 + K_H P_H + \frac{PF_{HC}}{F} \sum_j K_j w_j} \quad (4)$$

Expression (4) also reflects the fact that the catalyst deactivation, α_i, affects both the forward and the reverse reaction rates equally. An extensive study of the kinetic behavior of the reformer reactions for a typical reformer feed, A-216, (67.5% P, 8.2% CP, 10.1% CH, 14.2% A) over *fresh* catalyst has been completed and the rate constants (ks) are incorporated into the reformer model.

Catalyst deactivation kinetics

The catalyst deactivation term, α_i, appearing in equation (2), is given by:

$$\frac{d \ln \alpha_i}{dt_d} = -k_{id}^{o} \left[\frac{P_H}{P_{HC}}\right]_d^{\delta_i} \exp(-E_{id}/RT_d) \quad (5)$$

where the subscript d refers to the conditions of deactivation. Reforming catalysts are known to have two types of active sites, acid and metal. The rate-limiting steps for the cracking and ring-closure reactions (see (1); P → C_{5-} and P ⇌ CP) involve the acid sites, whereas the isomerization and dehydrogenation reactions (CP ⇌ CH and CH ⇌ A) are limited by the metal activities. Thus, α_1 and α_2 are expected to take on approximately the same values (and similar temperature and P_H/P_{HC} dependencies). Likewise α_3 and α_4 should be similar.

THE COMPUTER PROGRAM

The module is written in C and FORTRAN languages. It uses some IMSL routines for solving systems of linear, non-linear and ordinary differential equations. The program can simulate a pilot plant at steady or unsteady states. For 'experiments', the output results are randomly perturbed to simulate experimental error, based on a variation parameter set by the instructor.

The program can run on any machine that supports the X-Window System. At Purdue, it runs on Sun Sparc workstations with 12 MB of memory. Each module uses less than 10 MB of disk space.

An important feature of the program is its menu-driven graphical user interface. This enables any person to use it regardless of his or her knowledge of computers. An on-line help facility is provided to further assist the user to navigate through the program. The user can exit the program at any time.

STUDENT ASSIGNMENT

Budget and experiments

In the measurements part of the Mobil project, students are required to determine the following:

1. Constants k_{ad}^{o}, E_{ad} and δ_a for the acid sites of the catalyst.
2. Constants k_{md}^{o}, E_{md} and δ_m for the metal sites of the catalyst.

To determine these quantities, the students must prepare deactivated catalyst samples and then run the reformer pilot plant.

Contributing a sense of realism in this module is a requirement that the students work within a

Table 1. Expenses[a] and duration

Activity	Cost (US$)	Duration (h)
Preparation of deactivated catalysts	45,000	3000
Catalyst evaluation studies		
Start up	1400	24
Sample analysis, per run	500	–
Reactor lineout (clean up)	500	12
Consultation	500	?

[a] All expenses are to be multiplied by 1.5 and 2 for Saturday and Sunday runs, respectively.

budget of $115,000 (simulated money, of course). Table 1 shows the relevant costs.

Preparation of deactivated catalyst samples. Before they can run any experiments, the students must prepare catalyst samples. A total of 1300 cm^3 of catalyst is provided, from which eighteen 71 cm^3 catalyst samples may be prepared. Samples are deactivated under varying conditions in six automatic deactivation rigs in the Mobil Paulsboro Laboratory. Each rig can hold a maximum of 225 cm^3 of catalyst and is designed to run at constant temperature, P_H and P_{HC} for long periods of time (up to 3000 h). Periodically, catalyst may be added to or removed from the rig, and the operating conditions changed.

Since the catalyst deactivation conditions in the rigs are constant (for each sample), equation (5) can be readily integrated for use in the determination of deactivation parameters. See Table 2 for the allowed ranges of deactivation conditions.

Catalytic reformer pilot plant. An isothermal, plug flow, fixed catalyst bed, U-shaped reactor (shown in Figure 3) is used for the experiments. The reactor, containing 71 cm^3 of catalyst, is immersed in a fluidized sand bath to achieve isothermal conditions. Five sample taps are spaced along the reactor so that the stream composition profiles can be determined over a wide range of catalyst contact times. Samples are also taken at the reactor inlet, making a total of six sampling points along the reactor length. Gas samples are withdrawn at each tap through capillary flow restrictors into a heated manifold and then fed to an on-line gas chromatograph. Details are provided in [5].

For use in the pilot plant runs, sufficient quantities of A-216 feed, and pure P, CP, CH and A are available. Mixtures of these samples may, of course, also be fed to the reactor. During any pilot plant run, the following conditions are assumed along the length of the reactor.

1. Constant temperature.
2. P_H is constant since it is fed in large excess.
3. Although the amounts of individual hydrocarbon species are changing, P_{HC} may be assumed to be constant.
4. The pressure drop is negligible.
5. αs will be constant, since the time required for the catalyst to deactivate is very large compared to the duration of a single run.

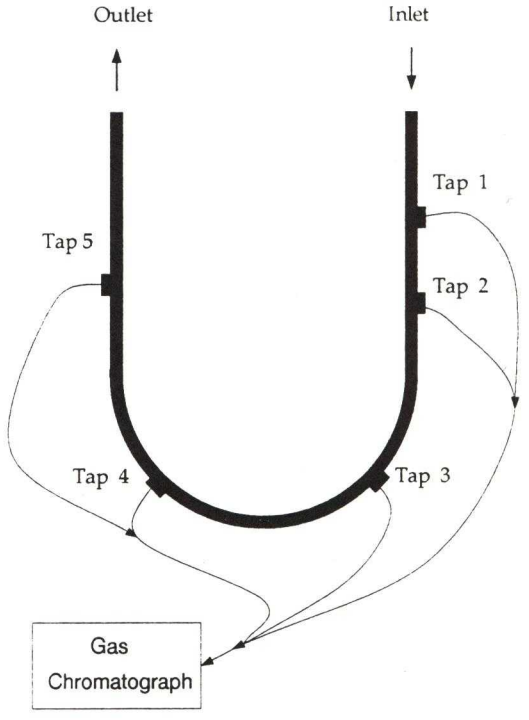

Fig. 3. Isothermal reformer reactor (from [5] © 1987 Academic Press, Inc.).

Table 2 lists the ranges of allowable deactivation conditions. After samples from a run have been collected, the task of estimating the deactivation coefficient (αs) would require integration of equations (such as (4), for all the components) for a fixed set of coefficients and choosing the set that closely fits the measured data. However, it was decided to relieve the students of this work, since the time and effort required could be disproportionately high while needlessly digressing from the aim of the project. The computer has been programmed to do these calculations, and hence directly provides the values of the αs after each run.

Validity of the computer-predicted αs. As indicated earlier, αs are predicted by finding a set of kinetic parameters that best fit the data. These predicted values, therefore, can be no better than the estimated values of the kinetic parameters. The simulator is programmed to check whether the data are sufficiently reliable so that the calculated

Table 2. Summary of allowed operating conditions

Variable	Pilot plant	Pre-run deactivation	Simulation
Temperature (°F)	100–980	840–980	≤980
Pressure (p.s.i.a.)	100–500	100–500	350
P_H/P_{HC}	2–10	4–10	2–10
Space velocity (h^{-1})	0.5–20	NA	1

kinetic parameters are meaningful. For example, if the reaction conditions cause the reactions to occur so rapidly that almost all of the conversion occurs before the second tap of the reactor, the data from the other downstream taps become useless and none of the predicted values can be trusted.

While numerous such cases can be envisioned, a simpler criterion that reasonably encompasses them all is the following: the α_i predicted for reaction i may be trusted only if, for at least three pairs of adjacent taps, the weight fractions of the reactant and product (of reaction i) change by at least 0.005. Clearly, since the catalyst deactivation coefficients depend solely on the (past) pre-run deactivation conditions, the pilot plant operating conditions must be chosen to ensure the validity of the predicted αs.

Validity of the student-estimated deactivation parameters. Apart from the pilot plant experiments, a pilot plant 'simulator' is provided that will accept as initial input, the parameters of the catalyst deactivation model determined from the series of experiments. Students can run the simulator at the same conditions and feed as those of representative experiments. A good match of the simulated and actual outcomes indicates that the determined deactivation parameters are correct within limits of experimental error.

Application problem: optimization of reformer performance

In general, the *application* problem requires using the parameters estimated from the experiments to study an existing or new process focusing on aspects such as efficient startup, effect of scale up on heat transfer requirements, controllability at desired steady states, or simply analyzing the performance. In the Mobil project, the problem is to optimize the catalyst regeneration schedule.

Referring to Fig. 2, higher P_H/P_{HC} ratios favor longer cycle length that reduces the costs of downtime and catalyst regeneration, while lower P_H/P_{HC} ratios increase gasoline yield and product values. Thus, there is an economic trade-off between the two competing trends. The objective is to determine the P_H/P_{HC} ratio that optimizes the annual profit of the unit.

The reformer model for this problem, which simulates an isothermal plug flow reactor, is designed to predict the operation of a reformer with 20,000 barrels/day feed of A-216 naphtha. Other operating conditions (see Table 2) that cannot be changed are pressure (350 p.s.i.a.) and the space velocity (1 h^{-1}). P_H/P_{HC} can be varied from 2 to 10. Once the students enter their deactivation constants and a P_H/P_{HC} value, the program calculates the initial temperature of the reactor to achieve a desired product octane number, in this case, corresponding to 31% aromatics.

For optimization, the reformer model is run in the *manual mode*. The aromatics content in gasoline (product) is to be controlled between 30.5 and 31.5%. As the aromatics content falls to the lower level, the feed temperature will have to be increased, but only enough to keep the aromatics content to below 31.5%. This manipulation has to be repeated until the temperature reaches 980°F. The simulator will also terminate automatically if the output aromatics content is not in the 30–32% range. An example of an actual complete manual run is given in Figure 4. The annual profit function (given to students) not only accounts for the cost of raw materials and products but also includes the costs of operating the reformer and catalyst regeneration (labor and chemicals).

The simulator can also be run in *automatic mode* where the computer controls the process. After the students determine an optimal P_H/P_{HC} for profitable operation, they are required to run the simulator in *automatic mode* for this derived pressure condition, and compare the results of the cycle time and gasoline yield from the two modes of operation.

Recall that the application problem is attempted by students *after* they determine the catalyst deactivation parameters. In the event that they are unable to obtain reasonable parameter estimates, the computer program has the option of allowing them to perform the optimization using the *instructor's data* (with the permission of the instructor).

COMMENTS

Apart from the undergraduate design laboratory, the computer modules developed at Purdue have also been used successfully in reactor design and process control courses in several schools (see, for example, [6]). This is partly due to the flexibility in proposing the problem or stressing only part of the problem. For example, in a course that can allow only three weeks for the Mobil project, the task of preparing the deactivated catalysts can be skipped. For this reason, a default set of deactivated catalysts is included for the students to start with.

In fact, the accreditation requirements for chemical engineering education have recently been revised and they recommend that the design component be spread throughout the curriculum rather than the current practice of including design primarily in the final year. Schools seeking to follow these new guidelines can easily find ways to adapt our modules in different chemical engineering courses.

A project to port these modules from Sun workstations to other Unix platforms like HP, DEC, IBM and Silicon Graphics is expected to begin soon. Porting of the software onto personal computers is also being considered.

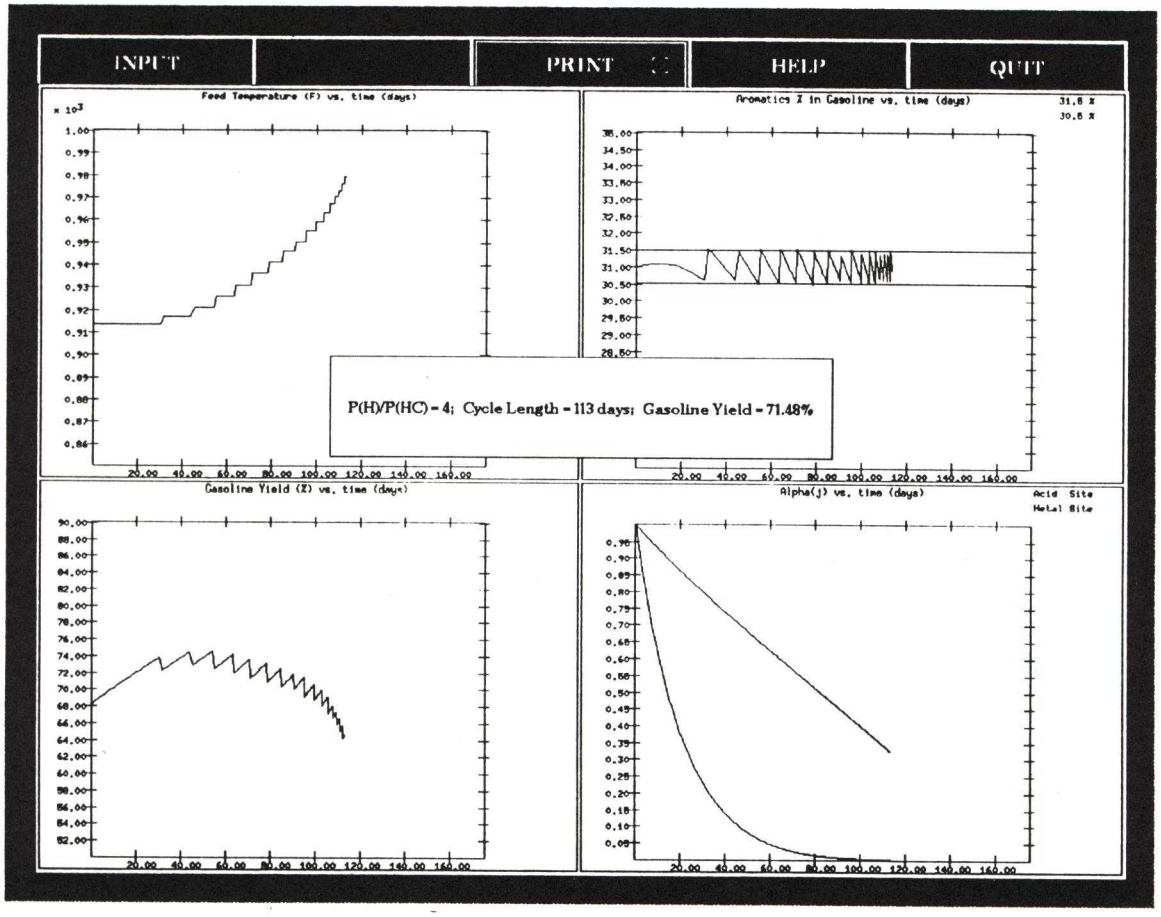

Fig. 4. A screen-dump of a manual run showing profiles of (clockwise from top left) feed temperature, product aromatics content, catalyst deactivation terms (α_is), and gasoline yield. At the end of the run, the cycle length and an average gasoline yield are displayed.

CONCLUSION

At the time of writing, the Mobil module has been used at Purdue for three years, and our experience has been positive. The commercial reality of the process (the process operates at multiple Mobil sites), the simplicity of its presentation and use, its applicability to both laboratory and lecture courses, and a true to life simulated budget, among other aspects, make projects of this kind very attractive in the chemical engineering curriculum. Future directions to improve the effectiveness of education via the use of computers must include efforts to incorporate state-of-the-art video-based technologies [7] into computer applications to make abstract transport phenomena and kinetic concepts more concrete.

NOMENCLATURE

α Catalyst deactivation term ($0 \leqslant \alpha \leqslant 1$)
E Activation energy (BTU/lb-mol)
F Flow rate (unsubscripted ⇒ total), (lb-mol/h)
K Adsorption equilibrium constant (p.s.i.a.$^{-1}$)
k Reaction rate constant (h^{-1})
k^o_{id} Deactivation pre-exponential factor (h^{-1})
k^o_{if} Reaction rate pre-exponential factor (p.s.i.a.$^{-n_{if}}h^{-1}$)
P Pressure (unsubscripted ⇒ total) (p.s.i.a.)
T Temperature (°R)
t Time (h)
V Total catalyst volume (ft^3)
v Fractional catalyst volume along length of reactor ($0 \leqslant v \leqslant 1$)
w Weight fraction of component in reactor ($0 \leqslant w \leqslant 1$)

Subscripts
d Deactivation
f Forward reaction
i ith reaction, $i = 1, 2, 3, 4$
j jth component, $j = C_{5-}$, P, CP, CH, A
H Hydrogen
HC All hydrocarbons

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