USE OF VISUAL INTERACTIVE DISPLAY IN PROCESS DESIGN

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Both ChE students in process design classes and practicing process engineers have long been plagued by the necessity of doing many tedious and methodical calculations before reaching the more interesting and creative aspects of design. The advent of high speed computers generated great hope that both the professional engineer and the student would be freed from tedium and would be able to concentrate on the heart of any engineering problem — the exercise of engineering judgment and innovation. Unfortunately, in practice this hope has not been totally realized. Even if one assumes that the programming and "debugging" are done by others, several crucial issues remain which detract from the real engineering meat of the problem.

• Although the usual process design calculations can be done in seconds, the actual time measured from the time of submitting input data to the receipt of the printed results can be many hours. The reason for this is simply that large computers in any organization are used by many people. Time sharing makes this use an orderly, efficient process, but some kind of priority system must be established which often relegates many problems to longer waiting periods. This is especially true in a university where involved research calculations may take a large portion of computer time.

• The results when obtained consist of the familiar long printout of masses of numbers which is essentially unintelligible until one produces some sort of graph that enables analysis of trends. This further delay is particularly annoying during the earlier stages of contact with the problem when the student or designer has little feel for the way variables interact to effect outcomes, and is anxious to overcome this deficiency. Chemical reactor design, because of the associated nonlinear systems of differential equations is an excellent example of a problem requiring detailed calculations merely to acquire a feel for the problem.

• In the early stages of a problem the designer must decide how the stated purposes are to be accomplished. It is during this aspect of the problem that he exercises his creative abilities and makes some of the most critical decisions of the project. Although the creative act remains essentially a mystery to psychologists and others who have attempted to study it, it seems rather clear that it usually occurs most successfully when one is totally immersed in the problem and is obtaining the results of tentative ideas in a rather rapid and orderly fashion. This climate is not provided by the usual mode of interacting with the digital computer as described above. Relatively long waiting periods for receiving results together with the presentation of these results in long printed format cause the mind to wander from the problem and require that one renew his interests and reestablish his previous viewpoints each time a series of results is received. Of course, one can submit a number of different designs at one time. In any real situation, however, one is apt to submit a number of cases which are trivial and do not necessarily converge to the desired result. This can be a very common and natural consequence of an inadequate intuition about the variables during the early stages of attack on a problem.

An obvious and much more desirable beginning on a design problem would involve toying with the variables and immediately observing the results in graphical form. An interactive visual display is ideally suited for this purpose. We have recently adapted such a unit for use by members of the senior class in process design, and the results have been most gratifying. Each student in two separate twenty minute periods was able to master rather complete understanding of the impact of the several variables on the problem and developed a feel for the issues which enabled him to make major engineering decisions. This encounter with the visual display of profiles of variables was then followed by an opportunity to accomplish study of a well planned series of cases using the more common procedure of submitting and receiving design cases from the digital computer in printout form. The second phase of work now, however, was intelligently planned and executed for the purpose of obtaining precise quantitative results for a rather well-defined system, major decisions on operating conditions having been fairly well decided by use of the visual display.

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The proof of the efficacy of this procedure can best be realized by observing the effect on students. The encounter with the visual display is essentially a teaching encounter in which the student teaches himself about the problem. It is rather inspiring and somewhat surprising to see how rapidly a student becomes very knowledgable about the important issues. Students seem to be overflowing with ideas at this stage and become most anxious to proceed with testing these ideas further. Even the average and below average students are stimulated and their abilities extended to the maximum. The use of visual interactive displays has received a great deal of attention in mechanical design, and it also now seems to possess equally exciting potential in process design.

In order to provide interested readers with some insight into the issues involved in planning and executing the use of visual interactive displays, we will present some of the details of a reactor design problem and the issues involved in selecting the variables for display.

THE DESIGN PROBLEM

The design problem was stated simply: Design a catalytic reforming unit for producing 20,000 BPSD of 95 research octane number reformate.

Hydrodesulfurized Feedstock Analysis

The feedstock has API gravity of 51.9° and volumetric composition of 43.4% paraffins, 40.0% naphthenes, and 16.4% aromatics. Data for the ASTM distillation are: IBP—240°F; 10%—262°F; 20%—272°F; 30%—279°F; 40%—284°F; 50%—292°F; 60%—302°F; 70%—311°F; 80%—322°F; 90%—335°F; 95%—346°F; and EP—369°F.

Catalyst

The catalyst is Sinclair-Baker RD 150 (0.6% Pt-on-alumina), 1/16″ extrudate and has bulk density of 0.78 gm/cc; surface area of 471 m²/gm; and pore volume of 0.42 cc/gm.

Catalyst characteristics: Poisoned by sulfur, arsenic, and nitrogen compounds. Coking occurs on the catalyst and deactivates it gradually. Regeneration by burning with air partially restores the activity. Catalyst life declines with increasing operating temperature and decreasing pressure.

Idealized Rate Equations[7]

A number of references on the process were supplied[1-10] including kinetic data.[7] The following equations apply:

Each of the three hydrocarbon classes is represented by a single compound having the average properties of that class.

1. Naphthene $\rightleftharpoons$ aromatic + $3H_2$; $\quad \Delta H_1 = 30,500 \dfrac{Btu}{\text{mole } H_2 \text{ liberated}}$

$$-r_1 = k_{p1}\left(P_N - \frac{P_A P_{H2}^3}{K_{p1}}\right)$$

$$k_{p1} = e^{\left(23.21 - \frac{34,750}{T}\right)}, \quad \frac{\text{lb-moles naphthene}}{(\text{hr})(\text{lb cat})(\text{atm})}$$

$$K_{p1} = e^{\left(46.15 - \frac{46,045}{T}\right)}, \quad \text{atm}^3$$

2. Naphthene + H_2 $\rightleftharpoons$ Paraffin; $\quad \Delta H_2 = -19,000 \dfrac{Btu}{\text{mole } H_2 \text{ consumed}}$

$$-r_2 = k_{p2}\left(P_N P_{H_2} - \frac{P_P}{K_{p2}}\right)$$

$$k_{p2} = e^{\left(35.98 - \frac{59,600}{T}\right)}, \quad \frac{\text{lb-moles naphthene}}{(\text{hr})(\text{lb cat})(\text{atm})^2}$$

$$K_{p2} = e^{\left(\frac{8,000}{T} - 7.12\right)}, \quad \text{atm}^{-1}$$

3. Paraffin + H_2 $\rightarrow$ Hydrocracked Products; $\quad \Delta H_3 = -24,300 \dfrac{Btu}{\text{mole } H_2 \text{ consumed}}$

Stoichiometry: $C_n H_{2n+2} + \frac{n-3}{3} H_2 \rightarrow \frac{n}{15}[c_1 + c_2 + c_3 + c_4 + c_5]$

$$-r_3 = k_{p3}\frac{P_P}{P_T} = k_{p3}Y_P$$

$$k_{p3} = e^{\left(47.97 - \frac{62,300}{T}\right)}, \quad \frac{\text{lb-moles paraffin}}{(\text{hr})(\text{lb cat})}$$

4. Naphthenes + H_2 $\rightarrow$ Hydrocracked Products; $\quad \Delta H_4 = -22,300 \dfrac{Btu}{\text{mole of } H_2 \text{ consumed}}$

Stoichiometry: $C_n H_{2n} + \frac{n}{3} H_2 \rightarrow \frac{n}{15}[c_1 + c_2 + c_3 + c_4 + c_5]$

$$-r_4 = k_{p4}\frac{P_N}{P_T} = k_{p4}Y_N$$

$$k_{p4} = \text{same as } k_{p3}$$

. . . the creative act remains a mystery, but it seems clear that it occurs most successfully when one is totally immersed in the problem and is obtaining the results of ideas in a rapid and orderly fashion . . . the visual display expedites the creative process . . .

The value of n is obtained from the molecular weight of the feed and the mole fractions of the feed component types as described by Smith.[7]

Balance Equations in Difference Form

Material:

$$(-r_1) \frac{\Delta W}{F_T} = \Delta x_1 \qquad (5A)$$

$$(-r_2) \frac{\Delta W}{F_T} = \Delta x_2 \qquad (5B)$$

$$(-r_3) \frac{\Delta W}{F_T} = \Delta x_3 \qquad (5C)$$

$$(-r_4) \frac{\Delta W}{F_T} = \Delta x_4 \qquad (5D)$$

Heat:

$$\frac{\Delta W}{F_T} [(-r_1)(-\Delta H_1)(3) + (-r_2)(-\Delta H_2) + (-r_3)(-\Delta H_3) \frac{n-3}{3}$$

$$+ (-r_4)(-\Delta H_4)(\frac{n}{3})] = \sum_{i=1}^{9} N_i C_{P_i} \Delta T \qquad (6)$$

The reason for use of adiabatic reactors in all industrial installations of this process was first established in discussions with the students. By proper choice of initial condition Reaction 1 is made to proceed to the right and Reaction 2 to the left. These events are both highly endothermic and demand staging and intermediate heating.

The balance equations were programmed for the iterative calculations necessitated by the coupling of Equation 5A-D and 6. Variables selected for appearance on the visual display are limited by the capacity of the oscilloscope to produce a readable graph. Thus, items were chosen that would contribute most to the students grasp of the problem and understanding of the sensitivity of the more important rates to changes in variables. The cumulative volume per cent aromatics in the C_5^+ reformate, which is correlated with octane number, and the rate profiles of aromatics production and paraffin hydrocracking were selected for visual display as a function of W/F (reciprocal space velocity). These rates have an overriding effect on octane number of the finished product. Volume per cent aromatics is not only affected by the amount of aromatics formed but also by the extent of hydrocracking, which acts to decrease the volume of C_5^+ paraffins in the product and thus increase the net volume per cent aromatics.

At the end of each trial design the designer also needs to know the yield, which is most desirably expressed for a product sold by volume, as volume of C_5^+ product divided by volume of feed.

Use of the Visual Interactive Display

These variables were plotted as shown in Figures 1 - 3. All are graphical except the yield figure which appears as a number at the end of each trial on the lower right hand corner of the screen. The user selected the number of reactors, the inlet temperature, average pressure and space velocity for each reactor by punching the keyboard as shown in Figures 4 and 5. This simple keyboard could be mastered by anyone, even a person not familiar with the problem. Thus, it was possible for a student to use the keyboard freely and let his ideas develop without inhibition.
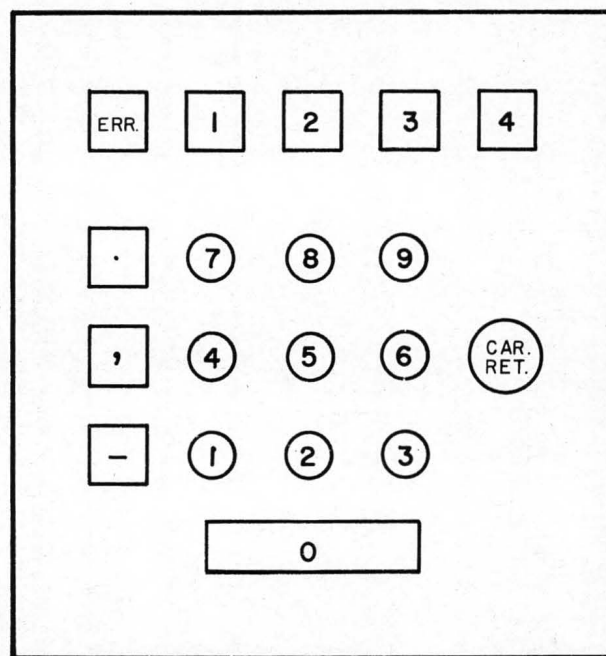

Fig. 4. Keyboard. The top row of keys is used to select the class of variable, e.g., temperature, pressure, W/F, and numbers of reactors. The particular reactor of interest and the magnitude of each variable is specified using the lower array of keys.

Typical Trial Run on the Display

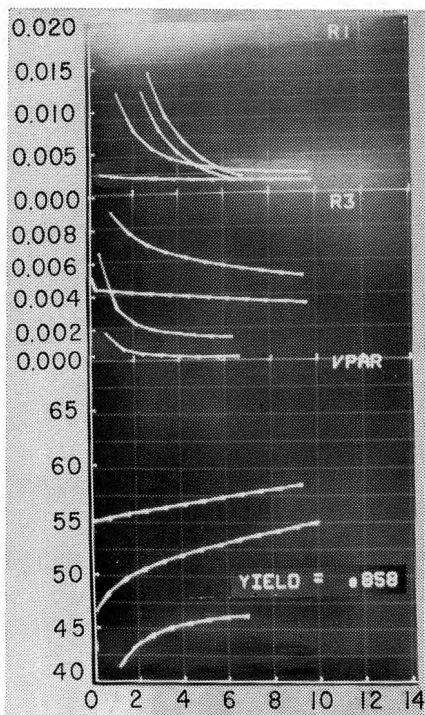After initial random trials or prior study of literature on existing reformer plants the stu-

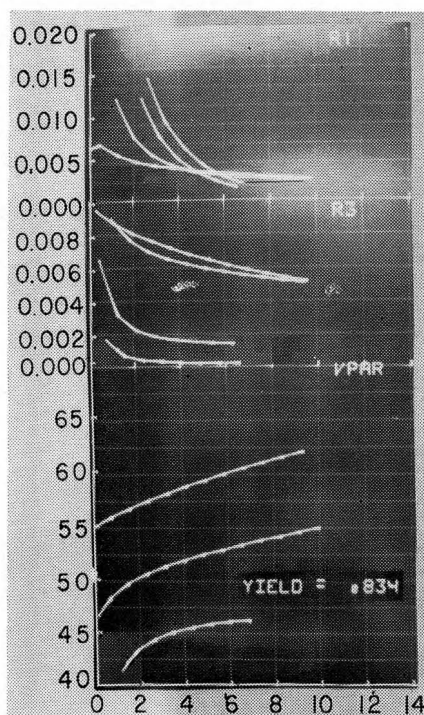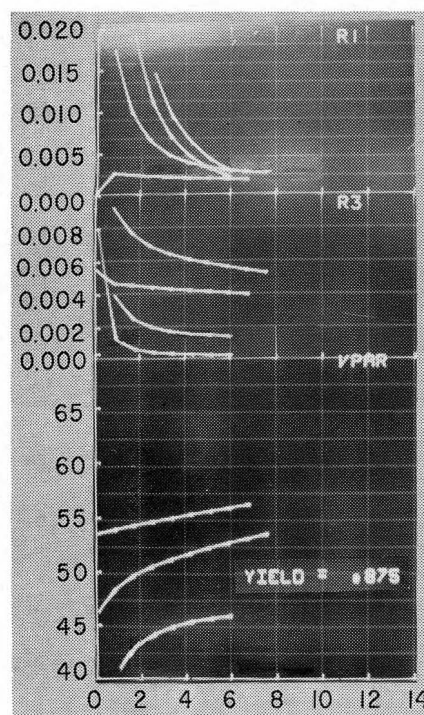Fig. 1. View of display for Trial 1.   Fig. 2. View of display for Trial 2.   Fig. 3. View of display for Trial 3.

X axis division 2. **Y axis division R1 = 0.005, R3 = 0.002, VPAR = 0.05 beginning at 0.4. R1 and R3 are rates of reactions 1 and 3 respectively. VPAR is volume per cent aromatics.**

dent decides that a reasonable set of input values would be as follows:

Trial 1: (Fig. 1) No. of Reactors 4

T	950	950	950	950
P	475	450	425	400
W/F	7	7	10	10

From the display the student realizes that a volume per cent aromatics (VPAR) of 62.9 at outlet of last reactor is above his product quality specification (57% required) and that his yield is not particularly good. The student reasons that possibly eliminating the re-heating between the 3rd and 4th reactor would cause less hydro-cracking of paraffins which would lower his product quality to a more acceptable value and also simplify the design of the reformer. From previous trials the student knows to expect a temperature drop of approximately 25°F in the third reactor. The student then changes the inlet temperature of the 4th reactor to give:

Trial 2: (Fig. 2) No. of Reactors 4

T	950	950	950	925
P	475	450	425	400
W/F	7	7	10	10

The student sees that the results of Trial 2 are a VPAR of 58.25 which is near the range of product quality desired. He also is pleased to see that the yield has increased to 85.8%.

Upon examining the rate of conversion of naphthenes to aromatics (the top-plot-R1) he sees that R1 has become quite low near the end of 1st and 2nd reactor. He, therefore, reasons that the 1st and 2nd reactor should be made smaller. Also, since the product quality could still be lower and be acceptable, he decides that he will need less cracking of paraffins and can therefore shorten both the 3rd and 4th reactors. These inferences lead to

Trial 3. (Fig. 3) No. of Reactors 4

T	950	950	950	925
P	475	450	425	400
W/F	6	6	7.5	7.5

The student notes that R1 has not fallen to as low a value as in Trial 2. He sees that his product quality has dropped to a VPAR of 57.0% which is quite acceptable to him and he is also rewarded with a much higher yields of 87.5%. He also recognizes that Reactors 3 and 4 can be
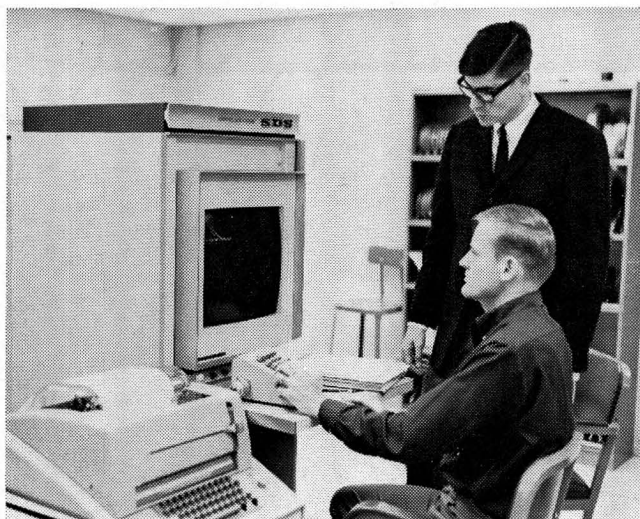
Fig. 5. Student operating display under observation of teaching assistant.

combined into a single reactor if vessel economics so indicate.

Description of Computer Equipment and Program

Equations 1 through 6 were programmed to calculate the rates of reaction, temperature profiles, and material balances through the length of fixed bed catalytic reactors. An iterative technique was used to balance the heats of reaction and reaction rates for small increments of catalyst bed based on an arithmetic average temperature for that increment. Once a balance was reached for one increment of catalyst bed, the outlet temperature and component flow rates were used as inlet values to the next increment of catalyst bed. The computation continued until the prespecified amount of catalyst had been used. The program allowed the student to specify the number of reactors and the inlet temperature, average pressure, and space velocity of each reactor.

The program was modified to run on a Scientific Data Systems Model 930 computer coupled to a Model 9185 Scope Display having vector and character generators. The unit had 32,000 words of memory. The program was operated under the special University of Texas Tape Monarch system containing a custom multigraphics package for the scope.

CONCLUSION

It can be seen from the description of a series of trials by a student that the student rapidly acquires knowledge about the process. He is motivated by the ease and rapidity to try new ideas of all types. We have found that great enthusiasm for the problem is generated by this encounter with the visual display, and many of the students have indicated genuine originality.

ACKNOWLEDGMENT

NOMENCLATURE

C_p = heat capacity
F_T = total fresh feed, lb-moles/hr
ΔH = heat of reaction, see text
k_p = velocity constant based on partial pressure, see text
K_p = equilibrium constant in pressure units, see text
n = number of carbon atoms
P = pressure, atm
r = reaction rate, $\dfrac{\text{lb-moles converted}}{\text{lb cat-hr}}$
W = weight of catalyst, conversion
x = conversion, $\dfrac{\text{moles converted}}{\text{mole total fresh feed}}$
Y = mole fraction

Subscripts:

A = aromatic
H_2 = hydrogen
i = any component in reaction mixture
N = naphtha
P = paraffin
T = total

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