CHEMICAL REACTOR DESIGN
FOR PROCESS PLANTS

Volume Two:
Case Studies and Design Data

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CASE STUDY 108

Catalytic Reforming

THIS CASE STUDY illustrates the effective use of pseudocomponents to simplify a complex reaction system with a feed containing numerous chemical entities. Again adiabatic-staged reactors are specified the first two of which involve net endothermic reactions and the last, a net exothermic effect. Reheating between stages is necessary. More detailed models than that used here have been described that include other important reactions such as deactivation by coking (e.g., Ref 4). The data for excellent studies of this type remain proprietary.

Problem Statement

Design a catalytic reforming unit for producing 20,000 BPSD of C_5+ reformate having a research octane number of 95.

Typical Hydrodesulfurized Feedstock Analysis

Gravity: 51.9 API

ASTM Distillation:

IBP	240°F	60%	302°F
10%	262	70	311
20	272	80	322
30	279	90	335
40	284	95	346
50	292	EP	369

Compound Type:

	Mole %
paraffins	39.4
naphthenes	40.7
aromatics	19.9
	100.0

molecular weight: 123; characterization factor: 11.7

VABP: 293°F

MABP: 285°F

Received at battery limits at 40 psig and 200°F.

Catalyst

The catalyst is a 0.6% Pt-on-alumina ($\frac{1}{16}$ in. × $\frac{3}{16}$ in. extrudate) with $\rho_b = 0.78$ g/cm^3, $\rho_p = 1.2$ g/cm^3, $a_m = 471$ m^2/g, and pore volume = 0.42 cm^3/g. Costs in 1968 were \$13.80/lb with an approximate royalty of \$35/bbl of capacity, and a recovery cost of \$3.25/lb for new support. In addition to the poisons shown in Table 2.13, coking deactivates the catalyst but can be removed by regenerating with air. The catalyst has a dual-function with an acidic function for carbonium-ion reactions and a metallic function for hydro-dehydrogenation reactions. The acidic characteristics are thought to occur by partial replacement of OH on the alumina and the corresponding enhancement of activity of the residual hydrogen atoms upon treatment with halogens or halogen compounds (1).

Chemistry

Dual-function catalysts, both Pt-on-alumina and Pt-on-silica-alumina, have been studied extensively using various pure compounds as typical examples of constituents in refinery naphtha streams (1). An overall reaction scheme is given in Fig. CS-8.1 for C$_6$ hydrocarbons, showing the acidic functions horizontally and the hydro-dehydrogenation function vertically. In addition to these reactions, hydrocracking (e.g., C$_7$H$_{16}$ + H$_2$ → C$_4$H$_{10}$ + C$_3$H$_8$) and coking are also important. Isomerization of straight-chain to branched paraffins, aromitization, and hydrocracking each enhance the octane number of the product, but aromitization plays the major role because of the high octane numbers for aromatics (in the range of 120–140). Some hydrocracking is often essential, however, to meet high octane requirements.
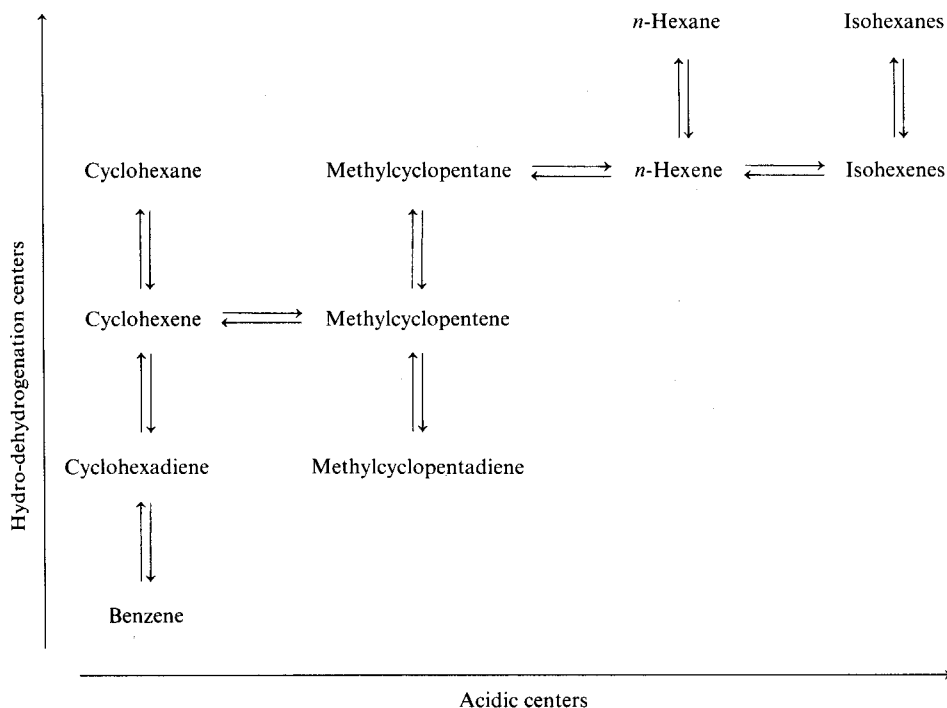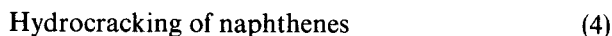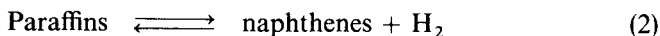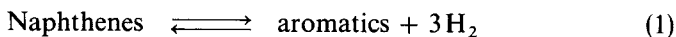
Fig. CS-8.1   Reaction paths for reforming C_6 hydrocarbons on dual-function catalysts. Reproduced by permission: J. H. Sinfelt, *Adv. Chem. Eng.,* **5**, 38 (1964). [Copyright by Academic Press.]

It breaks up large low-octane fragments into higher-octane molecules of smaller size. More importantly, it increases octane number by increasing the concentration of aromatics simply by reducing the specific volume of the nonaromatic fraction remaining in the liquid after flashing and distilling the reactor product. Octane number has been correlated with volume percent aromatics (VPAR) on the C_5 + reformate and is 58% for the 95-octane goal of this study (2). The effect of paraffin octane numbers (in the range of 40–60) is not significant.

Coking deactivates the catalyst, but it can be minimized by rapid hydrogenation of unsaturated coke precursors. Thus coking is prevented to a large extent by using high hydrogen partial pressures—high H_2/oil ratios and/or high pressures. Continuous catalyst use before regeneration of up to 26 mo has been reported (3). Newer forms of this catalyst will exceed this performance even with lower hydrogen partial pressures. Coking characteristics are always difficult to quantify, and the designer must often depend on

pilot-plant and plant operating data. Assume such data indicate that in the range of 425–575 psig that 1 yr of operating without regenerating is possible with a pure hydrogen-to-oil ratio of 5.9, which is a typical reported value (2). The catalyst activity at the end of the run will be 20% of the virgin activity; and to compensate for declining activity, operating temperature is raised gradually to a maximum allowable based on end-of-run conditions. Although aromatics yield will be improved at inlet pressures below 475 psig, coking will increase; but the data presented here do not define the lower pressure region. As coking rate increases it ultimately will become necessary to regenerate more frequently and require an extra or swing reactor. This mode of operation will be avoided by restricting the minimum pressure to 475 psia.
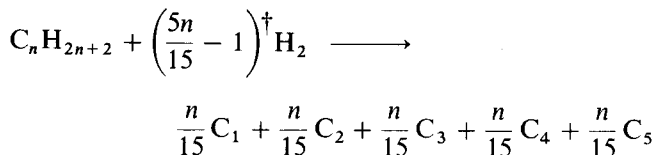
The complex feed mixture and product stream can be greatly simplified by considering four model reactions that are crucial in determining yield* and octane number (2).
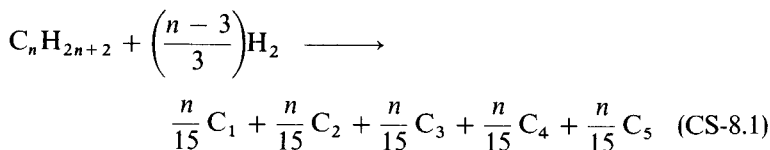
$$\text{Naphthenes} \quad \rightleftharpoons \quad \text{aromatics} + 3\,H_2 \qquad\qquad (1)$$

$$\text{Paraffins} \quad \rightleftharpoons \quad \text{naphthenes} + H_2 \qquad\qquad (2)$$

$$\text{Hydrocracking of paraffins} \qquad\qquad (3)$$

$$\text{Hydrocracking of naphthenes} \qquad\qquad (4)$$

The C_1 through C_5 fractions produced by hydrocracking were observed experimentally to occur in approximately equal molar portions (2). Thus for paraffin cracking the stoichiometric equation would be, for $C_{15}H_{32}$ as an example

$$C_{15}H_{32} + 4\,H_2 \quad \longrightarrow \quad C_1 + C_2 + C_3 + C_4 + C_5$$

or for the general case

$$C_n H_{2n+2} + \left(\frac{5n}{15} - 1\right)^{\dagger} H_2 \quad \longrightarrow$$

$$\frac{n}{15}\,C_1 + \frac{n}{15}\,C_2 + \frac{n}{15}\,C_3 + \frac{n}{15}\,C_4 + \frac{n}{15}\,C_5$$

or

$$C_n H_{2n+2} + \left(\frac{n-3}{3}\right) H_2 \quad \longrightarrow$$

$$\frac{n}{15}\,C_1 + \frac{n}{15}\,C_2 + \frac{n}{15}\,C_3 + \frac{n}{15}\,C_4 + \frac{n}{15}\,C_5 \quad \text{(CS-8.1)}$$
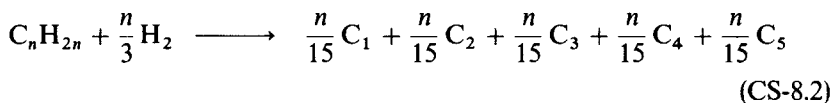
* Yield fraction for a product such as gasoline that is sold by volume is the volume of debutanized reformate produced per volume of liquid feed.

† Number of fragments minus one.

In like manner for naphthene cracking

$$C_nH_{2n} + \frac{n}{3}H_2 \longrightarrow \frac{n}{15}C_1 + \frac{n}{15}C_2 + \frac{n}{15}C_3 + \frac{n}{15}C_4 + \frac{n}{15}C_5$$

(CS-8.2)

Each of three hydrocarbon classes—paraffins, naphthenes, and aromatics—can be represented as a single compound having the average properties of that class (2). This reaction system is peculiarly amenable to this type of analysis because the major products have the same number of carbon atoms as the original feed constituents (e.g., heptane $\rightarrow$ methylcyclohexane $\rightleftarrows$ toluene). The nature of close boiling naphtha feed also suggests that each of the hydrocarbon classes in the original feed have the same number of carbon atoms. Hence (2)

$$M_F = n_P M_P + n_N M_N + n_A M_A$$

where n_P, n_N, and n_A designate moles of paraffin (C_nH_{2n+2}), naphthene (C_nH_{2n}), and aromatic (C_nH_{2n-6}) per mole of feed, respectively, n is the number of carbon atoms, and M_F is the molecular weight of the feed.

$$M_F = n_P(12n + 2n + 2) + n_N(12n + 2n) + n_A(12n + 2n - 6)$$

or

$$14n(n_P + n_N + n_A) = M_F - 2n_P + 6n_A$$

or

$$n = \tfrac{1}{14}(M_F - 2n_P + 6n_A)$$

(CS-8.3)

since $n_P + n_N + n_A = 1$ mole of feed. The average value of n characteristic of a given naptha feed can be determined from Eq. CS-8.3 and was calculated to be 8.82 for the feed in question.

Thermodynamics

The most important reactions are the hydrogenations of cycloparaffins to aromatics. These are rapid reactions that approach equilibrium in a short time. One can often assess complex systems such as this in a qualitative manner by considering a typical pure component such as cyclohexane ($C_6H_{12} \rightleftarrows C_6H_6 + 3H_2$). Calculations for cyclohexane at 500 psia pressure range and H_2-to-oil feed ratio of 5.9 indicate high equilibrium conversions in the range of 900°F.

Extensive experimental reforming runs using naphthas of the type being considered have yielded the following equilibrium constants for naphthenes being converted to aromatics and to paraffins (2):

$$K_{p_1} = \frac{P_A P_H^{3}}{P_N} = \exp\left(46.15 - \frac{46045}{T}\right), \qquad \text{atm}^3 \qquad \text{(CS-8.4)}$$

where $T = {}^\circ R$, P_A, P_N, and P_H are the partial pressures in atm of aromatics, naphthenes, and hydrogen, respectively.

$$K_{p_2} = \frac{P_P}{P_N P_{H_2}} = \exp\left(\frac{8000}{T} - 7.12\right), \qquad \text{atm}^{-1} \qquad \text{(CS-8.5)}$$

where P_P is the partial pressure of paraffins.

When based on moles of H_2 consumed or liberated in a particular reforming reaction, the heat of reaction is essentially independent of molecular weight in the range normally encountered in reforming (2). The values are listed with the corresponding rate equations. The adiabatic factors and heat generation potentials shown in Table 6.4 for the dehydrogenation steps are moderately negative and confirm the need for staged reactors with reheating.

Kinetics

The model reactions 1–4 were used as a basis for empirical rate equations, the constants for which were evaluated from laboratory and plant data (2).

Naphthenes to Aromatic

$$(-\hat{r}_1) = \hat{k}_{p_1}\left(P_N - \frac{P_A P_{H_2}^{3}}{K_{p_1}}\right), \qquad \frac{\text{moles naphthene converted to aromatics}}{\text{(hr)(lb cat.)}}$$

(CS-8.6)

$$\hat{k}_{p_1} = \exp\left(23.21 - \frac{34{,}750}{T}\right), \qquad \frac{\text{moles}}{\text{(hr)(lb cat.)(atm)}} \quad \text{(CS-8.6A)}$$

$$\Delta H_1 = 30{,}500 \text{ BTU/mole of } H_2 \text{ liberated}$$

Naphthenes to Paraffins

$$(-\hat{r}_2) = \hat{k}_{p_2}\left(P_N P_{H_2} - \frac{P_P}{K_{p_2}}\right), \qquad \frac{\text{moles naphthenes converted to paraffins}}{\text{(hr)(lb cat.)}}$$

(CS-8.7)

$$\hat{k}_{p_2} = \exp\left(35.98 - \frac{59{,}600}{T}\right), \qquad \frac{\text{moles}}{\text{(hr)(lb cat.)(atm)}^2} \text{(CS-8.7A)}$$

$$\Delta H_2 = -19{,}000 \text{ BTU/mole of } H_2 \text{ consumed}$$

(Under properly chosen conditions the reverse reaction, paraffins to naphthenes, will become more important.)

Hydrocracking of Paraffins

$$(-\hat{r}_3) = \hat{k}_{p_3} \frac{P_P}{P}, \quad \frac{\text{moles paraffins converted by hydrocracking}}{(\text{hr})(\text{lb cat.})} \quad \text{(CS-8.8)}$$

where P is the total system pressure.

$$\hat{k}_{p_3} = \exp\left(42.97 - \frac{62,300}{T}\right), \quad \frac{\text{moles}}{(\text{hr})(\text{lb cat.})} \quad \text{(CS-8.8A)}$$

$$\Delta H_3 = -24,300 \text{ BTU/mole of } H_2 \text{ consumed}$$

Hydrocracking of Naphthenes

$$(-\hat{r}_4) = k_{p_4} \frac{P_N}{P}, \quad \frac{\text{moles naphthenes converted by hydrocracking}}{(\text{hr})(\text{lb cat.})}$$

$$\text{(CS-8.9)}$$

$$\hat{k}_{p_4} = \exp\left(42.97 - \frac{62,300}{T}\right), \quad \frac{\text{moles}}{(\text{hr})(\text{lb cat.})} \quad \text{(CS-8.9A)}$$

$$\Delta H_4 = -22,300 \text{ BTU/mole of } H_2 \text{ consumed}$$

Operating Conditions and Reactor Type

Pressure

We must confine our range of interest to the values (475–575 psig) already presented as acceptable for activity maintenance. The optimum pressure within this range will be determined by a study of catalyst cost, compressor cost, and vessel cost. The reaction is a net producer of hydrogen, and plant hydrogen pressure is not a major factor.

Temperature

Based on pure component data, it is apparent that the operating temperature must be 900°F or above in order to assure negligible reverse reaction and maximize aromatics production. More precise temperatures will be selected on studying the rate characteristics. There will be merit in limiting the maximum reactor temperature to 1000°F in order to safely select a low alloy, 1.25 Cr − 0.5 Mo, steel. This means that the end-of-run temperature should not exceed this temperature. Maximum virgin catalyst temperature is most logically based on the hydrocracking reaction since it is the major cause of

catalyst deactivation. Using an activity at the end-of-run of 20% of the virgin activity, the initial maximum temperature will be from Eq. CS-8.8A.

$$(\hat{k}_{p_3})_0 = 0.2\hat{k}_{p_3}$$

or

$$\exp\left(42.97 - \frac{62,300}{T_0}\right) = 0.2 \exp\left(42.97 - \frac{62,300}{1460}\right)$$

Solving for T_0:

$$T_0 = 947 \text{ or } \approx 950°F$$

Thus it appears that we only need explore the range 900–950°F.

Conversion and Yield

Fractional yield for a product sold by volume is most usefully expressed simply as the volume of debutanized reformate per volume of liquid feed. This type of yield does nothing to describe the quality of the product. Quality is specified by a separate statement on the octane number or the % aromatics in the product (58% in this case).

Knowledge of the yield is not essential initially since we can begin with calculations based on W/F only for an adiabatic reactor. Yield data, however, are usually known prior to the design stage from pilot plant studies. For this system a yield of approximately 88% is a reasonable goal, and it is convenient for computer calculations to use preliminary values of component feed rates based on this value which can be adjusted iteratively to give the desired production rate of reformate.

Recycle Ratio

Reactor product gas will be cooled and flashed to separate the hydrogen-rich gases for recycle. For initial calculations one can assume pure hydrogen as recycle, and the composition of the recycle can then be established by successive flash and reactor calculations. For illustrative purposes we will assume a typical recycle composition that has been reported (2) (Mole %: $H_2 = 85.3$, $CH_4 = 8.0$, $C_2H_6 = 5.0$, and $C_3H_8 = 1.7$).

Total recycle ratio: (5.9)/(0.853) = 6.9. The preliminary feed material balance is based on 88% yield (see Table CS-8.1).

Reactor Type

Based on the rough adiabatic factor ($-286°F$) for the aromatization reaction it appears that a temperature change of this magnitude would require a

Table CS-8.1   Computer Results for Alternate 1

W/F	Temp., F	Component Flow Rates, Lb Moles/Hr										
		Paraffins	Naphthenes	Aromatics	Hydrogen	Methane	Ethane	Propane	Butane	Pentane	VPAR	Yield
Reactor 1 (P = 475 psia, MW = 20.16)												
0	950	816.56	843.50	412.43	12198.07	1144.02	715.01	243.10	0	0	.—	—
6.03	834.2	843.72	376.77	830.16	13359.91	1156.86	727.85	255.94	12.84	12.84	36.67	96.38
Reactor 2												
0	950	(Outlet from reactor 1, press. 450 psia)										
6.03	886.6	822.10	105.07	1077.38	13987.75	1183.94	754.94	283.03	39.93	39.93	49.15	93.39
Reactor 3												
0	950	(Outlet from reactor 2, press. 425 psia)										
9.90	932.6	607.50	35.58	1205.81	14130.26	1275.42	846.53	374.51	131.41	131.41	58.08	88.51

Basis: 20,000 BPSD C_5t reformate.

series of adiabatic fixed-bed reactors with intermediate reheating. Reaction 1 is not excessively temperature sensitive, for a 100°F change in temperature produces only a 7.5-fold change in the velocity constant, and temperature drops of 50–100° might be permissable before reheating is necessary.

Design Model

The following equations apply.

Material Balance

$$(-\hat{r}_1)\left(\frac{\Delta W}{F_T}\right) = \Delta X_1 \tag{CS-8.10}$$

and similar equations for reactions 2, 3, and 4. X_1 is the conversion in reaction 1, moles naphthenes converted per mole of total feed.

Heat Balance

$$\Delta W\left[(-\hat{r}_1)(-\Delta H_1)(3) + (-\hat{r}_2)(-\Delta H_2) + (-\hat{r}_3)(-\Delta H_3)\left(\frac{n-3}{3}\right) \right.$$
$$\left. + (-\hat{r}_4)(-\Delta H_4)\left(\frac{n}{3}\right) \right] = \sum \mathscr{F}_j c_{p_j} \Delta T \tag{CS-8.11}$$

Heat capacities from the *API Data Book* based on nearest true compounds to value of n were used.

Products

C_5 and lighter hydrocarbons are obtained from the calculated conversions X_3 and X_4 and the stoichiometry expressed by Eqs. CS-8.1 and CS-8.2.

Volume % Aromatics

$$\text{VPAR} = \frac{M_A \mathscr{F}_A/\rho_A}{(M_A \mathscr{F}_A/\rho_A) + (M_P \mathscr{F}_P/\rho_P) + (M_N \mathscr{F}_N/\rho_N) + (M_{C_5} \mathscr{F}_{C_5}/\rho_{C_5})}$$

Volume % Yield

This is simply 100 times the volumetric flow of C_5 + reformate divided by the volumetric liquid feed rate all measured at 60°F.

It was assumed that differences between catalyst surface and bulk fluid conditions were negligible. The reactor configuration will be selected to validate this assumption.

The algorithm was similar to that used for Case 102A.

Design Procedure

Preliminary Studies

The exact number of reactors and the operating scheme must be determined by calculating various cases. The several simultaneous and consecutive reactions make qualitative reasoning rather fruitless. In this preliminary stage of process design, however, it is most valuable to obtain an intuition about the variables and their effects on reactor design just as rapidly as is possible for less complex systems. For only by this means of rapidly testing tentative ideas does one obtain useful new approaches. A visual interactive display associated with a digital computer makes such interplay possible. One can, for example, follow with position in the reactor (W/F_T), volume % aromatics and rates of reactions 1 and 3 (aromatics production and hydrocracking of paraffins), which are crucial in setting VPAR and thus octane number.

Hence these two rates together with a plot of the cumulative volume % aromatics, all as a function of W/F were chosen for display. At the end of each trial design the yield was also displayed. A series of preliminary studies by this method using an inlet pressure of 475 psig are shown in sequence in Figs. CS-8.2–CS-8.4, which are line drawings made directly from photographs of the display oscilloscope. If oscilloscope capacity permits, plots of temperature versus W/F_T for each reactor are also useful.

Typical Trial Runs on the Display

Trial 1. Use 900°F inlet and 475 psia pressure and observe behavior in a single reactor. This temperature is too low, the rate of aromatics formation ($\hat{r}_1$) declines too rapidly.

Trial 2. Use 950°F inlet and 475 psia (Fig. CS-8.2). This is a good starting temperature, but it appears that the aromatics production rate declines to a low value such that the first reactor ought to be terminated at $W/F_T \approx 7$. Note also that hydrocracking is negligible.

Trial 3. Use two reactors of same size $W/F_T = 7$ (Fig. CS-8.3; curves 1 and 2). Reheat between reactor 1 and 2 and allow 25 psi for total reheat furnace and reactor pressure drop. Inlet for reactor 1 is 475 psia and 950°F and for reactor 2, 450 psia and 950°F. The volume % aromatics of 49.4 is inadequate, and it is clear that reheating and another reactor are needed.

Trial 4. Add a third reactor of undesignated W/F_T with reheat to 950°F and inlet pressure of 425 psi. (Fig. CS-8.3; curves 1, 2, and 3).
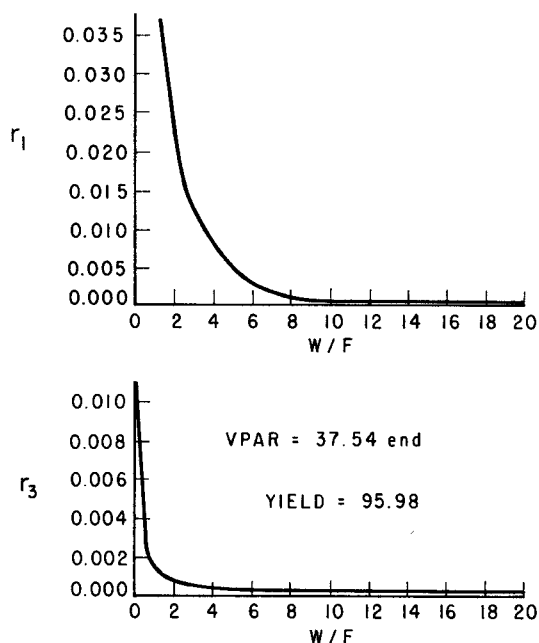
Fig. CS-8.2 Trial 2.

The target percentage aromatics is reached in reactor 3 at $W/F_T \approx 10$. By examining the progress of the rate curves it is apparent that hydrocracking ($\hat{r}_3$), which occurs primarily in reactor 3, is essential for reaching the desired aromatics content, since the aromatics rate is too low in the third reactor to accomplish this goal by additional conversion to aromatics. It must be done instead by reducing the nonaromatics content of the product through hydrocracking. Trial 4 can be further improved in catalyst utilization by reducing the size of reactors 1 and 2 by a W/F_T of 1, for the last increment of W/F_T is not of much value at the low rate indicated for $\hat{r}_1$ (the volume % aromatics changes imperceptibly in this region in reactor 2).

Trial 5.   (Fig. CS-8.4)

	1	2	3
Inlet temp. °F	950	950	950
Inlet pressure, psia	475	450	425
W/F_T	6	6	10

This seems to be a good basis for beginning detailed design studies. The nature of the display is such that these initial studies are approximate only,
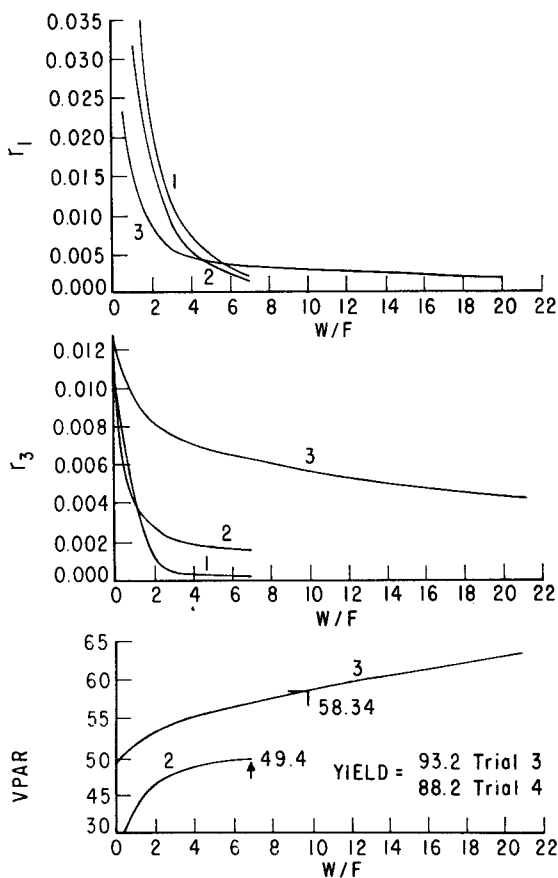
Fig. CS-8.3   Trials 3 and 4.

but at this point the designer has a good feel for the behavior of the variables
and has essentially completed the most creative part of the effort, that of
selecting the reactor style and arrangement. Further work will involve detailed
calculations of various cases including costs of associated equipment in
order to obtain the most economical design.

Final Design for First Alternate

The result of computer calculations for the first detailed alternate decided by
the preliminary work on the iterative display (Trial 5) are shown in Table
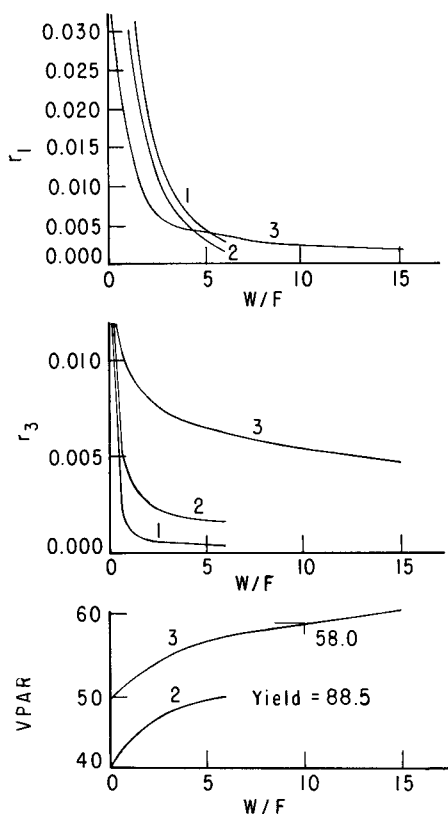CS-8.1. The marked decline in aromitization as the naphthene concentration

Fig. CS-8.4   Trial 5.

diminishes is evident in the third reactor, as is the corresponding increase in hydrocracking evidenced by the decline in paraffins.

   Pressure drop through the reactor beds was considered negligible, but this must be checked on deciding the reactor configuration. The pressure drop between reactors is that required for the furnace coil. This together with total pressure is subject to further study involving furnace, recycle-compressor and catalyst costs. In making such a study various cases can be calculated and the optimum sought.* Engineering judgment must be applied with a strong hand, for the problem as stated lacks good quantitative data on activity

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* Furnace coils of the type required in this unit can be designed for as low as 5 psi drop. This lower ΔP will reduce compressor costs and must be studied in comparison with increased furnace costs caused by the special coil design.

maintenance. Lower pressures improve the aromatics production rate but adversely affect activity. Because of the lack of precise expressions for activity, an elaborate optimization study is not indicated and, in fact, could lead to erroneous conclusions if the designer lost sight of the limited nature of the data. In fact a conservative decision in this particular situation might be to design the reactor and associated equipment for operating at the higher pressure range (575 psig), but purchase initially an amount of the expensive catalyst based on calculations for the lower pressure range (425 psig). The reactor design temperature shall, of course, be based on the end-of-run temperature (1000°F).

Reactor Configuration

Select a G such that ΔT between catalyst surface and bulk fluid is minimized, and at the same time ΔP for the bed is not excessive. It is clear based on preliminary calculations that the L/D will be low and great care in designing distributors and outlet collectors will be necessary.

Reactor 1

$$Z = \left(\frac{W}{F_T} G\right) \frac{1}{\rho_b M_F} = \frac{6.03\,G}{(48.7)(159)} = 7.79 \times 10^{-4} G, \qquad \text{ft}$$

$$D = \sqrt{\left(\frac{\text{total mass flow}}{G}\right) \frac{4}{\pi}} = \sqrt{\frac{329,335}{G} \frac{(4)}{\pi}} = 647.6(G)^{-0.5}, \qquad \text{ft}$$

Thus for $G = 3000\,\text{lb/hr ft}^2$, $Z = 2.34\,\text{ft}$ and $D = 11.8\,\text{ft}$. Using the procedures shown in Case Study 105 the corresponding $\Delta P = 2.44$ psi and the ΔT between catalyst and bulk fluid is 14°F (8°C) at the inlet, which is high. By increasing G to 6000 this is reduced to approximately 8°F (4.4°C), which is within accuracy of rate data. The corresponding dimensions will then be 8.36 ft in diameter and 4.67 ft of bed with a ΔP of 18.1 psi. This ΔP is less than 10% of the operating pressure and the larger bed height will reduce the problem of flow distribution. Final selection of bed dimensions for each reactor must be based on a more thorough study of costs including compression costs as in Case Study 105. Vessel costs may be lowered by specifying a refractory lining so that the design metal wall temperature may be lowered.

Adding additional catalyst to extend run length must be approached with caution in this complex reaction system. In addition to the disadvantage of higher catalyst cost with this expensive catalyst, more catalyst in the first bed will increase aromatics content of the effluent, which is desirable; but the paraffin content will increase further, which is undesirable.

Parametric Sensitivity

Several parameters were varied to ascertain the effect of possible errors on the final values of product quality. Selecting 943°F as a base temperature, activation energies were varied $\pm 10\%$ and the preexponential factor altered so that values of rate constants would remain the·same at 943°F. These changes produced variations of only 1 % in volume % aromatics and yield. This simply illustrates that if the rate constant is "correct" at a temperature close to the average temperature where most of the conversion occurs (entrance of reactors), small errors in the activation energy do not effect the result for this system.

The model was found to be highly sensitive to the hydrogen content of the reaction mixture which in turn depends on the accuracy of the flash equilibrium at the separator where recycle gas is removed. A variation of hydrogen content of the recycle gas from 75.8 to 100 mole % produced a variation in volume % aromatics from 65.1 to 57.7%. For illustrative purposes this program used an arbitrary split at the separator. Ideally a flash calculation with precise equilibrium data together with a recycle material-balance routine should be included. The sensitivity of the model and the process to hydrogen pressure is caused by its strong effect on the aromatics reaction. Not included in the model, but also important, is the effect of hydrogen in reducing coking.

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