

ER 1404

KINETIC AND MATHEMATICAL MODELS

FOR A CATALYTIC REFORMER

By

Rodrigo Varela Villegas

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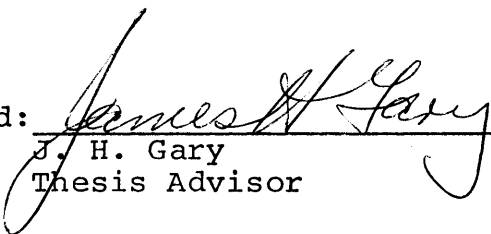
ER 1404

A Thesis submitted to the Faculty and the Board of Trustees of Colorado School of Mines in partial fulfillment of the requirements for the degree of Master of Engineering in Chemical and Petroleum Refining Engineering.

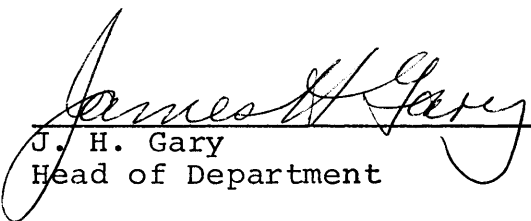
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ABSTRACT

Using Smith's kinetic information, a kinetic model able to predict the products and their properties when a feedstock is catalytically reformed at specified operating conditions was developed.

By computer simulation, with different feedstocks and at different operating conditions, relationships of research octane number versus volume percent of reformate as a function of characterization factor, have been established.

With the results of computer-simulation, a linear-regression-computer program was used to find a linear model for the catalytic reformer.

The models developed in this report can be used by everybody to study the effect that the operating condition and the properties of the feedstock have on the yields and on their properties.

All the computer programs presented in the Appendixes were written in Fortran IV, and run in the PDP-10 of Colorado School of Mines, under the Monitor 503-B.

To my wife, Constanza, and to my mother, Lola,
who with their help and encouragement, have made this
possible.

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INTRODUCTION

Catalytic reforming is today's most important refinery process for octane improvement. It has also become a basic process for production of aromatics and liquefied petroleum gases (LPG).

By the end of 1971, catalytic reformers will be capable of processing about 3 million barrels per day (bpd), which is equivalent to about 22% of the total crude oil capacity in U.S. refineries.

Refiners will continue to convert greater portions of crude oil into fuel oil and motor fuels. Cracking processes make the conversion, but they need cat-reforming to meet the antiknock quality of finished motor fuel blends. Furthermore, the drive to reduce or omit lead antiknock additives puts extra emphasis on cat-reforming. Also the growing need for aromatics in petrochemical production demand more catalytic reforming capacity.

During the last four years, many changes in cat-reforming have occurred: process improvement and optimization, after-treatments of reformate, extension of the process to new applications, and new or improved reforming catalysts.

Despite its importance there is not a published model capable of predicting the average products and their

average properties for specified operating conditions. So the basic goal of this work is to try to develop a model able to predict products, properties, and effect of operating conditions which can be used for preliminary evaluation of feedstocks and in preliminary design of cat-reformers.

Also, if similar models are developed for the different units, it can be used to optimize the whole refinery.

The results of these models will not match completely with all the commercial results, but they will give average values.

BACKGROUND

Catalytic reforming is a regenerative-heterogeneous catalytic process, involving the use of dual-functional catalysts to produce high-octane gasoline and pure hydrocarbons from virgin and cracked naphthas.

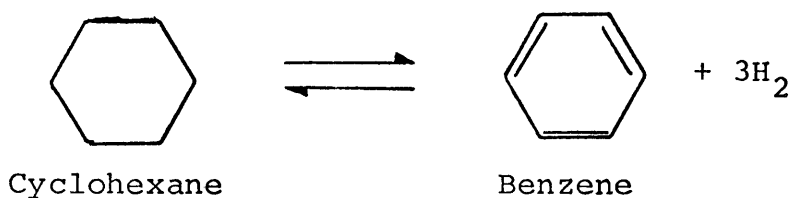
It is a rather complex process, not only because the feed-stocks contain a mixture of different hydrocarbon types - paraffins aromatics, naphthenes -, but also because of the number of reactions occurring.

Kinetics

The reactions can be classified as either octane improving reactions or supporting reactions.

Octane improving reactions,

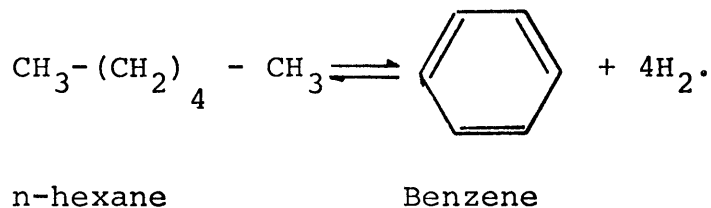
1 - Dehydrogenation of naphthenes to aromatics,



The dehydrogenation of six membered ring naphthenes - cyclohexane derivatives - to aromatics is the primary octane improving reaction in cat-reforming. Net octane gain, however, is not so great as in the dehydrocyclization

aromatics easily with high yields, five membered ring naphthenes are more difficult to convert and give lower aromatic yields due to side reactions producing paraffins.

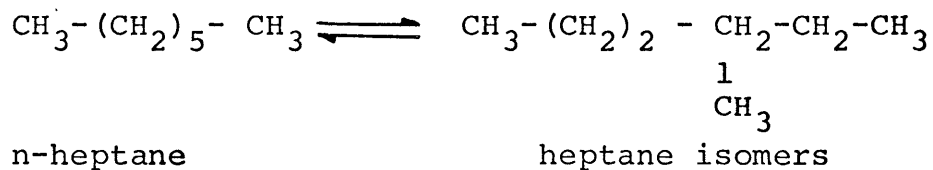
3 - Paraffin dehydrocyclization,



Aromatization of paraffins is achieved by the dehydrocyclization of straight-chain paraffins having at least six carbon molecules. This reaction converts some naphtha components with octanes as low as ten into aromatics with octanes up to 130. This reaction produces a substantial density increase with volumetric yields around 70%.

Supporting reactions,

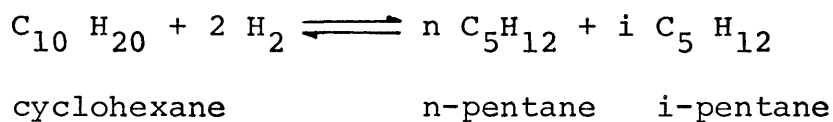
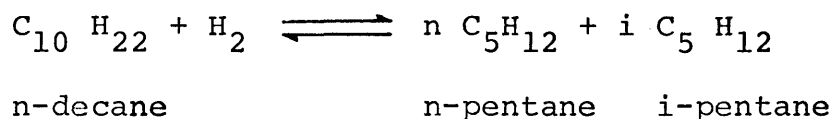
4 - Paraffin Isomerization,



Paraffin isomerization for increasing octane is of little value as the sole catalytic reforming process, but it is

important as a supporting reaction along with naphthene and paraffin aromatization. Although generally the larger part of naphtha feedstock is paraffinic, only a small portion can be converted to aromatics - leaving an appreciable amount of naphtha within the 10-20 octane range. Upgrading 10-20 octane material by isomerization, even if only to 50-60 octane, allows far more of this material to remain in the final product and still meet 90-100 octane specifications.

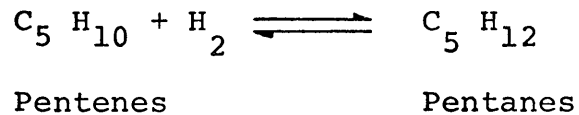
5 - Paraffin and naphthene hydrocracking.



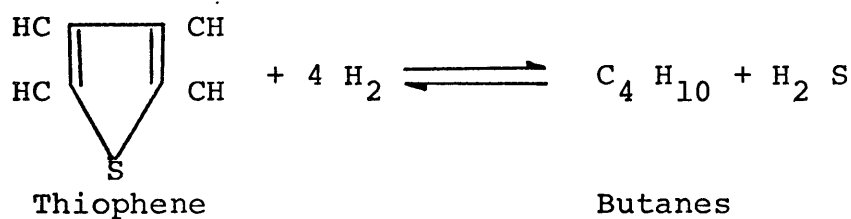
Hydrocracking as a supporting reaction can be useful when reforming feedstocks containing high boiling fractions. It breaks long chains or rings into shorter chains to reduce the overall reformat boiling point, increase product volatility, and off-set some of the density yield losses resulting from the aromatization of naphthenes and paraffins. Volumetric yields from hydrocracking are high, with very good octane gain. The 100% hydrocracking of decane into two

pentane molecules gives a volumetric yield of 118% and an octane gain of more than 100 units.

6 - Olefin hydrogenation.



7 - Hydrodesulfurization.



Olefin dehydrogenation and hydrodesulfurization do not have a large effect on the process because they generally occur in the hydro-treating unit, which is placed before the cat-reformer.

8 - Formation of Highly Aromatic Polymers.

These polymers must be removed from the reformat prior to gasoline blending.

9 - Carbon Laydown.

It occurs in any catalytic process and appreciably reduces the catalyst activity. Recirculation of hydrogen is used to decrease the carbon formation.

Table 1, taken from Marshall (Petrol Ref. 1955), presents a general resume of the principal reactions and their effects on the products.

Process

Description. After the feed leaves the hydrotreating unit, it is combined with the recycle hydrogen stream. The mixture is heated and passed through the three or four reactors containing catalysts, which are connected in series. Since the overall reforming process is endothermic, reheaters are used between reactors to bring the mixture back to reaction temperature. The effluent from the final reactor is cooled and separated into reformat and butane and lighter components. The gases split into hydrogen rich gas which is recirculated and C1 - C4 gases, which are separated to recover the butanes. (See Figure 1).

TABLE 1

SOME BASIC RELATIONSHIPS IN CATALYTIC REFORMING

	Reaction Rate	Reaction Heat Effect	Effect of High Pressure	Effect of High Temperature	Effect of High Space Velocity	Effect on Hydrogen Production	Effect on Reid Vapor Pressure	Effect on Density	Effect on Volumetric Yield	Effect on Octane
Hydro-cracking	Slowest	Exother	Aids	Aids	Hinders	Absorb	Increase	Decrease	Decrease	Increase
Isomerization	Rapid	Mildly Exotherm	None	Aids	Hinders	None	Increase	Slight Decrease	Slight Increase	Increase
Cyclization	Slow	Mildly Exotherm	Hinders	Aids	Hinders	Evolve	Decrease	Increase	Decrease	Increase
Naphthene Isomerization	Rapid	Mildly Exotherm	None	Aids	Hinders	None	Decrease	Slight Increase	Slight Decrease	Slight Decrease
Naphthene Dehydrogenation	Very Fast	Quite Endotherm	Hinders	Aids	Hinders	Evolve	Decrease	Increase	Decrease	Increase

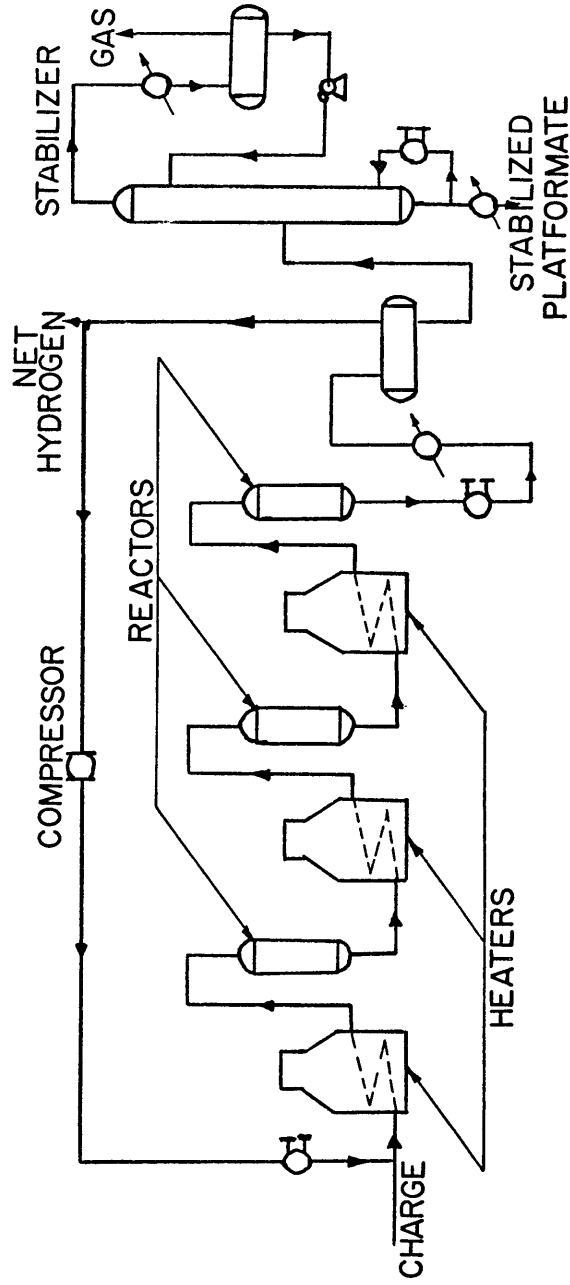


Figure 1
Catalytic Reformer Flow Diagram

Feedstocks. Typical feedstocks to catalytic reformers are virgin naphthas; however, the use of cracked naphthas is increasing because of the increase in demand for high-octane gasoline. Materials boiling below 200°F are not usually included in the reformer feed for gasoline because they already have a relatively high octane number, basically contain molecules with less than five atoms of carbon, which cannot be converted to aromatics, or in other words, they cannot be reformed. Materials boiling above 400°F are not included, because of greater coke deposition, which causes deactivation of the catalyst.

Catalyst. Catalytic reforming uses a dual-function catalyst, generally platinum supported on a silica-alumina base. In new catalyst, rhenium is combined, to form a more stable catalyst, which permits operation at lower pressure. Platinum is thought to serve as a catalytic site for hydrogenation and dehydrogenation reactions, and chlorinated alumina provides an acid site for isomerization, cyclization, and hydrocracking. Reforming catalyst activity is a function of its surface area, pore volume, and active platinum and chlorine content. Catalyst activity is reduced during operation by coke deposition and chlorine lost.

Operating Variables

Traditionally, the operating variables for the cat-reformer have been temperature, pressure, space velocity and hydrogen-to-hydrocarbon ratio. However, new designs such as the Magnaforming process show that the profile of the variables has a big influence on the products and their properties.

Temperature. The temperatures limited on the lower side by the equilibrium that exists among paraffins, naphthenes, and aromatics; that is to say, higher temperature will enhance the formation of aromatics; however, very high temperature will increase hydrocracking and decrease reformate yield. Generally the temperature has to be increased over the operating period to compensate for catalyst deactivation caused by carbon laydown.

Pressure. Increasing pressure causes higher rates of hydrocracking because it is not equilibrium controlled. Also it adjusts the equilibrium among paraffins, aromatics, and naphthenes, in the direction of the more saturated compounds. Higher pressures decrease carbon laydown and increase the residence time of reactants on the catalyst surface. Reducing pressure allows increases in dehydrocyclization of paraffins, dehydrogenation of naphthenes,

and less hydrocracking.

Space velocity. The time of contact among the reactants, intermediate products, and catalyst, has a marked effect on the product distribution. Faster reactions will tend to predominate in a shorter residence time. These are the dehydrogenation of naphthenes, isomerization of paraffins, and hydrocracking of the heavier paraffin reactants. Conversely, longer residence time tends to enhance the slow reactions such as: hydrocracking of lighter hydrocarbons and dehydrocyclization of paraffins. Short residence times are generally preferred for producing maximum amounts of aromatics and hydrogen, with the minimum paraffin destruction. An increase in space velocity (at constant severity) requires higher temperatures but increases catalyst life.

Hydrogen to hydrocarbon ratio. The effect of increasing hydrogen-to-hydrocarbon ratios is primarily that of preventing catalyst carbonization. However, it has been proposed recently that hydrogen not only affects the carbon laydown rate, but also reduces mass transfer resistance at the catalyst-hydrocarbon interface by reducing the partial pressure of hydrocarbon.

It is easy to see that there are compromises among all

the operating conditions to get better yields and longer catalyst life.

One of the latest developments in reforming of naphthas is the use of profiles for temperature, catalyst charge, and hydrogen-to-hydrocarbon ratio, through the reactors. This is the basis of the Magnaforming design licensed by Atlantic-Richfield Company, which gives better catalyst life and increases reformate yields for a given severity.

The Magnaforming design uses an increasing temperature profile, a decreasing space velocity profile, an increasing hydrogen-to-hydrocarbon ratio profile through the reactors, to decrease the side reactions, to get better reformate yield and better cycle length.

The effect of catalyst charge in the reactors will be analyzed later in this report.

The general optimum conditions in a catalytic reformer to get better yields and cycle life are shown in Table 2.

TABLE 2

Optimum Operating Conditions

	<u>Best Yields</u>	<u>Best Cycle Life</u>
Front reactor(s)		
Space Velocity	High	High
H ₂ /HC Mol Ratio	Low	-
Temperature	-	Low
Terminal reactor(s)		
Space Velocity	Low	Low
H ₂ /HC Mol Ratio	High	High
Temperature	High	-

KINETIC MODEL

Reaction models for the reforming process have been suggested by many authors. Some of them are: Smith's (1959), Krane's (1959), Burnett's (1965), Henningsen's (1970).

Logically a good engineering model will be the one which is easy to use, gives good results and requires only data at hand.

The Smith model requires a PONA analysis and has four simultaneous differential equations to solve. It has all the kinetic information required to consider temperature effects and is for naphtha feed stocks.

Burnett's model has the big disadvantage that it is for pure hydrocarbons, not for naphthas.

Krane's model requires a complete analysis of the feed stock, (C5-C10, for aromatics, paraffins, naphthenes, plus isomers) and is not an easy model to use (20 simultaneous differential equations). It, also does not contain the effect of temperature on the rate constants.

Henningsen's model takes into account the fact that the C5-C6 ring naphthenes react according to different patterns, but requires a good analysis of the feedstock (PONA, isomers, C5-C6 naphthene rings). It has good kinetic information and is able to consider activity of the catalyst.

As the kind of information about feedstocks available generally includes only PONA analysis, the model proposed by Smith was selected and was used in all the simulations.

SMITH'S MODEL

Basic assumptions.

a) The four major reactions occurring in reforming petroleum naphthas over platinum catalyst are:

1. Naphthenes \rightleftharpoons Aromatics
2. Paraffins \rightleftharpoons Naphthenes
3. Hydrocracking of naphthenes
4. Hydrocracking of paraffins

b) The complex naphtha mixture is idealized so that each of the three hydrocarbon classes - paraffins, naphthenes, aromatics - is represented by a single compound having the average properties of that class. This assumption supports the fact that isomerization is not considered.

c) Generally the naphtha will consist of hydrocarbons with different numbers of carbon atoms per molecule. However, since reformer feedstocks have a rather narrow molecular weight distribution, a reasonable simplification can be obtained by substituting for the naphtha in question a naphtha containing only hydrocarbons with an average number of carbon atoms in the molecules.

d) Although the reactions are heterogeneous, experimental results have shown that satisfactory results are obtained if the system is treated as though it were homogeneous.

e) Experimental data show that C1, C2, C3, C4, and C5 are produced in approximately equal molal proportions in the hydrocracking reactions.

Kinetic Data. The equilibrium and reaction rate constants were obtained from data derived from reforming runs over an extreme range of space velocity with platinum catalyst of virgin activity.

a) Conversion of naphthenes to aromatics.

$$-\frac{dN_n}{dV_r} = \frac{k_f P_n}{K_p} \left(K_p - \frac{P_a P_{H_2}^3}{P_n} \right)$$

$$K_p = \left(\frac{P_a P_{H_2}^3}{P_n} \right)_{eq} = \text{EXP} \left(46.15 - \frac{46045}{T} \right) (\text{atm}^3)$$

$$K_f = \text{EXP} \left(23.21 - \frac{34750}{T} \right) \frac{\text{moles}}{\text{hr (lb cat) atm}}$$

$$\frac{dT}{dV_r} = \frac{dN_n}{dV_r} \left(\frac{91500}{N_t C_p} \right)$$

b) Conversion of paraffins to naphthenes

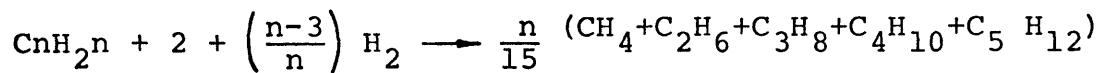
$$\frac{dN_n}{dV_r} = \frac{Kf_1}{K_{P_1}} P_n P_{H_2} \left(K_{P_1} - \frac{P_p}{P_n P_{H_2}} \right)$$

$$K_{P_1} = \left(\frac{P_p}{P_n P_{H_2}} \right)_{e_q} = \text{EXP} \left(\frac{8000}{T} - 7.12 \right) (\text{atm}^{-1})$$

$$K_{f_1} = \text{EXP} \left(35.98 - \frac{59600}{T} \right) \frac{\text{moles}}{\text{hr (lb cat) atm}}$$

$$\frac{dT}{dV_r} = \frac{dN_n}{dV_r} \left(\frac{-19000}{N_t C_p} \right)$$

c) Hydrocracking of paraffins

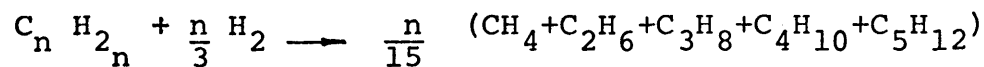


$$\frac{-dN_p}{dV_r} = \frac{K_c P_p}{\pi}$$

$$K_c = \text{EXP} \left(42.97 - \frac{62300}{T} \right) \frac{\text{moles}}{\text{hr (lb cat)}}$$

$$\frac{dT}{dV_r} = \frac{dN_p}{dV_r} \left(\frac{-24300}{N_t C_p} \right) \left(\frac{n-3}{3} \right)$$

d) Hydrocracking of naphthenes



$$\frac{-dN_n}{dV_r} = \frac{K_{c1}}{\pi} P_n$$

$$K_{c1} = \text{EXP} \left(42.97 - \frac{62300}{T} \right) \frac{\text{moles}}{\text{hr (lb cat)}}$$

$$\frac{dT}{dV_r} = \frac{dN_n}{dV_r} \left(\frac{-22300}{N_t C_p} \right) \frac{n}{3}$$

Information required. The following data are required:

- a) PONA analysis.
- b) Operating conditions for each reactor.
- c) Number of reactors.
- d) Molecular weight of the feedstock.

Properties Predictions.

Smith's model is not able to predict volumetric yields, Reid vapor pressure, and octane number in a direct way, and it is necessary to include some kind of correlation of these properties in the model. Because the model is based on an average number of carbon atoms, it requires correlations of average values of octane number, specific gravity, and Reid vapor pressure versus the number of carbon atoms, for the three kinds of hydrocarbons-paraffins, naphthenes aromatics. These relationships are presented in Table 3 and Figures 2, 3,4. They were calculated by using arithmetic averages of all the values found in "API, project #44".

To get mathematical expressions for these relationships, two curve-fitting programs were used. They appear in Appendixes 2 and 3, and were made using least-square theory.

The first-order program was used to fit two kinds of curves:

a) $Y = A + BX$

$$b) \quad Y = C \text{ EXP } (DX)$$

The second-order program was used to fit the parabolic curve:

$$Y = E + FX + GX^2$$

The general criteria used to select one fitting or another were the standard error of the estimate.

TABLE 3

AVERAGE PROPERTIES' VALUES

Number of Carbon Atoms	Paraffins			Naphthenes			Aromatics		
	Specific Gravity	Reid Vapor Pressure	Research Octane Number	Specific Gravity	Reid Vapor Pressure	Research Octane Number	Specific Gravity	Reid Vapor Pressure	Research Octane Number
5	0.6176	23.97	79.83	0.7505	9.914	101.3			
6	0.6623	7.016	73.6	0.7460	3.884	87.15	0.8845	3.224	
7	0.6903	2.591	68.8	0.7630	1.988	78.82	0.8719	1.032	120.1
8	0.7134	0.944	69.36	0.7768	0.780	69.15	0.8722	0.326	113.76
9	0.7334	0.392	93.70	0.7870	0.252	70.94	0.8752	0.118	95.61

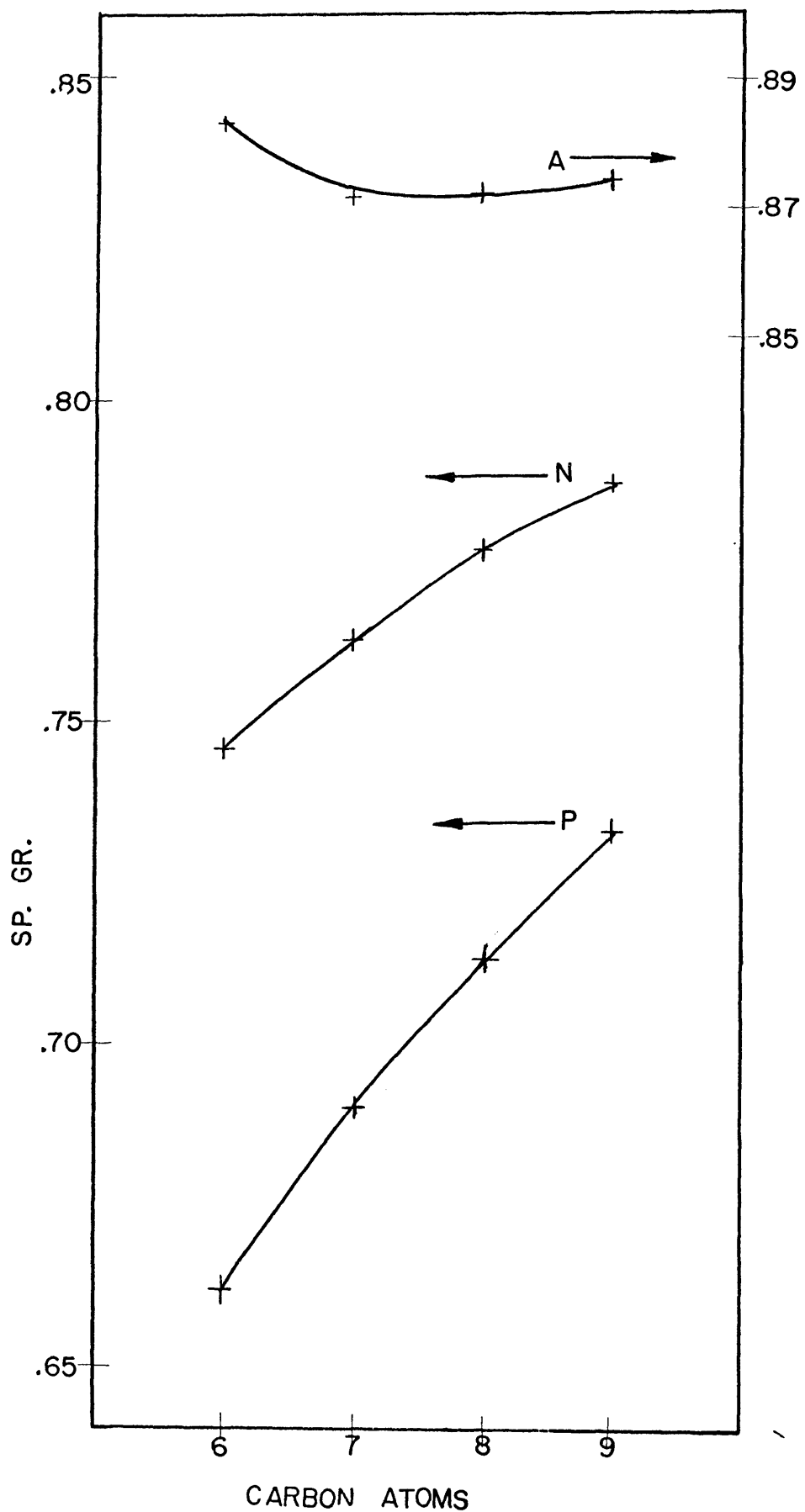


Figure 2

Specific Gravity Versus Number of Carbon Atoms for
Paraffins, Aromatics, and Naphthenes

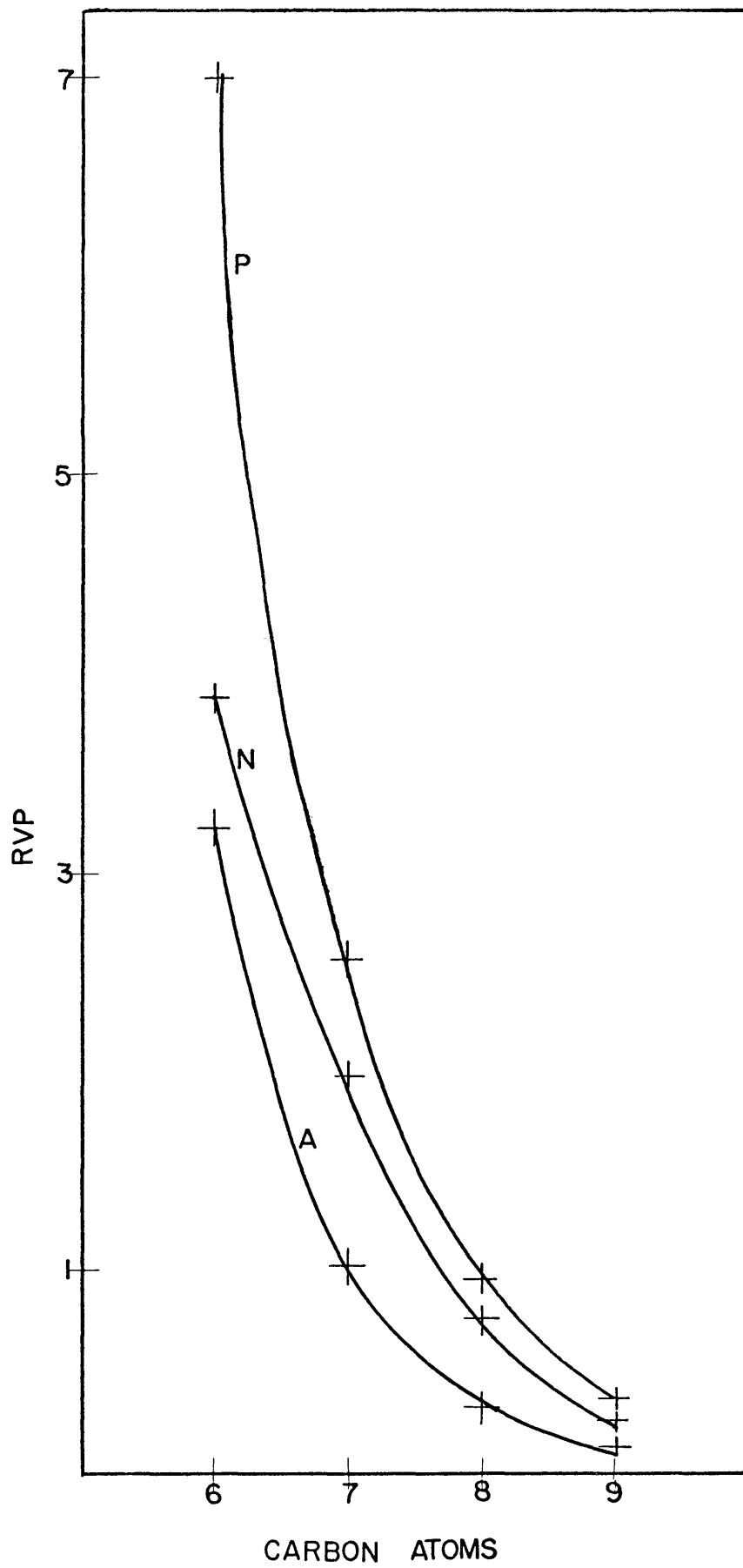
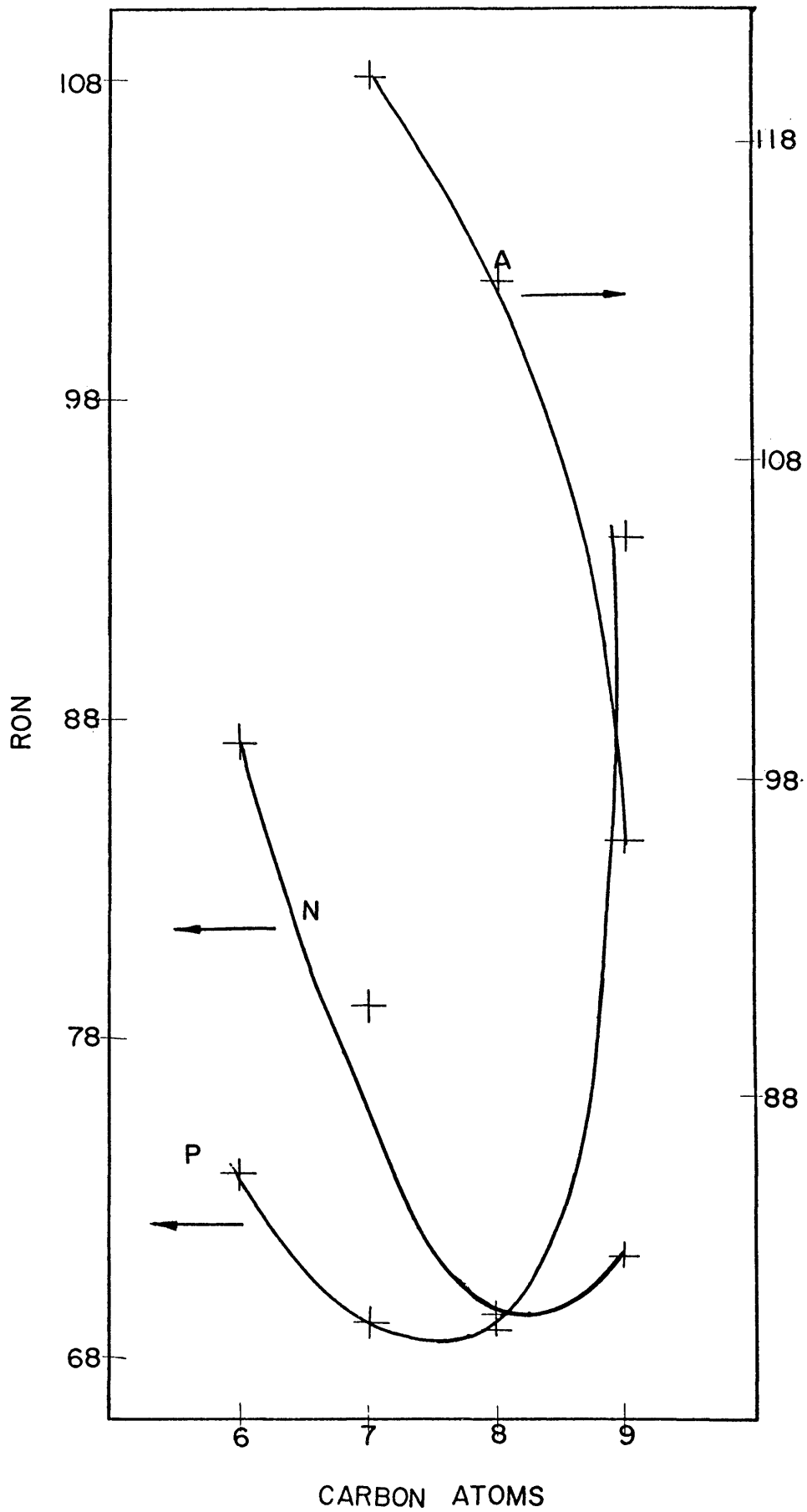


Figure 3

Reid Vapor Pressure Versus Number of Carbon Atoms for Paraffins, Aromatics, and Naphthenes



CARBON ATOMS

Figure 4

Research Octane Number Versus Number of Carbon Atoms
for Paraffins, Aromatics, and Naphthenes

The results of the fittings are shown in Table 4.

To predict the specific gravity of the reformat the equation that was used was

$$\text{Sp. gr.} = \frac{\sum_{i=1}^j m_i}{\sum_{i=1}^j \frac{m_i}{(\text{Sp.gr.})_i}}$$

To predict research octane number of the reformat the equation that was used was

$$\text{RON} = \sum_{i=1}^j (\text{RON})_i X_i$$

To predict Reid Vapor Pressure of the Reformat, the equation that was used was

$$\text{RVP} = \sum_{i=1}^j (\text{RVP})_i Y_i$$

The computer program (CATREF.F4) was developed by considering each reactor as composed of a number of nodes (this number is a data input for the program). A copy of the program and a print-out are presented in Appendix 1.

Comparison of Results. Unfortunately there is not a large amount of information in the literature about all the operating conditions and the yields in a cat-reformer. Generally it is only possible to find some yields and some operating conditions. This is the reason for only comparing the calculated results as these were the only ones reported which contained all the information needed. (See Table 5).

TABLE 4
Curve Fitting Coefficient to Predict Properties
As a Function of the Number of Carbon Atoms

Variable	Kind of Hydrocarbons	A	B	C	D	E	F	G
Specific Gravity	Paraffins	0.52255	0.02364					
	Naphthenes	0.66560	0.01368			1.11116	-0.0611	0.00389
	Aromatics							
Clear Research Octane Number	Paraffins					431.397	-103.168	7.286
	Naphthenes					259.384	-43.770	2.530
	Aromatics					116.188	82.180	-5.913
Reid Vapor Pressure	Paraffins			2275.6	-0.97	29.614	-6.340	0.342
	Naphthenes			2416.3	-1.11			
	Aromatics							

TABLE 5

Comparison of Results

	Run #1		Run #2	
	<u>Commercial</u>	<u>CATREF.F4</u>	<u>Commercial</u>	<u>CATREF.F4</u>
PVR5	81.2	79.7	84.3	76
RONR5	95.5	97.5	93.1	93.5
RVPR5			3.7	3.7
SGR5			0.7949	0.7915
PVIC4			1.0	5.27
PVNC4			1.2	5.08
PVAC5	63.2	61.96		

In run No. 2, there is a big difference in volume percent of reformat, but one of the reasons for this difference is the low percentage of butanes reported for this severity, so it may be the difference is caused by the splitter they used. If C4⁺ reformat yields are compared the agreement is good.

However, in a general sense, the kinetic model gives a good agreement with the commercial results.

The models developed in this report can be used by everybody to study the effect that the operating condition and the properties of the feedstock have on the yields and on their properties.

All the computer programs presented in the Appendixes were written in Fortran IV, and run in the PDP-10 of Colorado School of Mines, under the Monitor 503-B.

SIMULATION

To have relationships between research octane number and volume percent of reformat as a function of characterization factor, it is necessary to simulate the catalytic reformer process at different severities with different feedstocks. To get different severities it is necessary to use different operating conditions.

To select the feedstocks to be used in the simulation, information was taken from Zielinsky (1957), Emmett (1958), Petroleum Refinery (1955), which present different feedstocks with the kind of data required for CATREF. F4. From 23 feedstocks, six were selected to cover a wide range of characterization factor and they appear in Table 6 with their basic specifications.

Table 7 shows the ranges in the different properties which are used in the computer simulation.

To select the operating conditions the information given in Hydrocarbon Processing (Sept. 1970) on all the processes was used to fix the ranges of the different variables (see Table 8).

Within the ranges of operating variable shown in Table 8, seventeen runs were made with each feedstock. The operating conditions for each run are presented in Table 9.

TABLE 6

Feedstocks' Specifications

Name Speci- fications	Venezuelan		Gulf Coast	Venezuelan	Mixed	Mid- Continent	Mid- Continent
API°	47.4		48.1	48.6	52.2	51.8	54.3
T Mean	281		296	306	283	295	284
K	11.44		11.56	11.64	11.76	11.8	11.9
%P	31		26	33.8	44.5	54	55.2
%A	33		18.5	22.9	16.0	19	16.4
%N	36		55.5	43.3	39.5	27	28.4
· MW	115		125	126	122	125	123

TABLE 7

Selected Feedstocks' Range

Mean Boiling Point	281	-	306 °F
API°	47.4	-	54.3
K	11.44	-	11.9
% Paraffins	26	-	55.2
% Aromatics	16	-	33
% Naphthenes	27	-	55.5

TABLE 8

Selected Operating Condition's Range

Temperature	850°	-	1000°F
Pressure	200	-	500 Psia
Recycle Ratio	5	-	8
Hydrogen Purity			85%
Weight hourly space velocity (overall)	2	-	<u>4 lb fresh feed</u> hr lb catalyst

TABLE 9

Operating Conditions for the Runs

Run	A	B	C	D	E	F	G	H	I
T (°F)	850	900	950	1000	900	900	900	900	900
P (Psia)	300	300	300	300	200	400	500	300	300
RC	6	6	6	6	6	6	6	5	7
WHSV	3	3	3	3	3	3	3	3	3
Run	J	K	L	M	N	O	P	Q	
T (°F)	900	900	900	900	900	900	950	1000	
P (Psia)	300	300	300	300	300	300	200	200	
RC	8	6	6	6	6	6	6	6	
WHSV	3	4	2	3*	3*	3*	3	3	

To make these runs the following assumptions were made:

- a) Four reactors
- b) 500 nodes
- c) Pressure drop in each reactor was considered zero, because the effect of a small pressure drop is negligible.
- d) The reactor inlet temperatures were equal to each other.
- e) To calculate reciprocal molar space velocity an average-molecular weight was calculated with the molecular weight of the 23 feedstocks.
- f) For runs A to L reciprocal molar space velocity was distributed as 10%, 20%, 30%, 40%, of the total for the first, second, third, fourth reactors, respectively.
- g) For run M, 25% to each reactor; for run N, 40%, 30%, 20%, 10% of the total; for the first, second, third, fourth reactor, respectively; for run O, 30%, 20%, 20%, 30% of the total for the first, second, third, fourth reactor, respectively.
- h) For run P and Q, the same distribution than in run A was used.

Many runs were necessary to check the effect of all the variables and to establish enough points for the relationship.

Runs A, B, C, D	Temperature effect
Runs B, E, F, G	Pressure effect
Runs B, H, I, J	Hydrogen recycle ratio effect
Runs B, K, L	Space velocity effect
Runs B, M, N, O	Catalyst distribution effect
Runs P, Q	High-temperature and low-pressure effect

The results of these 17 runs for each feedstock are plotted in Figures 5, 6, 7, 8, 9, 10 and some of the results are in Table 10.

Figures 5, 6, 7, 8, 9, 10 show the relationships between research of reformat as a function of characterization factor.

Figure 11 shows the relationship between weight percent of hydrogen and volume percent of reformat. The points are scattered so there is not a direct relationship. Similar behavior is given by methane, ethane, propane, n-butane, i-butane, and this is the reason for not including those figures in this work.

The curves drawn on Figures 5, 6, 7, 8, 9 and 10, are not fitting curve lines, they were just drawn to show the trend of the relationship.

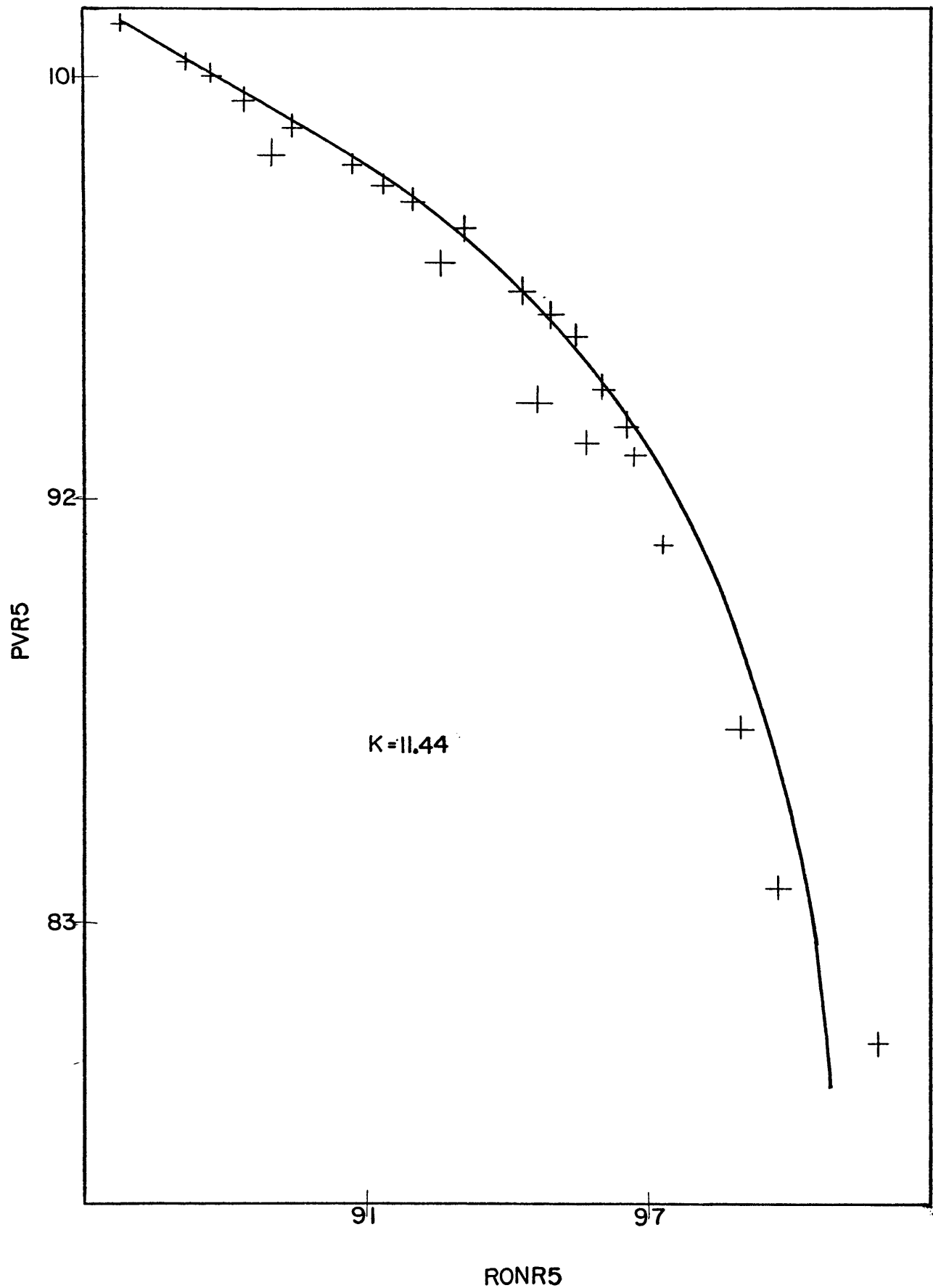
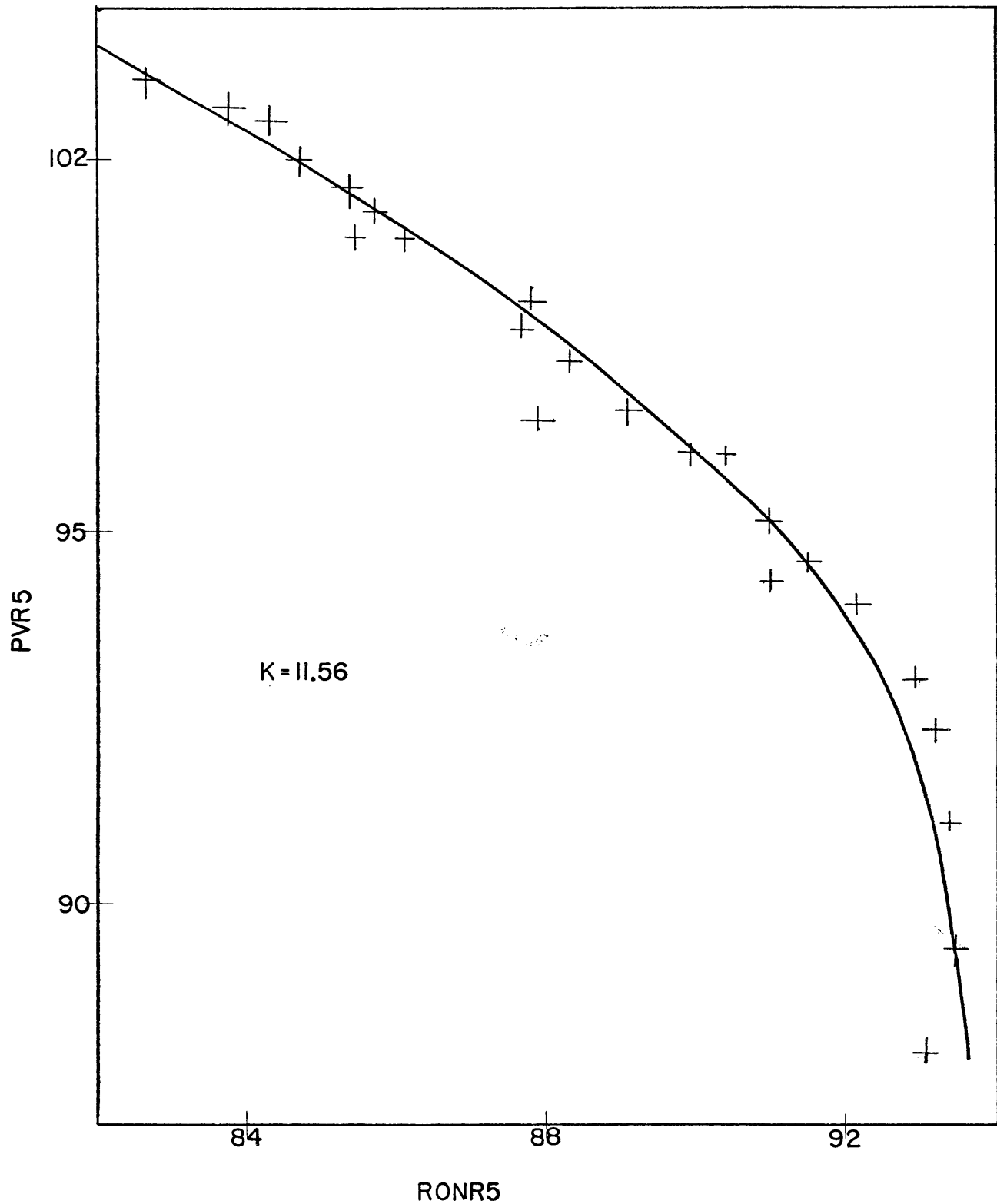
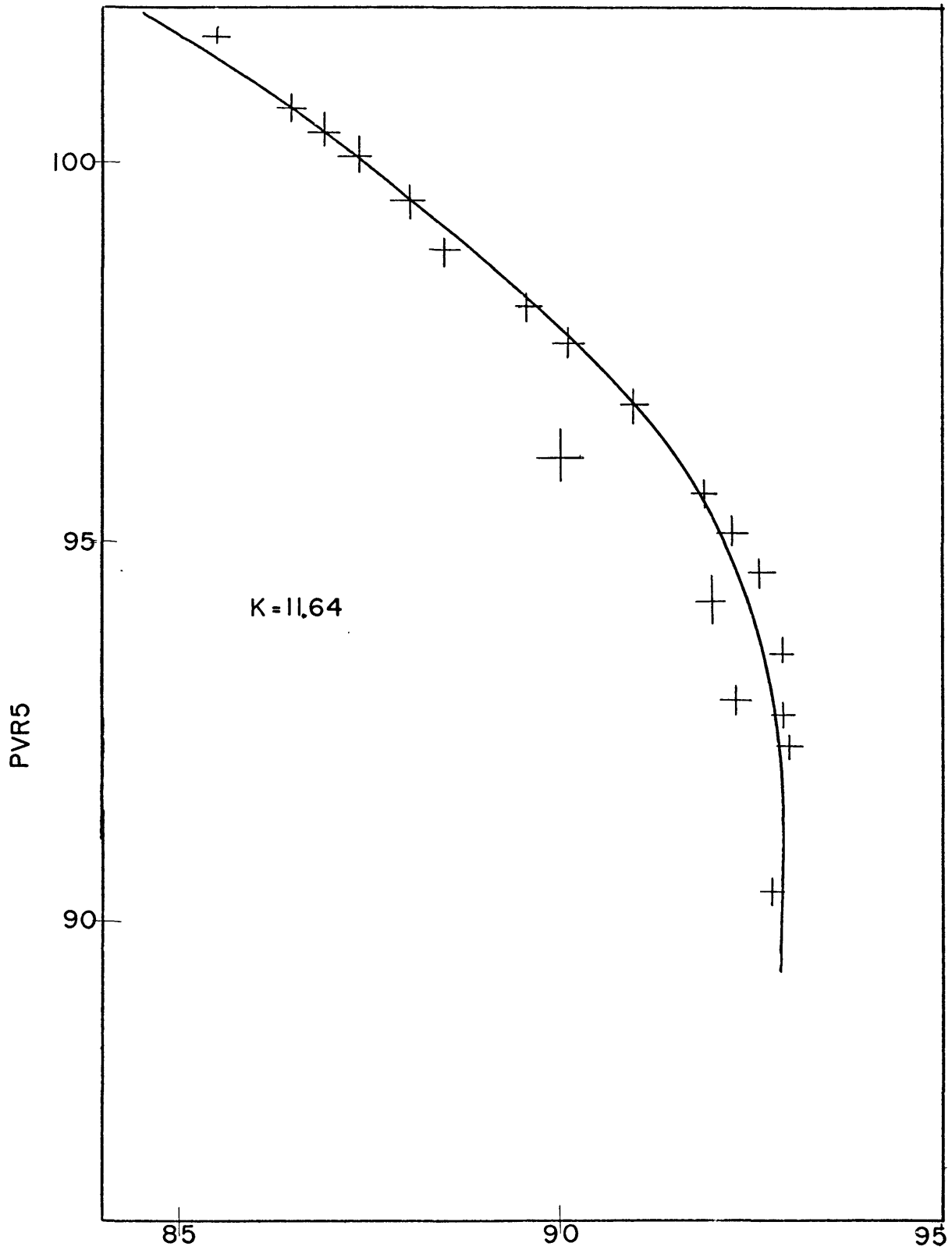


Figure 5

Volume Percent of Reformate Versus Research Octane Number
of Reformate for a Characterization Factor of 11.44



RONR5
Figure 6
Volume Percent of Reformate Versus Research Octane Number of
Reformate for a Characterization Factor of 11.56



RONR5
Figure 7

Volume Percent of Reformate Versus Research Octane Number of Reformate for a Characterization Factor of 11.64

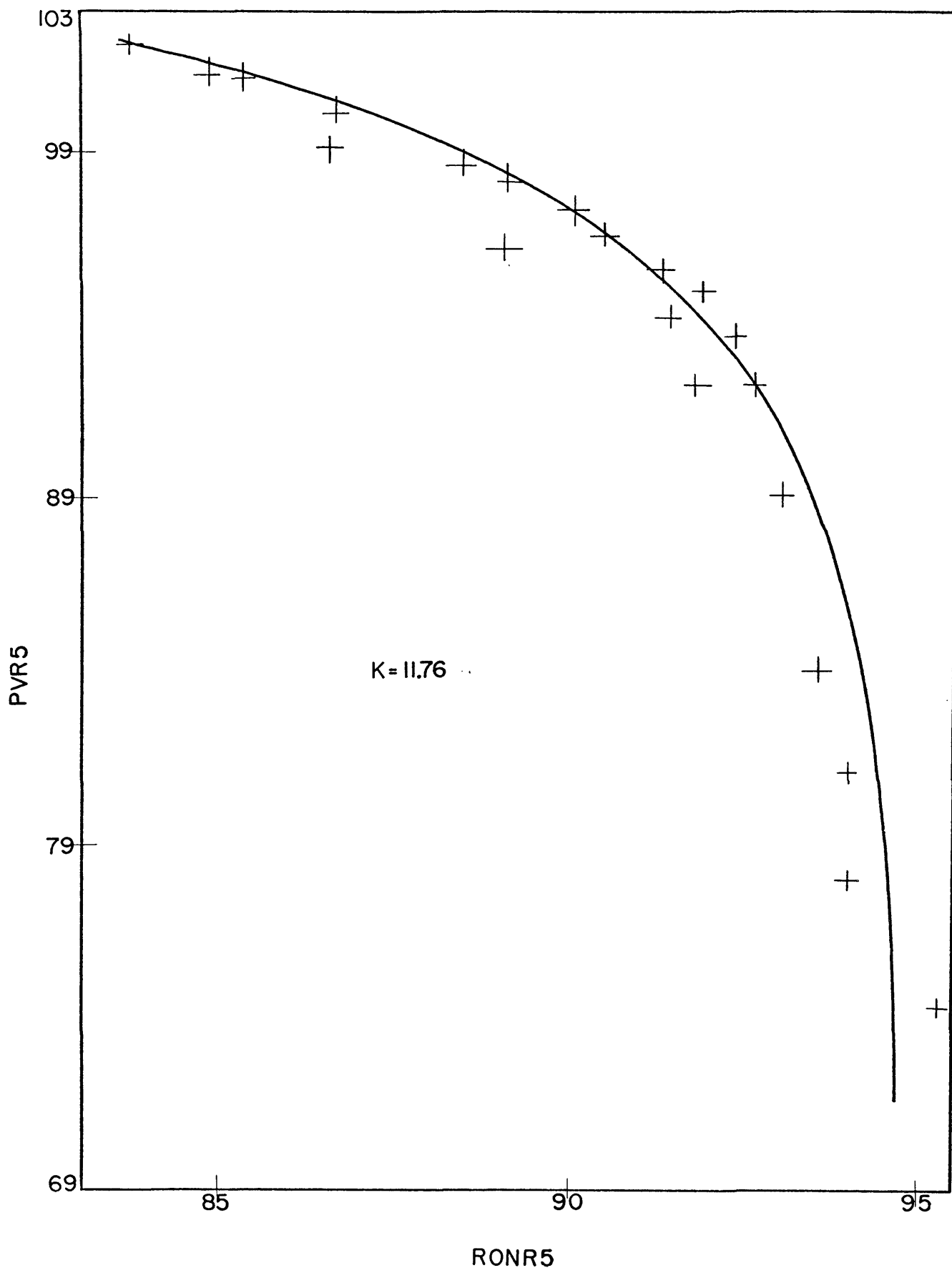
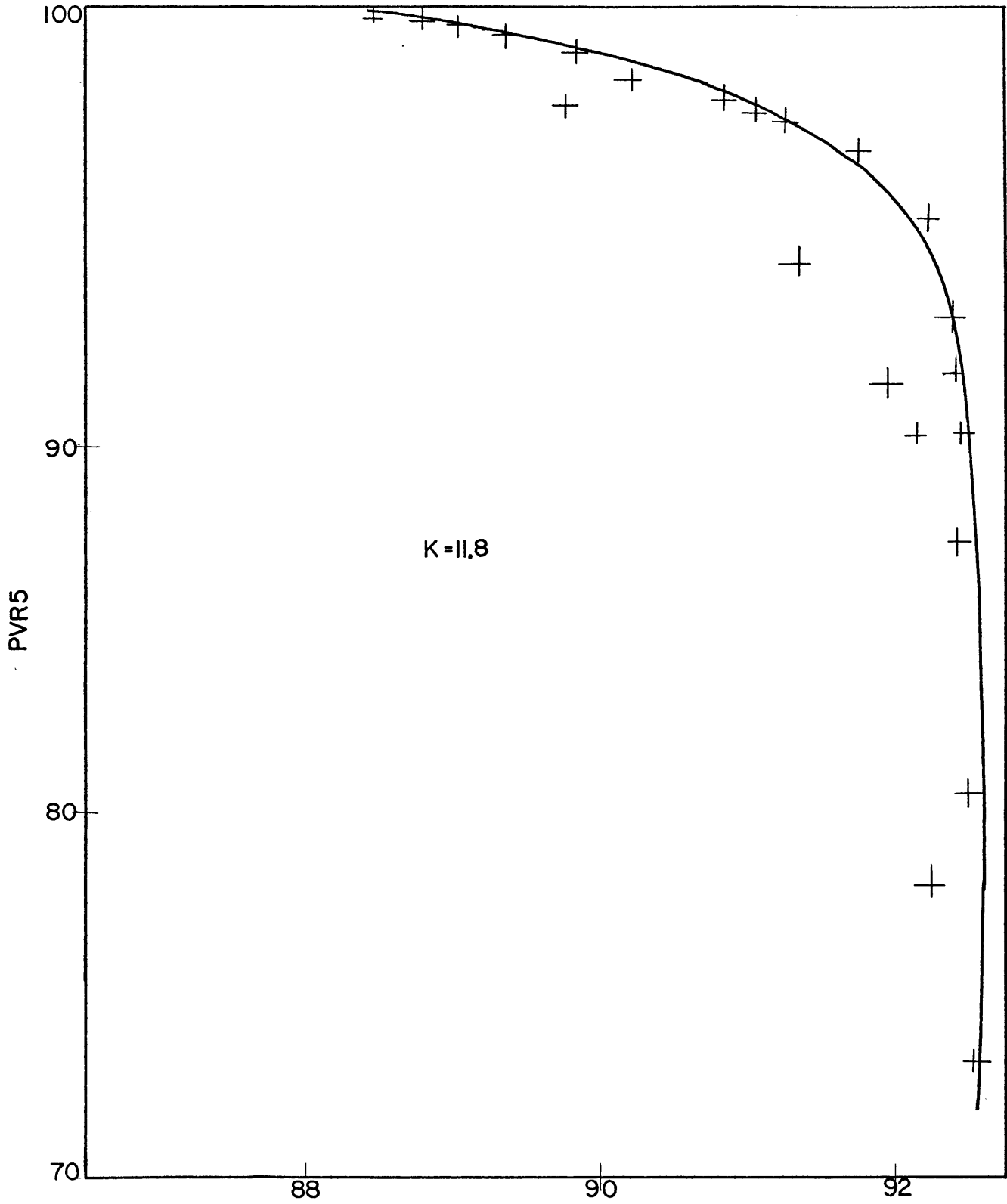


Figure 8

Volume Percent of Reformate Versus Research Octane Number of Reformate for a Characterization Factor of 11.76



RONR5
Figure 9

Volume Percent of Reformate Versus Research Octane Number of Reformate for a Characterization Factor of 11.80

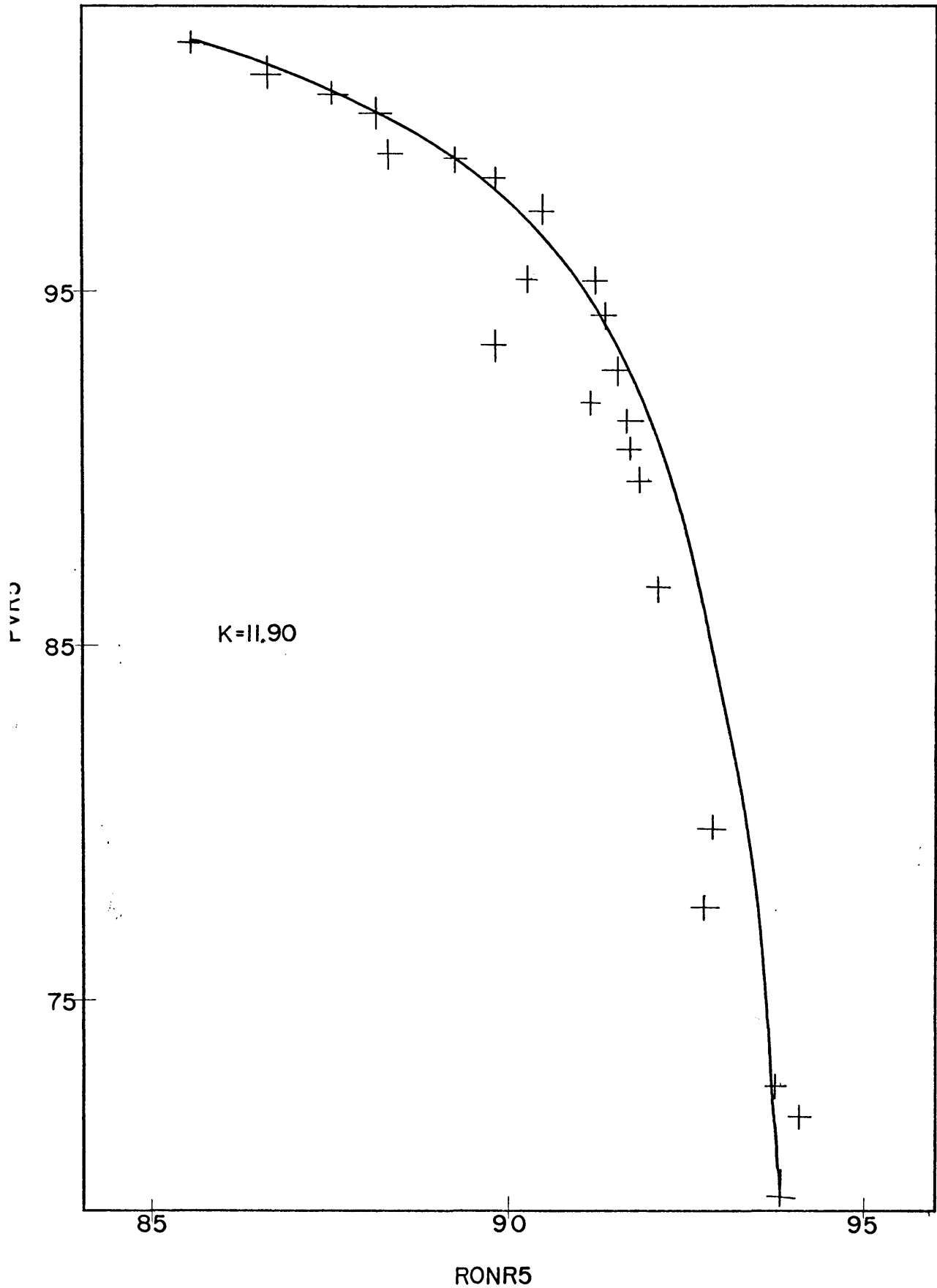


Figure 10
Volume Percent of Reformate Versus Research Octane Number of
Reformate for a Characterization Factor of 11.90

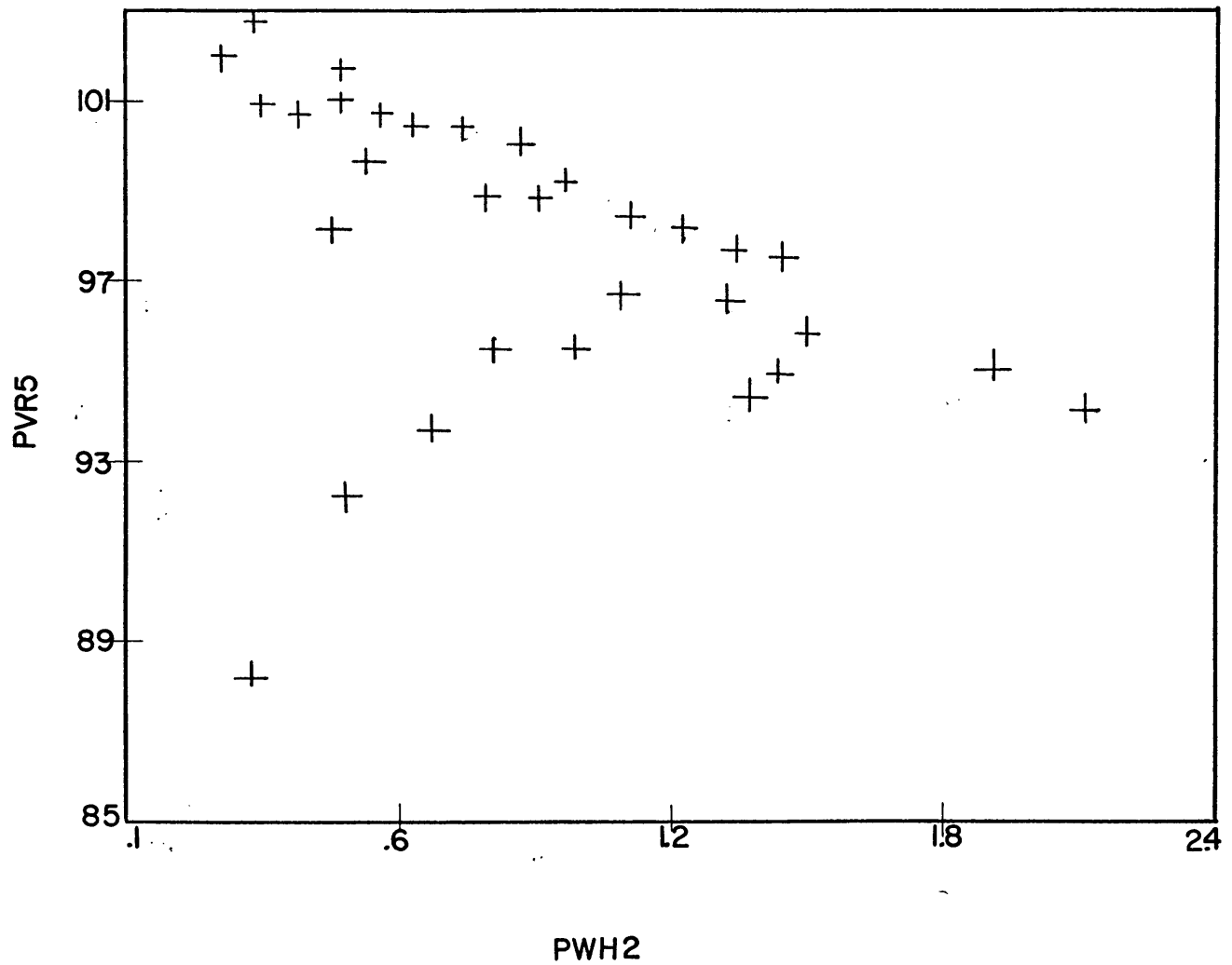


Figure 11
Volume Percent of Reformate Versus
Weight Percent of Hydrogen Produced

COMPUTER SIMULATION RESULTS

Table 10 presents some of the results obtained by computer simulation with different feed stocks at different operating conditions.

For some feed stocks a small increase in octane represents a big decrease in reformat yields because of the increase in hydrocracking, therefore optimum reforming octanes numbers have been selected and they are presented in Table 10. As can be seen from these data, it is possible to sometimes obtain the optimum octane in the first reactor and sometimes it is necessary to use four reactors.

The criteria to select the final reactor was the maximization of incomes from reformat. This was made using the data shown in Table 11, which gives the increase in value for an increase in octane number.

Computer Simulation Results

K = 11.44

Run Reactor	RONR5	PVR5	SGR5	RVPR5	PWH2	PWC1	PWC2	PWC3	PVNC4	PVIC4
A4	93.01	97.86	0.7907	0.534	1.331	0.090	0.169	0.248	0.221	0.229
B3	94.99	95.97	0.7963	0.666	1.510	0.202	0.378	0.555	0.495	0.513
C2	95.25	95.02	0.7965	0.810	1.453	0.310	0.580	0.851	0.759	0.788
D1	92.44	96.97	0.7871	0.767	1.091	0.260	0.487	0.714	0.637	0.661
E3	94.85	95.83	0.7961	0.695	1.482	0.223	0.418	0.613	0.547	0.568
F3	94.13	96.44	0.7929	0.688	1.368	0.212	0.392	0.582	0.519	0.539
G2	90.71	99.23	0.7822	0.566	0.966	0.097	0.183	0.268	0.239	0.248
H3	95.07	95.91	0.7966	0.668	1.521	0.203	0.381	0.559	0.499	0.518
I3	94.90	96.05	0.7960	0.664	1.498	0.199	0.374	0.548	0.489	0.507
J3	94.80	96.13	0.7956	0.661	1.487	0.197	0.368	0.540	0.482	0.500
K3	94.42	96.56	0.7945	0.625	1.458	0.167	0.313	0.459	0.410	0.425
L3	95.61	95.01	0.7984	0.760	1.555	0.276	0.517	0.758	0.676	0.702
M3	95.40	95.52	0.7977	0.699	1.549	0.229	0.429	0.630	0.562	0.583
N3	95.47	95.45	0.7979	0.704	1.555	0.233	0.437	0.640	0.571	0.593
O3	95.21	95.80	0.7971	0.673	1.537	0.208	0.390	0.572	0.511	0.530
P2	94.97	94.56	0.7958	0.903	1.372	0.377	0.707	1.037	0.925	0.960
Q1	92.10	96.14	0.7865	0.919	0.978	0.370	0.695	1.019	0.909	0.943

K = 11.56

Run Reactor	RONR5	PVR5	SGR5	RVPR5	PWH2	PWC1	PWC2	PWC3	PVNC4	PVIC4
A3	87.92	97.67	0.7917	0.281	1.457	0.042	0.080	0.117	0.104	0.108
B3	91.53	94.61	0.8058	0.393	2.020	0.132	0.248	0.363	0.323	0.335
C1	86.04	98.90	0.7825	0.348	1.036	0.080	0.15	0.220	0.195	0.203
D1	88.19	96.79	0.7890	0.504	1.292	0.193	0.361	0.53	0.471	0.489
E2	87.54	97.52	0.7899	0.361	1.349	0.096	0.179	0.263	0.233	0.242
F3	91.11	95.20	0.8022	0.391	1.889	0.128	0.239	0.351	0.312	0.324
G3	90.39	96.08	0.7956	0.426	1.633	0.145	0.273	0.400	0.355	0.369
H3	91.49	94.65	0.8057	0.386	2.021	0.127	0.239	0.350	0.311	0.323
I3	91.54	94.59	0.8057	0.399	2.016	0.136	0.255	0.374	0.332	0.345
J3	91.53	94.59	0.8055	0.403	2.008	0.139	0.260	0.382	0.339	0.352
K3	90.92	95.14	0.8032	0.376	1.919	0.118	0.221	0.325	0.289	0.300
L3	92.18	93.95	0.8086	0.427	2.121	0.158	0.297	0.435	0.386	0.401
M3	92.04	94.14	0.8081	0.408	2.107	0.145	0.271	0.397	0.353	0.362
N3	92.15	94.05	0.8085	0.411	2.125	0.147	0.276	0.405	0.359	0.373
O3	91.84	94.34	0.8072	0.398	2.077	0.137	0.257	0.377	0.335	0.342
P1	85.45	98.94	0.7805	0.401	0.925	0.114	0.214	0.314	0.279	0.290
Q1	87.60	96.25	0.7875	0.639	1.171	0.283	0.531	0.778	0.692	0.718

K = 11.64

Run Reactor	RONR5	PVR5	SGR5	RVPR5	PWH2	PWC1	PWC2	PWC3	PVNC4	PVIC4
A1	85.49	101.70	0.7686	0.256	0.391	0.012	0.023	0.034	0.030	0.031
B1	86.85	100.48	0.7742	0.284	0.647	0.037	0.070	0.102	0.090	0.094
C1	88.45	98.86	0.7803	0.365	0.906	0.098	0.185	0.271	0.240	0.249
D1	90.25	96.53	0.7863	0.576	0.118	0.247	0.462	0.678	0.601	0.624
E1	86.39	100.68	0.7724	0.305	0.556	0.050	0.094	0.177	0.122	0.126
F1	87.03	100.46	0.7746	0.275	0.672	0.031	0.058	0.086	0.076	0.079
G1	86.95	100.64	0.7736	0.273	0.634	0.029	0.054	0.079	0.070	0.073
H1	86.89	100.45	0.7744	0.282	0.657	0.036	0.068	0.099	0.088	0.091
I1	86.80	100.51	0.7739	0.286	0.635	0.038	0.072	0.105	0.093	0.097
J1	86.75	100.55	0.7737	0.288	0.623	0.039	0.073	0.107	0.095	0.099
K1	86.50	100.77	0.7727	0.283	0.577	0.035	0.065	0.095	0.084	0.088
L1	87.31	100.09	0.7762	0.286	0.740	0.041	0.076	0.112	0.099	0.103
M1	87.83	99.65	0.7785	0.289	0.844	0.045	0.084	0.123	0.109	0.113
N1	88.20	99.34	0.7801	0.292	0.915	0.048	0.091	0.133	0.118	0.122
O1	87.99	99.52	0.7792	0.290	0.875	0.046	0.086	0.126	0.112	0.116
P1	87.91	98.82	0.7785	0.427	0.802	0.139	0.260	0.381	0.338	0.352
Q1	89.70	95.74	0.7853	0.747	0.999	0.359	0.674	0.988	0.876	0.909

K = 11.76

Run Reactor	RONR5	PVR5	SGR5	RVPR5	PWH2	PWC1	PWC2	PWC3	PVNC4	PVIC4
A4	90.24	97.44	0.7714	0.465	1.439	0.106	0.199	0.291	0.253	0.262
B2	89.10	98.13	0.7671	0.480	1.238	0.112	0.209	0.306	0.266	0.276
C1	87.16	99.29	0.7602	0.505	0.900	0.120	0.225	0.330	0.287	0.298
D1	89.25	96.60	0.7658	0.765	1.100	0.309	0.580	0.850	0.738	0.766
E2	88.38	98.25	0.7650	0.527	1.114	0.142	0.266	0.390	0.339	0.352
F2	89.08	98.32	0.7666	0.466	1.224	0.100	0.188	0.276	0.240	0.249
G2	88.57	98.77	0.7638	0.474	1.105	0.103	0.192	0.282	0.245	0.254
H1	85.34	100.97	0.7548	0.407	0.656	0.043	0.081	0.118	0.103	0.107
I1	85.20	101.05	0.7543	0.411	0.628	0.045	0.085	0.125	0.108	0.112
J2	88.92	98.22	0.7664	0.486	0.203	0.115	0.215	0.316	0.274	0.285
K2	88.46	98.61	0.7650	0.468	0.139	0.100	0.188	0.276	0.240	0.249
L1	85.86	100.6	0.7565	0.411	0.740	0.049	0.091	0.134	0.116	0.125
M1	86.54	100.15	0.7580	0.414	0.851	0.054	0.101	0.148	0.129	0.134
N2	90.57	96.88	0.7723	0.529	1.458	0.153	0.286	0.419	0.364	0.378
O1	86.74	100.00	0.7595	0.416	0.885	0.056	0.104	0.153	0.133	0.138
P1	86.58	99.17	0.7585	0.577	0.788	0.169	0.316	0.463	0.402	0.418
Q1	88.80	95.54	0.7648	0.972	0.971	0.450	0.844	1.238	1.075	0.116

K = 11.80

Run Reactor	RONR5	PVR5	SGR5	RVPR5	PWH2	PWC1	PWC2	PWC3	PVNC4	PVIC4
A1	87.65	102.81	0.7475	0.324	0.286	0.018	0.033	0.048	0.042	0.044
B1	88.85	101.60	0.7519	0.377	0.496	0.059	0.111	0.163	0.142	0.148
C1	90.21	99.65	0.7568	0.537	0.690	0.174	0.328	0.481	0.419	0.434
D1	91.49	95.78	0.7622	0.015	0.792	0.502	0.940	1.379	1.201	1.246
E1	88.43	101.72	0.7504	0.404	0.410	0.076	0.143	0.210	0.183	0.189
F1	89.04	101.59	0.7523	0.364	0.522	0.051	0.096	0.14	0.122	0.126
G1	88.99	101.72	0.7517	0.361	0.499	0.048	0.090	0.132	0.115	0.119
H1	88.93	101.54	0.7522	0.376	0.510	0.059	0.110	0.162	0.141	0.146
I1	88.77	101.66	0.7516	0.378	0.476	0.060	0.112	0.164	0.143	0.148
J1	88.69	101.72	0.7512	0.378	0.461	0.060	0.112	0.164	0.142	0.148
K1	88.53	101.88	0.7507	0.370	0.433	0.053	0.100	0.147	0.128	0.133
L1	89.30	101.21	0.7536	0.386	0.575	0.068	0.127	0.186	0.162	0.168
M1	89.82	100.75	0.7555	0.399	0.668	0.078	0.147	0.215	0.199	0.195
N1	90.19	100.39	0.7570	0.412	0.735	0.089	0.166	0.244	0.213	0.221
O1	89.98	100.60	0.7562	0.403	0.697	0.082	0.154	0.226	0.197	0.204
P1	89.25	99.34	0.7554	0.632	0.589	0.239	0.447	0.656	0.571	0.592
Q1	91.13	93.92	0.7616	0.355	0.654	0.723	0.355	0.987	0.730	1.796

K = 11.90

Run Reactor	RONR5	PVR5	SGR5	RVPR5	PWH2	PWC1	PWC2	PWC3	PVNC4	PVIC4
A2	87.53	100.65	0.7487	0.404	0.643	0.044	0.083	0.122	0.104	0.108
B1	86.90	100.94	0.7464	0.429	0.520	0.059	0.110	0.162	0.139	0.148
C1	88.47	99.01	0.7514	0.580	0.729	0.171	0.321	0.471	0.405	0.426
D1	90.07	95.29	0.7507	1.066	0.847	0.484	0.907	1.331	0.103	1.186
E1	86.43	101.02	0.7449	0.456	0.433	0.076	0.143	0.209	0.180	0.186
F1	87.11	100.92	0.7469	0.415	0.554	0.050	0.094	0.138	0.118	0.123
G1	87.07	101.04	0.7465	0.411	0.535	0.046	0.087	0.128	0.110	0.114
H1	86.99	100.89	0.7468	0.427	0.538	0.058	0.109	0.160	0.137	0.142
I1	86.41	101.00	0.7461	0.430	0.504	0.059	0.111	0.163	0.140	0.145
J1	86.73	101.06	0.7458	0.430	0.488	0.059	0.111	0.163	0.140	0.145
K1	86.54	101.23	0.7452	0.423	0.458	0.053	0.100	0.146	0.125	0.130
L1	87.42	100.55	0.7482	0.436	0.607	0.067	0.125	0.183	0.158	0.164
M1	88.01	100.08	0.7502	0.447	0.706	0.077	0.144	0.211	0.181	0.188
N1	88.45	99.72	0.7517	0.458	0.777	0.086	0.162	0.237	0.204	0.211
O1	88.19	99.94	0.7508	0.451	0.736	0.080	0.150	0.221	0.189	0.196
P1	87.98	98.72	0.7499	0.674	0.624	0.235	0.440	0.646	0.555	0.576
Q1	89.77	93.51	0.7561	1.350	0.708	0.699	1.310	1.921	1.650	1.713

TABLE 11

Scale of Octane Differentials

Research Octane	\$/bbl per Octane
86 to 87	.0336
87 to 88	.0370
88 to 89	.0403
89 to 90	.0437
90 to 91	.0479
91 to 92	.0521
92 to 93	.0572
93 to 94	.0630
94 to 95	.0689
95 to 96	.0756
96 to 97	.0840
97 to 98	.0941
98 to 99	.1058
99 to 100	.1210

DISCUSSION OF RESULTS

As it would be very tedious to discuss the results of each of the different cases, the results of $K = 11.44$ will be analyzed to observe the effect of the operating variables on the yields and properties predicted by the computer simulation and to analyze the results from the view point of the reaction kinetics. All the comparisons will be made of the outlet products of the fourth reactor. The data are shown in Table 12.

a. Temperature effect (runs A,B,C,D.)

- 1) Octane number increases with temperature.
- 2) Percent volume of reformate decreases with temperature.
- 3) Reid vapor pressure increases with temperature.
- 4) C1, C2, C3, C4's increase with temperature.
- 5) Hydrogen yield decreases for temperature increases above 900F.

b. Pressure effect (runs B, E, F, G.)

- 1) Octane decreases with pressure.
- 2) Percent volume of reformate increases with pressure.
- 3) Reid vapor pressure increases with pressure.
- 4) C1, C2, C3, C4's increase with pressure.
- 5) Hydrogen decrease with pressure.

TABLE NO. 12
Computer Simulation Results for K = 11.44 After Four Reactors

	RONR5	PVR5	SGR5	RVPR5	PWH2	PWC1	PWC2	PWC3	PVIC4	PVNC4
A	93.01	97.86	0.7907	0.534	1.331	0.090	0.169	0.248	0.229	0.221
B	96.52	93.22	0.8018	0.9551	1.568	0.426	0.798	1.171	1.084	1.044
C	101.98	80.80	0.8250	2.533	1.486	1.539	2.886	4.233	3.919	3.776
D	104.34	75.27	0.8336	3.417	1.299	2.094	3.926	5.758	5.331	5.137
E	96.73	93.16	0.8023	0.9477	1.595	0.422	0.791	1.16	1.074	1.034
F	95.60	93.52	0.7977	1.015	1.393	0.463	0.867	1.272	1.178	1.135
G	94.18	93.71	0.7901	1.19	1.052	0.576	1.08	1.584	1.466	1.514
H	96.68	92.90	0.8025	0.988	0.574	0.451	0.846	1.241	1.149	1.102
I	96.38	93.50	0.8012	0.926	1.562	0.403	0.756	1.110	1.027	0.990
J	96.26	93.74	0.8006	0.900	1.557	0.384	0.720	1.055	0.977	0.941
K	96.03	94.36	0.7998	0.824	1.567	0.326	0.611	0.897	0.831	0.800
L	97.34	91.06	0.8052	1.217	1.548	0.621	1.165	1.709	1.582	1.524
M	96.42	93.62	0.8014	0.899	1.583	0.385	0.721	1.065	0.979	0.943
N	96.01	94.58	0.7998	0.90	1.582	0.309	0.564	0.827	0.765	0.737
O	96.43	93.59	0.8015	0.904	1.582	0.388	0.727	1.067	0.987	0.951
P	101.81	80.12	0.8229	2.718	1.347	1.654	3.101	4.548	4.210	4.057
Q	104.00	74.27	0.8301	3.72	1.08	2.268	4.252	6.236	5.773	5.56

- c. Hydrogen recycle ratio (runs B, H, I, J.)
- 1) Octane decreases with an increase of hydrogen recycle ratio.
 - 2) Reformate volume increases with hydrogen recycle ratio.
 - 3) Hydrogen yield decreases with hydrogen recycle ratio.
 - 4) C1, C2, C3, C4 yields decrease with hydrogen recycle ratio.
 - 5) Reid vapor pressure decreases with hydrogen recycle ratio.
- d. Reciprocal hourly molal space velocity (runs B, K, L.)
- 1) Octane increase with an increase of reciprocal molal space velocity.
 - 2) Reformate volume decrease with reciprocal molal space velocity.
 - 3) Hydrogen yield decreases with reciprocal molal space velocity.
 - 4) C1, C2, C3, C4's yields increase with reciprocal molal space velocity.
 - 5) Reid vapor pressure increases with reciprocal molal space velocity.

- e. Catalyst distribution (runs B, M, N, O.)
 - 1) The higher octane number is obtained with an uphill profile, and the lower with a downhill profile. The other two cases (constant and down-up) give practically the same results.
- f. Effects of low-pressure and high-temperature (runs P-C, Q, D.)
 - 1) The largest effect of these conditions is the high rate of hydrocracking. Octane number decreases, reformate volume decreases, and Reid vapor pressure of reformate increases.

From the information given in "Background", it is possible to see the agreement between the results given by the computer simulation and the theory.

The Magnaforming-catalyst profile has been checked and it agrees with the Magnaforming data which predict higher yields at a given severity.

Runs P and Q give an idea of the compromise existing among the different operation variable although the cycle life effect has not been considered.

The general information given by the simulation can be condensed as follows:

- 1) Research octane number and volume percent of reformate are inversely proportional except at extreme conditions where hydrocracking increases rapidly.

- 2) C4's and lighter are proportional to Reid vapor pressure of reformat.
- 3) C4's and lighter are not a unique function of RONR5 or PVR5, but are functions of the operating conditions.

LINEAR MODEL

Using the results presented in "Computer Simulation Results", a stage-wise linear-regression program (SWMLR. SAV [7000, 303]) was used to derive a linear equation that can predict the yields and their properties when given the operating conditions and characterization factor of the feed.

For each correlation 102 data points were used, considered as independent variables: temperature (°F), pressure (atms), hydrogen-to-hydrocarbon recycle ratio, cumulative reciprocal molar space velocity and characterization factor.

The computer program used has the ability to select the more significant variables for the correlation, find their coefficients and give some statistical information which can be used to check the fit.

The results of the linear regression are presented in Table 13 and the program using these equations is given in Appendix 5.

Information concerning the linear regression program is given in Appendix 4.

TABLE 13
Linear Model Coefficients

Pre- dicted Variable	Temp °F	Pres- sure atm.	RMSV lb cat-hr lb mol Fresh F	H ₂ RC	Charac- teriza- tion Factor	Constant Term.	Coeffi- cient of Multiple Determi- nate	Coeffi- cient of Multiple Correla- tion	Stan- dard Error of Es- timate	F Test
RONR5	0.02562		0.17836		-4.83464	120.321	0.677	0.823	1.606	68.54
PVR5	-0.04779		-0.19447		2.11664	119.784	0.851	0.922	0.988	186.35
SGR5	0.00008		0.00065		-0.09177	1.76135	0.897	0.947	0.0065	284.94
RVPR5	0.00471	-0.00381	0.00958		0.22408	-6.463	0.593	0.770	0.138	35.29
PWH2	0.0039	0.00513	0.03641		-0.73946	5.53089	0.807	0.898	0.218	101.12
PWC1	0.00316	-0.0029	0.00607		0.10938	-4.04392	0.719	0.848	0.071	62.08
PWC2	0.00593	-0.00545	0.01139		0.20451	-7.57225	0.719	0.848	0.132	62.06
PWC3	0.00867	-0.00811	0.01662		0.29658	-11.04432	0.718	0.847	0.194	61.91
PVNC4	-0.00120	-0.03689		0.56244		-0.71487	0.849	0.921	0.463	183.5
PVIC4	-0.002	-0.04081		0.52875	-0.33253	4.16136	0.857	0.926	0.475	145.15

CONCLUSIONS

The developed kinetic model is able to give good values in accordance with average values obtained from already existing real plants, regarding yields and their properties, when all the operating conditions and the analysis of the feedstock are given. It will not give exact results for each process, catalyst and feedstocks, but it will give average values and shows the trend of the process.

The model also predicts yields and properties when reactor temperature, catalyst charge and hydrogen-to-hydrocarbon recycle ratio profiles are used. However, the computer program has to be slightly modified to use a hydrogen-to-hydrocarbon recycle ratio profile.

The linear model is not able to give as good approximation to commercial results as the kinetic model does, but it is an improvement over the existing linear model (Belt'stov, 1967) because this model covers a wider range in operating conditions, a more realistic range of octane numbers, and the standard error of the estimate is lower.

Either of the two models proposed in this paper can be used to evaluate a given feedstock without costly and time-consuming pilot plant runs.

The kinetic model can be used for preliminary design work in order to observe the general trend of the product

yields and their properties as well as operating conditions to determine the number of reactors required to obtain the desired octane number and to predict the heat required in the inter-heaters, evaluate performance, and as a control algorithm.

The kinetic model can be used with a confidence of 80% to predict products and properties and with a 95% confidence to predict the number of reactors required to get a specific octane number. The kinetic model can give an error less than one unit, when predicting octane number.

The linear model can give an error less than two units, when predicting octane number.

There is still one large area of investigation on catalytic reformer; it is to determine the variation in the kinetic data, as the new catalysts are more selective than the old ones.

NOTATION

A, B, C, Q	Name for the simulation runs
A, B.....G	Constant used in curve fitting
API°	API gravity
API	American Petroleum Institute
C1, C2, C3, C4	Methane, Ethane, Propane, Butane
Cp	Average heat capacity
H2RC	Hydrogen to hydrocarbon recycle ratio
k_f	Rate constant
Kp	Equilibrium constant
K	Characterization factor
m_i	Mass of each component
n	Number of carbon atoms
Nt, Nn, Np, Na	Number of moles: total, naphthenes, paraffins, aromatics respectively
P, Pa, Pn, Pp, PH ₂	Pressure: total, aromatics, naph- thenes, paraffins, hydrogen, respectively. (atms)
PONA	Paraffins, olefins, naphthenes, and aromatics in a naphtha or petroleum fraction.
PVAR5, PVIC4, PVNC4, PVR5	Volume percent of: aromatics in reformate, iso-butane, normal-butane, reformate, respectively.

PWC1, PWC2, PWC3, PWH2	Weight percent of methane, ethane propane and hydrogen, respectively.
RONR5	Clear research octane number of reformate.
RMSV	Reciprocal molal hourly space velocity.
RVPR5	Reid vapor pressure of reformate
T	Temperature (°F).
Tm	Mean average boiling point.
Vr	RMSV
WHSV	Weight hourly space velocity.
Xi	Volume fraction.
Yi	Molar fractions.
Numbers	
5	At the end means: reformate including C5 and heavier materials.

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APPENDIX No. 1

Kinetic Model

CATREF.F4

CATREF.F4 (LISTING)

C CATALYTIC REFORMER SIMULATION
 C ROBRIGO VARELA V
 C THIS PROGRAM COMPUTES: TEMPERATURE DROP THROUGH EACH REACTOR, YIELDS
 C AND THEIR PROPERTIES , FOR THE CATALYTIC REFORMING PROCESS OF ANY KIN
 D OF NAPHTHA, AT SOME GIVEN OPERATING CONDITIONS.
 C LAG IS USED TO RUN AS MANY SET OF DATA AS YOU WANT. IT MUST BE ZERO I
 F A NEW SET OF DATA IS GOING TO BE PROCESSED, IT MUST BE -1, IF THERE AR
 E NOT MORE DATA.
 C

DIMENSION TEMP(6), PRESS(6), PDIFF(6),

1 RMSV(4)

111 READ (4,400)LAG

IF(LAG.EQ.-1) GO TO 50

READ(4,800)I,J

READ(4,801)YA,YP,YN,AMW,API

READ(4,803)RC,PH

READ(4,802)(TEMP(K),PRESS(K),PDIFF(K),

1 RMSV(K),K=1,J)

PRINT 804,YA,YP,YN,RC,PH,AMW,API

PRINT 802,(TEMP(K),PRESS(K),PDIFF(K),RMSV(K),K=1,J)

C=2.71828183

YH=RC*PH

YT=RC+1.

E=I

AN=(AMW-2.*YP+6.*YA)/14.

YHI=YH

YLEI=YT-YA-YP-YN-YH

ER 1404

66

SGF=141.5/(CFI+131.5)

K=1

D0 40 M=1,J

IF=I

T=TEMP(K)

PT=PRESS(K)

PD=FDIFF(K)

VR=RMSV(K)

DVR=VR/B

PRINT 902,K

PRINT 900

L=0

PRINT 901,L,YA,YN,YP,YH,PT,T

1 D0 30 LL=1,I

PA=YA*PT/YT

PP=YP*PT/YT

PN=YN*PT/YT

PHY=YH*PT/YT

CK1=C**((46.15-46045./T)

R1=C**((23.21-34750./T)

D1=(R1*PN/CK1)*(CK1-PA*PHY**3/PN)

CK2=C**((8000./T-7.12)

R2=C**((35.98-59600./T)

D2=(R2*PN*PHY/CK2)*(CK2-PP/(PN*PHY))

R3=C**((42.97-62300./T)

D3=R3*PP/PT

R4=C**((42.97-62300./T)

D4=R4*PN/PT

DELA=D1*DVR

DELP=(D2-D3)*DVR

```

DELN = -(D1+D2+D4)*DVR
DELNH = (-D2+3.*D1-(((AN-3.)/3.)*D3)-(AN/3.)*D4)*DVR
YA = YA+DELA
YP = YP+DELP
YN = YN+DELN
YH = YH+DELH
DELYT = (-D2+3.*D1-D4)*DVR
YT = YT+DELYT
YLE = YT-YA-YP-YN-YH
CPA = 2.52 + (68.2*T*1.E-3) - (15.*T**2*1.E-6)
CPP = 7.66 + (87.5*T*1.E-3) - (18.3*T**2*1.E-6)
CFN = -7.77 + (103.*T*1.E-3) - (22.8*T**2*1.E-6)
CFH = 6.9 + (0.0033*T*1.E-3) + (0.086*T**2*1.E-6)
CPLE = 3.21 + (36.*T*1.E-3) - (6.96*T**2*1.E-6)
CP = (YA*CPA+YN*CFN+YP*CPP+YH*CFH+YLE*CPLE)/YT
DELT = ((-D1*91500.+D2*19000.+D3*8100.*(AN-3.)
1      +D4*22300.*AN/3.)/(YT*CP))*DVR
T = T+DELT
PT = PT-PD/B
IF (IP-LL) 10, 10, 30
10  PRINT 901, LL, YA, YN, YP, YH, PT, T
    IF (LL-I) 30, 31, 31
30  CONTINUE
31  YHF = YH - YHI
    YLEP = YLE - YLEI
    FWH2 = YHF * 200. / AMW
    FWC1 = YLEP * 320. / AMW
    FWC2 = YLEP * 600. / AMW
    FWC3 = YLEP * 880. / AMW
    FWC4 = YLEP * 580. * SCF / (0.5844 * AMW)

```

$$FVIC4=YLEF*560.*SGF/CO.5631*AMW)$$

$$FWNC4=YLEF*560./AMW$$

$$FWIC4=FWNC4$$

$$FVIC5=YLEF*960.*SGF/(.6248*AMW)$$

$$FWNC5=YLEF*480.*SGF/(.6312*AMW)$$

$$FWIC5=YLEF*960./AMW$$

$$FWNC5=YLEF*480./AMW$$

$$FVN=YN*1400.*AN/AMW$$

$$FVA=YA*(14.*AN-6.)*100./AMW$$

$$FVP=YP*(14.*AN+2.)*100./AMW$$

$$D=YA*(14.*AN-6.)/(1.1112-.0611*AN+.0039*AN**2)$$

$$1 + YP*(14.*AN+2.)/(.52+.02*AN)+YN*14.*AN/(.67+$$

$$1 + 0.01*AN)$$

$$SGR6=(YA*(14.*AN-6.)+YP*(14.*AN+2.)+YN*14.*AN)/D$$

$$PWR6=PVN+FVP+FVA$$

$$PVR6=PWR6*SGF/SGR6$$

$$PVNR6=YN*14.*AN/((.67+.01*AN)*D)$$

$$PVAR6=YA*(14.*AN-6.)/((1.1112-.061*AN+.0039*($$

$$1 AN**2))*D)$$

$$FVPR6=YP*(14.*AN+2.)/((.52+.02*AN)*D)$$

$$PWF5=PWR6+3.*FWNC5$$

$$D7=D+YLEF*14.4/.6270$$

$$SGR5=(YA*(14.*AN-6.)+YP*(14.*AN+2.)+$$

$$1 + YN*14.*AN+YLEF*14.4)/D7$$

$$PVR5=PWR5*SGF/SGR5$$

$$FVNR5=PVR6*D/D7$$

$$FVAR5=FVAR6*D/D7$$

$$FVPR5=FVPR6*D/D7$$

$$FVCSF5=YLEF*14.4/(.627*D7)$$

$$FVNF7=(FVPR6*(431.4-103.17*AN+7.28*AN**2))+$$

1 PVAR65=(-166.19+82.18*AN-5.91*AN**2)+

1 PVNR6=(259.38-43.77*AN+2.53*AN**2)

R0NR5=PVPR5*(431.4-103.17*AN+7.28*AN**2)+

1 PVAR5*(-166.19+82.18*AN-5.91*AN**2)+

1 PVNR5*(259.38-43.77*AN+2.53*AN**2)+

1 PVC5R5=82.8

TM=YA+YP+YN

RVPR6=YP*2275.6*(C**(-.97*AN))

RVPR6=RVPR6+YA*2416.3*(C**(-1.11*AN))

RVPR6=RVPR6+YN*(29.614-6.34*AN+.342*AN**2)

RVPR6=RVPR6/TM

TM5=TM+YLEP/5.

RVPR5=(YA*2416.3*(C**(-1.11*AN))+YP*2275.6*

1 (C**(-.97*AN))+YN*(29.614-6.34*AN+.342*

1 AN**2)+YLEP*18.8/5.)/TM5

PRINT 903

PRINT 904,YHP,YLEP,YA,YN,YP

PRINT 905,CP

PRINT 333,PWH2,PWC1,PWC2,PWC3,PWNC4,

1 PWIC4,PWIC5,PWNC5,PWR6,PWR5,PWA,PWN,PWP,

1 PVNC4,PVIC4,PVIC5,PVNC5,SGR6,SGR5,PVR6,

1 PVR5,PVNR6,PVAR6,PVPR6,PVNR5,PVPR5,PVAR5,

1 PVC5R5,R0NR6,R0NR5,RVPR5,RVPR6

K=K+1

IF(K-J)40,40,20

40 CONTINUE

800 FORMAT(2I3)

801 FORMAT(5F)

803 FORMAT(2F)

804 FORMAT(1H1/7F)

```

802 FORMAT(4F)
900 FORMAT(//22X,24HMØLES/MØLE OF FRESH FEED,14X,5HPRESS,9X,4HTEMP/6X
1,4HNODE,2X,9HAROMATICS,2X,10HNAPHTHENES,2X,9HPARAFFINS,2X,8HHYDRØG
2EN,7X,3HATM,9X,5HDEG R)
400 FORMAT(I2)
901 FORMAT (/7X,I3,3X,F8.3,3X,F8.3,3X,F8.3,3X,F8.3,3X,F8.3,3X,F8.1)
902 FORMAT(//30X,14HREACTØR NUMBERI4)
903 FORMAT(//6X,43HTØTAL MØLES PRØDUCED PER MØLE OF FRESH FEED)
904 FORMAT(//18X,8HHYDRØGENF16.3/18X,15HC1 THRU C5 SAT
1 F9.3/18X,9HAROMATICSF15.3/18X,10HNAPHTHENESF14.3
1 /18X,9HPARAFFINSF15.3)
905 FORMAT(//6X,37HMØLAR HEAT CAPACITY REACTØR EFFLUENT=F10.2,2X,17HBT
1U/LB MØLE/DEG F)
333 FORMAT(' PWH2='F9.4,8X,' PWC1='F9.4,8X,' PWC2='F9.4,/' PWC3='F9.4,
18X,' PWC4='F9.4,7X,' PWIC4='F9.4,/' PWIC5='F9.4,7X,' PWC5='F9.4,
17X,
2' PWR6='F9.4,/' PWR5='F9.4,8X,' PWN='F9.4,9X,' PWA='F9.4,/' PWF='
3F9.4,9X,' PWC4='F9.4,7X,' PVIC4='F9.4,/' PVIC5='F9.4,7X,' PWC5='
4F9.4,7X,' SGR6='F9.4,/' SGR5='F9.4,8X,' PVR6='F9.4,8X,' PVR5='F9.4
5,/' PVNR6='F9.4,7X,' PVAR6='F9.4,7X,' PVPR6='F9.4,/' PVNR5='F9.4,
57X
6 ,' PVFR5='F9.4,7X,' PVAR5='F9.4,/' PVC5R5='F9.4,6X,' RØNR6='F9.4,
7 7X,' RØNR5='F9.4,/' PVFR5='F9.4,7X,' RVPR6='F9.4)
20 GO TO 111
50 STOP
FND

```

CATREF.F4 (DATA)

\$
0
500 4
.33/.31/.36/115./47.7
6./85
1310./20.4/0.0/4.167
1310./20.4/0.0/8.334
1310./20.4/0.0/12.501
1310./20.4/0.0/16.668

CATREF.F4 (RESULTS)

	0.3300000	0.3100000	0.3600000	6.0000000	0.85000
00	115.0000007	47.6999998			
	1309.9999961	20.3999998	0.0000000	4.1670000	
	1309.9999961	20.3999998	0.0000000	8.3340000	
	1309.9999961	20.3999998	0.0000000	12.5009999	
	1309.9999961	20.3999998	0.0000000	16.6679999	

REACTOR NUMBER 1

TEMP	MØLES/MØLE ØF FRESH FEED					PRESS
DEG R	NØDE	ARØMATICS	NAPHTHENES	PARAFFINS	HYDRØGEN	ATM
0.0	0	0.330	0.360	0.310	5.100	20.400 131
7.1	500	0.402	0.286	0.311	5.311	20.400 126

TOTAL MØLES PRØDUCED PER MØLE ØF FRESH FEED

HYDRØGEN	0.211
C1 THRU C5 SAT	0.004
ARØMATICS	0.402
NAPHTHENES	0.286
PARAFFINS	0.311

MOLAR HEAT CAPACITY REACTOR EFFLUENT=		20.77	BTU/LB MØLE/DEG
PWH2= 0.3673	PWC1= 0.0122	PWC2= 0.0229	
PWC3= 0.0336	PWNC4= 0.0222	PWIC4= 0.0222	
PWIC5= 0.0367	PWNC5= 0.0183	PWR6= 99.4646	
PWR5= 99.5197	PWN= 38.5888	PWA= 28.8906	
PWP= 31.9852	PVNC4= 0.0299	PVIC4= 0.0311	
PVIC5= 0.0463	PVNC5= 0.0229	SGR6= 0.7699	
SGR5= 0.7698	PVR6= 102.0073	PVR5= 102.0766	
PVNR6= 0.2970	PVAR6= 0.3419	PVPR6= 0.3608	
PVNR5= 0.2967	PVPR5= 0.3606	PVAR5= 0.3417	
PVC5R5= 0.0007	RØNR6= 85.7337	RØNR5= 85.7317	
RVPR5= 0.4911	RVPR6= 0.4750		

REACTOR NUMBER 2

TEMP DEG R	NØDE	MØLES/MØLE ØF FRESH FEED				PRESS ATM	
		ARØMATICS	NAPHTHENES	PARAFFINS	HYDRØGEN		
0.0	0	0.402	0.286	0.311	5.311	20.400	1
2.3	500	0.482	0.202	0.311	5.545	20.400	1

TOTAL MØLES PRØDUCED PER MØLE ØF FRESH FEED

HYDRØGEN	0.445
C1 THRU C5 SAT	0.011
ARØMATICS	0.482
NAPHTHENES	0.202
PARAFFINS	0.311

MOLAR HEAT CAPACITY REACTOR EFFLUENT=		20.07	BTU/LB MØLE/DEG
PWH2= 0.7740	PWC1= 0.0296	PWC2= 0.0556	
PWC3= 0.0815	PWNC4= 0.0537	PWIC4= 0.0537	
PWIC5= 0.0889	PWNC5= 0.0444	PWR6= 98.8186	
PWR5= 98.9519	PWN= 46.2878	PWA= 20.4894	
PWP= 32.0414	PVNC4= 0.0726	PVIC4= 0.0753	
PVIC5= 0.1123	PVNC5= 0.0556	SGR6= 0.7785	
SGR5= 0.7783	PVR6= 100.2289	PVR5= 100.3968	
PVNR6= 0.2143	PVAR6= 0.4174	PVPR6= 0.3678	
PVNR5= 0.2140	PVPR5= 0.3672	PVAR5= 0.4167	
PVC5R5= 0.0017	RØNR6= 88.6596	RØNR5= 88.6498	
RVPR5= 0.4893	RVPR6= 0.4502		

REACTOR NUMBER 3

TEMP DEG R	NODE	MØLES/MØLE ØF FRESH FEED				PRESS	
		ARØMATICS	NAPHTHENES	PARAFFINS	HYDRØGEN	ATM	
0.0	0	0.482	0.202	0.311	5.545	20.400	12
0.6	500	0.549	0.133	0.311	5.738	20.400	12

TOTAL MØLES PRØDUCED PER MØLE ØF FRESH FEED

HYDRØGEN	0.638
C1 THRU C5 SAT	0.019
ARØMATICS	0.549
NAPHTHENES	0.133
PARAFFINS	0.311

MØLAR HEAT CAPACITY REACTOR EFFLUENT=			19.61	BTU/LB MØLE/DEG R	
PWH2=	1.1095	PWC1=	0.0540	PWC2=	0.1012
PWC3=	0.1485	PWNC4=	0.0979	PWIC4=	0.0979
PWIC5=	0.1620	PWNC5=	0.0810	PWR6=	98.1481
PWR5=	98.3910	PWN=	52.7284	PWA=	13.4126
PWP=	32.0070	PVNC4=	0.1322	PVIC4=	0.1372
PVIC5=	0.2047	PVNC5=	0.1013	SGR6=	0.7860
SGR5=	0.7855	PVR6=	98.5964	PVR5=	98.9024
PVNR6=	0.1426	PVAR6=	0.4834	PVPR6=	0.3735
PVNR5=	0.1422	PVPR5=	0.3724	PVAR5=	0.4819
PVC5R5=	0.0031	RØNR6=	91.2126	RØNR5=	91.1866
RVPR5=	0.5006	RVPR6=	0.4291		

REACTOR NUMBER 4

TEMP DEG R	NODE	MØLES/MØLE ØF FRESH FEED				PRESS	
		ARØMATICS	NAPHTHENES	PARAFFINS	HYDRØGEN	ATM	
0.0	0	0.549	0.133	0.311	5.738	20.400	12
3.8	500	0.595	0.084	0.309	5.865	20.400	12

TOTAL MOLES PRODUCED PER MOLE OF FRESH FEED

HYDRØGEN	0.765
C1 THRU C5 SAT	0.032
ARØMATICS	0.595
NAPHTHENES	0.084
PARAFFINS	0.309

MØLAR HEAT CAPACITY REACTØR EFFLUENT=

19.35 BTU/LB MØLE/DEG F

PWH2= 1.3307	PWC1= 0.0900	PWC2= 0.1688
PWC3= 0.2476	PWNC4= 0.1632	PWIC4= 0.1632
PWIC5= 0.2701	PWNC5= 0.1350	PWR6= 97.4315
PWR5= 97.8366	PWN= 57.1406	PWA= 8.5089
PWP= 31.7820	PVNC4= 0.2205	PVIC4= 0.2288
PVIC5= 0.3413	PVNC5= 0.1689	SGR6= 0.7916
SGR5= 0.7907	PVR6= 97.1878	PVR5= 97.6980
PVNR6= 0.0918	PVAR6= 0.5314	PVPR6= 0.3763
PVNR5= 0.0913	PVPR5= 0.3743	PVAR5= 0.5286
PVCSR5= 0.0052	RØNR6= 93.0632	RØNR5= 93.0096
RVPR5= 0.5335	RVPR6= 0.4139	

†Ø

1

†C

.K

CØNFIRM: K

JØB 11, USER [2700,324713] LØGGED ØFF TTY22 1054 22-JUL-71

DELETED 1 FILES (15. DISK BLØCKS)

SAVED 8 FILES (120. DISK BLØCKS)

RUNTIME 0 MIN, 28.02 SEC

APPENDIX No. 2

First Order Least Square Fitting Program

MNSQUARE.F4

MNSQUARE.F4 (LISTING)

```

00010      DIMENSION Y(100),X(100)
00020      SX=0.0
00030      SY=0.0
00040      SX2=0.0
00050      SXY=0.0
00055      SY2=0.0
00060      READ(5,6) N
00070      6  F0RMAT(I3)
00080      READ(5,10)(X(I),Y(I),I=1,N)
00090      D0 20 I=1,N
00100      SX=SX+X(I)
00110      SY=SY+Y(I)
00120      SX2=SX2+(X(I)**2)
00130      SXY=SXY+(X(I)*Y(I))
00135      SY2=SY2+(Y(I)**2)
00140      20  C0NTINUE
00150      A=(SY*SX2-SXY*SX)/(N*SX2-SX**2)
00160      B=(N*SXY-SX*SY)/(N*SX2-SX**2)
00170      WRITE(4,32) A,B
00180      32  F0RMAT(' A='F15.5/' B='F15.5)
00190      STDERR=SQRT((SY2-A*SY-B*SXY)/(N-2))
00200      WRITE(4,40) STDERR
00205      10  F0RMAT(6F)
00210      40  F0RMAT(' STANDARD ERR0R 0F THE ESTIMATE='F15.5)
00220      D0 28 I=1,N
00230
00240      EST=A+B*X(I)
00245
00250      WRITE(4,35) X(I),EST
00255      28  C0NTINUE
00260      35  F0RMAT(' X='F15.5,15X,' ESTIMATED VALUE='F15.5)
00270
00280      END

```

• EXE MNSQUARE.F4
LOADER 5K CORE
EXECUTION
*

ER 1404

77

MNSQUARE.F4 (LINEAR FIT)

DATA AND RESULTS

\$
4
6./7.7460/7./7.7630/8./7.7768
9./7.7870

A= 0.66560
B= 0.01368
STANDARD ERROR OF THE ESTIMATE=
X= 6.00000
X= 7.00000
X= 8.00000
X= 9.00000

$$Y = 0.6656 + 0.01368 X$$

0.00239
ESTIMATED VALUE= 0.74768
ESTIMATED VALUE= 0.76136
ESTIMATED VALUE= 0.77504
ESTIMATED VALUE= 0.78872

EXECUTION TIME: 0.23 SEC.
TOTAL ELAPSED TIME: 1 MIN. 4.15 SEC.
NO EXECUTION ERRORS DETECTED

EXIT

•
EXE MNSQUARE.F4
LOADING

LOADER 5K CORE
EXECUTION
*

@ MNSQUARE.F4 (EXPONENTIAL FIT)

DATA AND RESULTS

\$
4
6./1.9482/7./7.9536/8./-0.0576
9./-0.9365

A= 7.72590
B= -0.96653
STANDARD ERROR OF THE ESTIMATE=
X= 6.00000
X= 7.00000
X= 8.00000
X= 9.00000

$$Y = 2275.6 e^{-0.96653 X}$$

0.04720
ESTIMATED VALUE= 1.92672
ESTIMATED VALUE= 0.96019
ESTIMATED VALUE= -0.00634
ESTIMATED VALUE= -0.97287

EXECUTION TIME: 0.20 SEC.
TOTAL ELAPSED TIME: 1 MIN. 9.85 SEC.
NO EXECUTION ERRORS DETECTED

EXIT

APPENDIX No. 3

Second Order Least Square Fitting Program

SECOR.F4

SECOR.F4 (LISTING)

```

00010      DIMENSION Y(100),X(100)
00020      SX=0.0
00030      SY=0.0
00040      SX2=0.0
00050      SXY=0.0
00060      SY=0.0
00070      SX3=0.0
00080      SX4=0.0
00090      SYX2=0.0
00100      READ(5,6)N
00110      6  FØRMAT(I3)
00120      READ(5,10)(X(I),Y(I),I=1,N)
00130      DØ 20 I=1,N
00140      SX=SX+X(I)
00150      SY=SY+Y(I)
00160      SX2=SX2+(X(I)**2)
00170      SXY=SXY+(X(I)*Y(I))
00180      SX3=SX3+(X(I)**3)
00190      SX4=SX4+(X(I)**4)
00200      SYX2=SYX2+(Y(I)*(X(I)**2))
00210      20  CØNTINUE
00220      ANA=SY*(SX2*SX4-SX3**2)-SXY*(SX*SX4-SX2*SX3)+
00230      1      +SYX2*(SX*SX3-SX2**2)
00240      ANB=N*(SXY*SX4-SYX2*SX3)-SX*(SY*SX4-SYX2*SX2)+
00250      1      +SX2*(SY*SX3-SXY*SX2)
00260      ANC=N*(SX2*SYX2-SX3*SXY)-SX*(SX*SYX2-SX3*SY)+
00270      1      +SX2*(SX*SXY-SX2*SY)
00280      D=N*(SX2*SX4-SX3**2)-SX*(SX*SX4-SX2*SX3)+
00290      1      +SX2*(SX*SX3-SX2**2)
00300      A=ANA/D
00310      B=ANB/D
00320      C=ANC/D
00330      WRITE(4,32)A,B,C
00340      32  FØRMAT(' A='F15.5/' B='F15.5/' C='F15.5/)
00350      10  FØRMAT(6F)
00360      DIFF2=0.0
00370
00380      40  FØRMAT(' STANDARD ERROR ØF THE ESTIMATE='F15.5)
00390      DØ 28 I=1,N
00400      EST= A+B*X(I)+C*(X(I)**2)
00405      DIFF2=DIFF2+((Y(I)-EST)**2)
00410      WRITE(4,35) X(I),EST
00420      28  CØNTINUE
00425      STDERR=SQRT(DIFF2/(N-3))
00430      35  FØRMAT(' X='F15.5,15X,' ESTIMATED VALUE='F15.5)
00435      WRITE(4,40) STDERR
00440      END

```

EXE SECØR.F4
LØADING

LØADER 5K CØRE
EXECUTIØN

*

SECØR.F4 (PARABØLIC FIT)

DATA AND RESULTS

\$
4

6./87.15/7./78.82/8./69.15
9./70.94

A= 259.38438
B= -43.77031
C= 2.52969

$$Y = 259.38438 - 43.77031 X + 2.52969 X^2$$

X=	6.00000	ESTIMATED VALUE=	87.83125
X=	7.00000	ESTIMATED VALUE=	76.94688
X=	8.00000	ESTIMATED VALUE=	71.12188
X=	9.00000	ESTIMATED VALUE=	70.35625
STANDARD ERROR OF THE ESTIMATE=		2.86387	

EXECUTIØN TIME: 0.23 SEC.
TOTAL ELAPSED TIME: 1 MIN. 9.52 SEC.
NO EXECUTIØN ERRØRS DETECTED

EXIT

APPENDIX No. 4

Information about SWMLR.SAV

[7000,303]

.LOG

JOB 14 CSM #12 5S02C.38 TTY16

#2700,324713

PASSWORD:

PURPOSE: CR700

1026 19-JUL-71 MON

.TYPE R0NR5R.F4

SWMLR.SAVE7000,3031 (DATA)

CORREL. OF R0NR5 WITH T, P, H2RC, WHSV,K

5 102

TEMP	PRESS	H2RC	WHSV	K	R0NR5
------	-------	------	------	---	-------

(6F)

850./20.4/5.1/41.670/11.44/93.01

900./20.4/5.1/25.002/11.44/94.99

950./20.4/5.1/12.501/11.44/95.25

1000./20.4/5.1/4.1671/11.44/92.44

900./13.6/5.1/25.002/11.44/94.85

900./27.2/5.1/25.002/11.44/94.13

900./34.0/5.1/12.501/11.44/90.71

900./20.4/4.25/25.002/11.44/95.07

900./20.4/5.95/25.002/11.44/94.9

900./20.4/6.80/25.002/11.44/94.8

900./20.4/5.1/18.750/11.44/94.42

900./20.4/5.1/37.500/11.44/95.61

900./20.4/5.1/31.260/11.44/95.4

900./20.4/5.1/37.503/11.44/95.47

900./20.4/5.1/29.169/11.44/95.21

950./13.6/5.1/12.501/11.44/94.97

1000./13.6/5.1/ 4.167/11.44/92.1

†0

RUN DSK:SWMLR.SAVE7000,304\4\3J
 *5=R0NR5R.F4 6=TTY:\$

RESULTS

CORREL. OF R0NR5 WITH T, P, H2RC, WHSV,K

NO. OF INDEPENDENT VARIABLES 5
 NUMBER OF OBSERVATIONS 102

PRELIMINARY ANALYSIS OF DATA

STANDARD DEVIATIONS AND MEANS

VAR NO.	VAR NAME	DEV	MEAN
1	TEMP	37.61991	914.70588
2	PRESS	4.68780	20.40000
3	H2RC	0.49742	5.20000
4	WHSV	10.72019	12.27643
5	K	0.15499	11.68333
6	R0NR5	2.78512	89.45745

CORRELATION COEFFICIENTS

TEMP	VS	PRESS	-0.34358
TEMP	VS	H2RC	-0.07934
TEMP	VS	WHSV	-0.40606
TEMP	VS	K	-0.00003
TEMP	VS	R0NR5	0.06726
PRESS	VS	H2RC	0.00001
PRESS	VS	WHSV	0.10607
PRESS	VS	K	0.00003
PRESS	VS	R0NR5	-0.00463
H2RC	VS	WHSV	0.00425
H2RC	VS	K	0.00010
H2RC	VS	R0NR5	0.00144
WHSV	VS	K	-0.55962
WHSV	VS	R0NR5	0.69657
K	VS	R0NR5	-0.65324

NUMBER OF INDEPENDENT
VARIABLES IN REGRESSION 3

DEGREES OF FREEDOM 98

COEFFICIENTS OF THE REGRESSION EQUATION

VAR NO.	VAR NAME	COEFFICIENT	STD ERROR	T TEST
1	TEMP	0.02562	0.00487	5.25587
4	WHSV	0.17836	0.02064	8.64219
5	K	-4.83464	1.30447	3.70622

CONSTANT TERM 120.32100

COEFFICIENT OF MULTIPLE DETERMINATION 0.67723

MULTIPLE CORRELATION COEFFICIENT 0.82294

STANDARD ERROR OF ESTIMATE 1.60634

F TEST 68.54121

APPENDIX No. 5

Linear Model Program

FIN.F4

FIN.F4 LISTING

```

00005      REAL K
00010      1 READ(4,20) LAG
00020      IF(LAG)50,50,60
00030      50 READ(4,21)T,P,H2RC,RMSV,K
00040      R0NR5= 120.321 +(0.02562*T)+(0.17836*RMSV)-(4.83464*K)
00050      PVR5= 119.78416 -(0.04779*T)-(0.19447*RMSV)+(2.11664*K)
00060      SGR5= 1.76135 +(0.00008*T)+(0.00065*RMSV)-(0.09177*K)
00070      RVPR5= -6.46297 +(0.00471*T)-(0.00381*P)+(0.00958*RMSV)
00080      1+(0.22408*K)
00090      PWH2= 5.53089 +(0.0039*T)+(0.00513*P)+(0.03641*RMSV)
00100      1 -(0.73946*K)
00110      PWC1= -4.04392 +(0.00316*T)-(0.0029*P)+(0.00607*RMSV)
00120      1 +(0.10938*K)
00130      PWC2= -7.57225 +(0.00593*T)-(0.00545*P)+(0.01139*RMSV)
00140      1 +(0.20451*K)
00142      PWC3= -11.04432 +(0.00867*T)-(0.00811*P)+(0.01662*RMSV)
00144      1 +(0.29658*K)
00146      PVNC4= -0.71487 -(0.0012*T)-(0.03689*P)+(0.56244*H2RC)
00148      PVIC4= 4.16136 -(0.002*T)-(0.04081*P)+(0.52875*H2RC)
00150      1 -(0.33253*K)
00160      WRITE(5,24)R0NR5,PVR5,SGR5,RVPR5,PWH2,PWC1,PWC2,PWC3
00170      1 ,PVNC4,PVIC4
00180      20 F0RMAT(I2)
00185      21 F0RMAT(5F)
00190      24 F0RMAT(' R0NR5='F6.2/' PVR5='F6.2/' SGR5='F7.5/' R
00200      1VPR5='F7.4/' PWH2='F6.4/' PWC1='F6.4/' PWC2='
00210      1F6.4/' PWC3='F6.4/' PVNC4='F6.4/' PVIC4='F6.4/)
00220      G0 T0 1
00230      60 ST0P
00240      END
00250
00260

```

FIN.F4 D.RESULTS

EXE FIN.F4
LOADING

LOADER 5K CORE
EXECUTION

*S

00

935./32.6/4.8/51.3/11.9

RØNR5= 95.89

PVR5= 90.31

SGR5=0.77743

RVPR5= 0.9747

PWH2=2.4129

PWC1=0.4292

PWC2=0.8126

PWC3=1.1797

PVNC4=-.3398

PVIC4=-.4582

00

850./13.6/5.1/46.7/11.44

RØNR5= 95.12

PVR5= 94.30

SGR5=0.80986

RVPR5= 0.4996

PWH2=2.1566

PWC1=0.1374

PWC2=0.2656

PWC3=0.3839

PVNC4=0.6319

PVIC4=0.7988

10

EXECUTION TIME: 0.20

TOTAL ELAPSED TIME: 3 MI.

62 SEC.

NØ EXECUTION ERRØRS DETECTED

EXIT

INPUT GUIDE

- First card: 00
- Second card: Number of nodes, number of reactor, with
Format I3
- Third card: Molar fractions of aromatics, paraffins,
naphthenes, molecular weight of the feed-
stock, API gravity of the feedstock
(Free Format)
- Fourth card: Hydrogen to hydrocarbon recycle ratio,
purity in hydrogen of the recycle
(Free Format)
- Fifth card: Temperature, pressure, pressure drop,
reciprocal molal space velocity for the
first reactor, with free format.
- Sixth card: Equal to fifth but for second reactor.
- Seventh card: Equal to fifth but for third reactor.
- Final card: -1

See an example on Page 71.

OUTPUT GUIDE

For each reactor a complete information on yields and properties is printed, with the name for each one.

See an example on Pages 71 to 74.