COMPUTER MODEL OF A HOMOGENEOUS
CONTINUOUS STIRRED
TANK REACTOR

By

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NOMENCLATURE

A	frequency factor
$\hat{a}_j$	activity of component j
C_j	concentration of component j, $lbmole/ft^3$
C_{Pj}	specific heat of component j, Btu/lbmole °F
C_{ij}	interaction parameter for components i and j
D_I	impeller diameter, inches
D_{ij}	interaction parameter for components i and j
E	activation energy, Btu/lbmole
F_j	molar flow rate of component j, lbmole/hr
F_c	factor to account for molecular shapes and polarities of dilute gases
$\hat{f}_j$	fugacity of component j
f_j°	fugacity of component j at the standard state
K	equilibrium constant
m	dipole moment, debyes
N_j	number of moles of reacting component j
P	system pressure
P_r	reduced pressure
Q	volumetric flow rate, ft^3/hr
QG	rate of heat generated, Btu/hr
QR	rate of heat removed or added, Btu/hr
R_j	rate of component j, $lbmole/ft^3$ hr
r_i	rate of reaction i, $lbmole/ft^3$ hr

T_o	inlet temperature, °F
T_c	critical temperature, °K
t	time, hr
V	reactor volume, ft^3
V^*	pure component characteristic volume
V_s	saturated liquid volume
V_c	critical volume, $cm^3/mole$
w	accentric factor
X_j	conversion of component j
x_j	mole fraction of component j
y_j	mole fraction of component j
Z	compressibility factor
ρ	density of stream, lbm/ft^3
τ	space time, hr
ΔG^o	Gibb's free energy of reaction
$-\Delta H$	heat of reaction, Btu/lbmole
v	viscocity collision integral
r	dimensionless dipole moment
ϕ_{ij}	interaction parameter
μ_m	viscosity of mixture
γ_j	activity coefficient of component j

CHAPTER I

INTRODUCTION

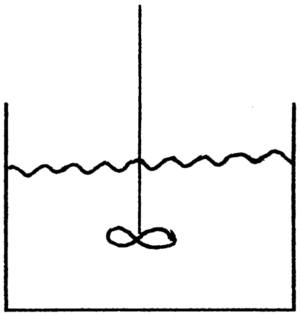
A mathematical model is a collection of equations that describes aspects of the behavior of a system being investigated. Generally, these equations are programed for solution by computer because this is the most convenient way of dealing with mathematical equations requiring numerical solution.

Much of today's industrial technology in petroleum refining, petrochemical processing and coal conversion centers around the use of chemical reactors. Due to the importance of chemical reactors in industry, simulation of these reactors has gained considerable attention. Mainly a reactor model is a set of mathematical relations describing the local production or consumption of chemicals, the physical properties of the chemicals, the thermodynamics of the system and the conservation laws. It is therefore important to summarize all the reactor information as mathematical expressions so that a proper optimization of the whole process can be achieved. This information can be used to simulate a full scale reactor or to improve the operation and control of an existing unit. A chemical reactor model can be available as one separate stand alone model or as one separate unit within a large simulator.

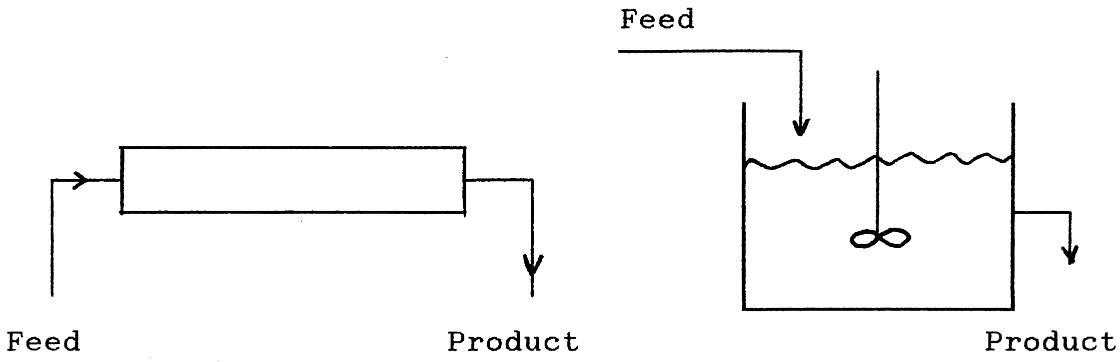
Developing a model demands a critical look at the system, the proposition of possible mechanisms and the comparison of importance of various steps occurring in the reactor. The model tests the possible mechanisms and reduces the number of possibilities. The discrepancies, which become evident during the fitting of the model, lead to changes in the mechanistic ideas. In this way modelling leads to a better understanding of the system (Rose, 1974).

Chemical reactors can be conveniently classified according to the method of operation. If there is not a continuous withdrawal of products and addition of reactants but instead a batch of reactants is added to the equipment at one time and the entire contents withdrawn at a subsequent time, the reaction system is termed batch or nonflow. Figure 1(a) depicts a batch reactor. This is an unsteady-state operation where composition changes with time; however, at any instant the composition throughout the reactor is uniform if the contents are well mixed.

The flow or continuous reactor is one in which products are removed continuously and reactants added continuously. A steady state flow reactor operates at steady state conditions. This means that there is no change in any of the properties of the reaction system with respect to time. The first of the two steady-state flow reactors is widely known by various names such as the plug flow, piston flow or an ideal tubular reactor, and is shown

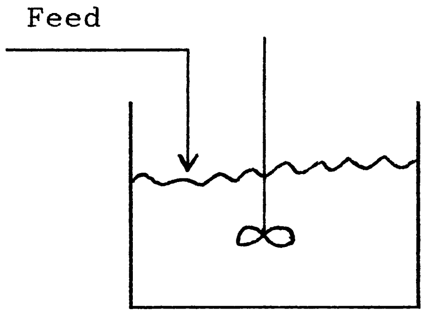


(a) Batch Reactor



(b) Plug Flow Reactor

(c) Continuous Stirred Tank Reactor (Steady State)



(d) Semi-Batch Reactor (Unsteady State)

Figure 1: The Types of Reactors

in Figure 1(b). Its main characteristic is the assumption of the absence of mixing or diffusion in the flow path. Therefore, the residence time in the reactor is the same for all fluid elements. The residence time is defined as the time required for a unit reactor volume to exit the reactor.

The other steady-state flow reactor is called the continuous stirred tank reactor (CSTR), or the backmix reactor, or the ideal stirred tank reactor. Figure 1(c) shows this kind of reactor. As the name indicates the contents are well mixed and uniform throughout. Thus the exit stream from this reactor has the same composition as the fluid within the reactor. In fact the most significant difference between batch and continuous flow reactors is that the temperature, pressure and composition may all vary with time in a batch operated system. Mathematically speaking, time is an independent variable in batch reactors. The corresponding variable in tubular flow reactors is position measured in the direction of flow in the reactor (Smith, 1956).

In some cases, the operation may be neither flow nor batch but a combination of the two. Such a case might be classified as a non steady state flow reactor or a semibatch reactor. Figure 1(d) shows such a reactor. The advantage of semi-batch operation is the possibility of maintaining a small concentration of one reactant at all times. This may be important when it is desired to obtain a predominant amount of one product out of several possibilities.

The purpose of this study is to simulate a homogeneous continuous stirred tank reactor which operates isothermally or adiabatically. The program is to be able to handle a maximum of twenty reacting or product components and fifteen reactions. The chemical reactions can be either elementary or non-elementary.

Once the model has been fully tested the user can use the model to do the following,

i) Design a new reactor for a given process.
ii) Evaluate the performance of an existing unit.
iii) Simulate a series of continuous stirred tank reactors.
iv) Estimate the power required for mixing.

CHAPTER II

LITERATURE REVIEW

Characteristics of a CSTR

The continuous stirred tank reactor consists of a well stirred tank into which there is a continuous flow of reacting material, and from which the partially reacted material passes continuously. It is because such vessels are squat in shape that good stirring of their contents is essential; otherwise there could occur a bulk streaming of the fluid between inlet and outlet and much of the volume of the vessels would be essentially dead space (Denbigh and Turner, 1984). With properly designed mechanical stirring equipment essentially complete mixing can be obtained. Efficient stirred tank reactors are difficult to construct for gaseous systems because of the mixing problem. However fixed baffles and mechanical stirrers can be used, although these do not ensure complete mixing in gaseous reaction mixtures (Smith, 1956).

An important characteristic of a CSTR is its stirring. The most appropriate first approximation to the estimation of its performance is based on the assumption that the contents are perfectly mixed. Under these conditions the mixing results in uniform composition, temperature and pressure throughout the reactor.

Advantages of a CSTR

The stirred tank reactor has certain advantages because of the uniform temperature, pressure and composition as a result of the mixing. First of all it is possible to operate such a reactor under isothermal conditions even when the heat of reaction is high. For example, when operation within a small temperature range is desired the opportunity for isothermal operation at the optimum temperature is a real advantage, in order to minimize side reactions or avoid unfavorable rates (Smith, 1956).

Another advantage of the tank flow reactor is the low cost of its construction. A particular advantage of the CSTR, apart from simplicity of construction, is the ease of temperature control. The reagents entering the first reactor plunge immediately into a large volume of partially reacted fluid and, because of the stirring, local hot spots do not tend to occur. Also the tanks offer the opportunity of providing a very large area of cooling surface. A further advantage is the openness of the construction. This makes it easy to clean the internal surfaces which is very important in some type of reactions (Denbigh and Turner, 1984).

It is often advantageous to have several CSTRs in series, the process stream flowing from one to the next. This results in a stepwise change in composition between successive tanks. This is the reason why it is usually necessary to use several tank reactors in series, especially if high conversion is required.

For these various reasons the typical fields of application of the CSTR are continuous processes such as sulphonation, nitration, polymerization, etc. CSTRs are used very extensively in the organic chemical industry and particularly in the production of plastics, explosives, synthetic rubber and so on. Certain gas phase reactions, e.g. combustion, chlorination of gaseous hydrocarbons, etc., are also sometimes carried out in reaction vessels which approximate to single stage CSTRs, although without having any mechanical stirring (Denbigh and Turner, 1984).

Design Equations

The design equation for a CSTR can be obtained from the material balance equation for any component j. Since the composition is uniform throughout, the accounting may be made about the reactor as a whole. A form of this equation is shown below (Levenspiel, 1972):

$$(-R_j)\,V = F_{j,o}\,(X_j - X_{j,o}) \tag{2.1}$$

where

R_j - rate of component j, lbmole/ft^3 hr

V - reactor volume, ft^3

$F_{j,o}$ - inlet molar flow rate of component j, lbmole/hr

$X_{j,o}$ - inlet conversion of component j

X_j - conversion of component j at exit

The space time, Γ , is an important design criterion and is defined as the time required to process one reactor volume of feed measured at specified conditions as presented in the equation below:

$$\Gamma = \frac{V}{Q} = \frac{C_{j,o}\ X_j}{-R_j} \qquad (2.2)$$

where

Q - inlet volumetric flow rate, ft^3/hr

$C_{j,o}$ - inlet concentration of component j, $lbmole/ft^3$

Mixing in a CSTR

Mixing is carried out in stirred tanks to meet a number of criteria. The incoming feeds must be well and quickly distributed in the bulk liquid. The whole reactor contents must be adequately mixed so that bypassing does not occur, and liquid in all parts of the reactor has the same residence time distribution and the same concentration. For certain high speed complex reactions particularly thorough mixing must be achieved to prevent local high concentrations. When the chemistry is complex, mixing is also more critical. Inadequate mixing of feeds can cause undesirable side reactions due to local concentration gradients. Mixing eliminates hot spots, so lower rates of reaction and correspondingly lower rates of heat generation can be obtained by operating at high outlet conversions. Thus temperature is easier to control (Rase, 1977).

Mixing can be done in standard vessels using agitators, and jet mixers can be used for fast reactions requiring only short contact time. Mixing devices such as tangential jets are usually used in gaseous systems in order to prevent localized high rates and explosions. One of the first principles in designing homogeneous CSTR systems is to select equipment and stirring procedures that will assure essentially perfect mixing. Of course the efficiency of stirring needs to be enhanced and the chemical literature abounds with useful hints: addition of baffles inside the reactor and employing a high speed paddle wheel stirrer appear to be effective and easy measures.

Recent studies on CSTRs showed that the rate of stirring can play a hitherto unsuspected role in the concentration inhomogeneities that are observed (Menzinger et al., 1986). A novel gas liquid stirred tank reactor is an example of a CSTR developed by Union Carbide in 1985 (Litz, 1985). The new design increases gas dissolution and chemical reaction rates and consumes less gas and power. It can be retrofitted into existing tanks.

CHAPTER III

DESIGN OF A CSTR

The CSTR is also called a backmix reactor or ideal stirred tank reactor. It is assumed that the contents of the tank are well mixed and the composition is uniform throughout the reactor. As a result the composition of the exiting stream is assumed to be the same as the fluid inside the reactor. Since steady state is assumed the mass rate of flow of feed and exit streams will be the same.

Material Balance

By performing a component j material balance over the whole reactor,

In - Out ± Generation = Accumulation

For a CSTR we get (Froment and Bischoff, 1979),

$$F_{j,o} - F_{j,e} + R_j * V = \frac{dN_j}{dt} \qquad (3.1)$$

Subscripts o and e refer to inlet and outlet streams respectively.

At steady state the accumulation term vanishes, giving,

$$F_{j,o} - F_{j,e} + R_j * V = 0 \qquad (3.2)$$

where

F_j - molar flow rate of component j, lbmole/hr

R_j - rate of component j, lbmole/ft^{3}hr.

Numerical Method

If the equation above is written for n components we get n non-linear simultaneous equations in n unknowns which can be solved using numerical methods.

Newton Raphson's method has been used for solving these equations. The linear equation solver package LINPAC was used for this purpose (Riggs, 1988).

Energy Balance

For non-isothermal operations we also need to consider the energy balance, which for a CSTR is as follows:

In - Out ± Generation = Accumulation

At steady state we get,

$$F_j * C_{P,j} * (T_o - T) + V * (\sum (-\Delta H_i) * r_i) + Q(T) = 0 \qquad (3.3)$$

where

T - temperature, °F

$C_{P,j}$ - specific heat of component j, Btu/lbmole °F

r_i - rate of reaction i, lbmole/ft^3 hr

H_i - heat of reaction i, Btu/lbmole

Q(T) - external heat addition or removal from reactor (e.g. $A*U*(T-T_s)$, where U and A are the heat transfer coefficient and area, T_s is the temperature of the surroundings.)

For adiabatic operation,

$$F_j*C_{P,j}*(T_o-T) + V*(\sum(-\Delta H_i)*r_i) = 0 \qquad (3.4)$$

This (n+1)th equation can be solved with the other equations using Newton Raphson's method.

Reaction Kinetics

The rate constant of a reaction is given by,

$$k = A * \exp(-E/RT) \qquad (3.5)$$

where

A - frequency factor , lbmole/ft^{3}hr

E - activation energy , Btu/lbmole

The rate expression is usually given in lbmole/ft^{3}hr.

Irreversible Reactions

For general kinetics the rate expression is,

$$r_i = A * \exp(-E/RT) * C_1^{\delta_1} * C_2^{\delta_2} * \circ\circ\circ * C_n^{\delta_n} \qquad (3.6)$$

The concentration of any component j, C_j, can be expressed as,

$$C_j = F_j/Q \qquad (3.7)$$

Substituting this value in equation (3.6) for each of the components we get,

$$r_i \;= A * \exp(-E/RT) * \left(\frac{F_1}{Q}\right)^{\delta_1} * \left(\frac{F_2}{Q}\right)^{\delta_2} * \;\circ\circ\circ\; * \left(\frac{F_n}{Q}\right)^{\delta_n} \qquad (3.8)$$

Rearranging the terms we get,

$$r_i \;= A * \exp(-E/RT) * \frac{(F_1^{\delta_1} * F_2^{\delta_2} * \;\circ\circ * F_n^{\delta_n})}{(Q^{\delta_1 + \delta_2 + \cdots\cdots + \delta_n})} \text{ lbmole/ft}^3\text{hr} \qquad (3.9)$$

Reversible Reactions

The chemical equilibrium constant, K, is generally related to the activities of the species in solution by the relation,

$$K = \prod_{j=1}^{n} (\;\hat{a}_j\;)^{\delta} \qquad (3.10)$$

where

$\hat{a}_j$ - activity of component j

For gas phase reactions,

$$\hat{a}_j \;= \frac{\hat{f}_j}{f_j^{\circ}} \qquad (3.11)$$

where

$\hat{f}_j$ - fugacity of component j

f_j° - fugacity of component j at the standard state

For a gas the standard state is the ideal gas state of pure component, j, at a pressure of 1 bar. Since the fugacity of an ideal gas is equal to pressure, f_j is set to unity for each component. Therefore from equations (3.10), and (3.11) we get,

$$K = \Pi (\hat{f}_j)^{\delta} \quad (3.12)$$

The fugacity is related to the fugacity coefficients by the relation,

$$\hat{f}_j = \hat{\phi}_j \ y_j \ P \quad (3.13)$$

where

P - system pressure

y_j - mole fraction of component j

$\hat{\phi}_j$ - fugacity coefficient of component j in mixture

Substituting this in equation (3.12) we get,

$$K * P^{-\delta} = \prod_{j=1}^{n} (y_j * \hat{\phi}_j)^{\delta_j} \quad (3.14)$$

Assuming ideal gas behavior the fugacity coefficients are set to one and we get,

$$K * P^{-\delta} = \prod_{j=1}^{n} (y_j)^{\delta_j} \quad (3.15)$$

where

δ - sum of the stoichiometric coefficients in the mixture

δ_j - stoichiometric coefficient of component j

If the mole fractions are expressed in terms of molar flow rates, we get,

$$K * P^{-\delta} (\Sigma F_j)^{\delta} - \prod_{j=1}^{n} F_j{}^{\delta_j} = 0 \quad (3.16)$$

For 1 ft^3 of the reactor we can express the component molar flow rates in the above equation as follows,

$$F_j = (F_{j,o}) + \delta_j * r_i \qquad (3.17)$$

Substituting this in equation (3.16) we can formulate the equilibrium criterion.

$$KP^{-\delta} \, (\Sigma[(F_{j,o} + \delta_j \, r_i])^{\delta} - \prod_{j=1}^{n} [(F_{j,o}) + \delta_j \, r_i]^{\delta_j} = 0 \qquad (3.18)$$

Equation (3.18) shows the equilibrium criterion for gas phase reactions.

For liquids the activity is expressed as,

$$a_j = \frac{\gamma_j \, x_j \, f_j}{f_j^{o}} \qquad (3.19)$$

Except for very high pressures, the ratio $f_j \,/\, f_j^{o}$ is taken as unity (Smith and Van Ness, 1987), and we get,

$$a_j = \gamma_j \, x_j \qquad (3.20)$$

Substituting in equation (3.10) we get,

$$K = \quad (x_j \, \gamma_j)^{\delta_j} \qquad (3.21)$$

Assuming the equilibrium mixture is an ideal solution, all the activity coefficients are set to one and we get,

$$K = \prod (x_j)^{\delta_j} \qquad (3.22)$$

If the mole fractions are expressed in terms of molar flow rates, we get

$$K \quad (\Sigma F_j)^{\delta} - \prod_{j=1}^{n} F_j^{\delta_j} = 0 \qquad (3.23)$$

For 1 ft^3 of the reactor we can express the component molar flow rates in the above equation as follows,

$$F_j = (F_{j,o}) + \delta_j * r_i \qquad (3.24)$$

Substituting this in equation (3.23) we can formulate the equilibrium criterion for liquid phase reactions.

$$K \ (\Sigma[(F_{j,o} + \delta_j \ r_i] \ )^{\delta} - \prod_{j=1}^{n} [(F_{j,o}) + \delta_j \ r_i]^{\delta_j} = 0 \qquad (3.25)$$

Equation (3.25) shows the equilibrium criterion for liquid phase reactions.

The chemical equilibrium constant in equations (3.18), and (3.25) can be expressed as a function of the standard Gibb's free energy of reaction, ΔG^o, as follows,

$$\ln K = - \frac{\Delta G^o}{R*T} \qquad (3.26)$$

where R is the ideal gas constant.

The above equation has been used to calculate the equilibrium constant at the reference temperature of 25°C, corresponding to the Gibb's free energy. Then Van Hoff's law is used to determine the equilibrium constant at any specified temperature T .

$$\ln \frac{K}{K_o} = - \frac{\Delta H}{R}\left(\frac{1}{T} - \frac{1}{T_o}\right) \qquad (3.27)$$

where the heat of reaction, ΔH, has been assumed to be independent of temperature.

After the value of the equilibrium constant has been calculated the only unknown remaining in equations (3.18) and (3.25) is the rate of the equilibrium reaction. In essence solving the equilibrium criterion is dependent on finding a numerical method to solve for the function f(x) = 0. The obvious method is the successive substitution method. This method has the advantage of hitting every root of the function. However, this method could be very slow in some cases, especially if the increment chosen is very small. Another method, called the bisection method, can be used to speed up the root finding task by evaluating the function at a lower and an upper limit, and comparing the respective signs. If there exists a sign change, the routine recognizes the existence of a root in between the limits, and therefore hunts for the zeros of the function. Obviously, such a method can diverge in some cases. In general the choice between such methods depends strongly on the problem at hand.

For this task a few observations can be made in order to facilitate the choice. In most cases four types of reactions in equilibrium are encountered:

A = B

A = B + C

A + B = C

A + B = C + D

All these reactions yield to an equilibrium criterion which is reasonably easy to solve. Also the bisection method is faster than the successive substitution method. Therefore the bisection method has been used in this work to solve for the equilibrium criterion.

Exothermic Reactions in a CSTR

For exothermic reactions in a CSTR an interesting situation may develop in that more than one reactor composition may satisfy the governing material and energy balance equations. This means that we may not know which conversion level to expect.

The general material balance for a CSTR can be used to define the rate of heat generated, QG, (Rase, 1977) given by

$$QG = (-\Delta H_i)(r_i)V \tag{3.28}$$

If this total rate of heat generation is plotted against temperature, T, for fixed values of the component feed rates to the reactor, then the curve will be seen to have the sigmoid shape, due to opposing effects of increased rate constant and diminished concentration of the components. At a high enough value of T the rate constant is so great that virtually no unreacted reagent remains in the outflow from the system and that a still higher value of T cannot make QG significantly greater, with the consequence that the curve must flatten off.

In contrast to the exponential character of the heat generation curve, the heat absorption or removal curve (QR) is linear, for constant C_P, for an adiabatic reactor.

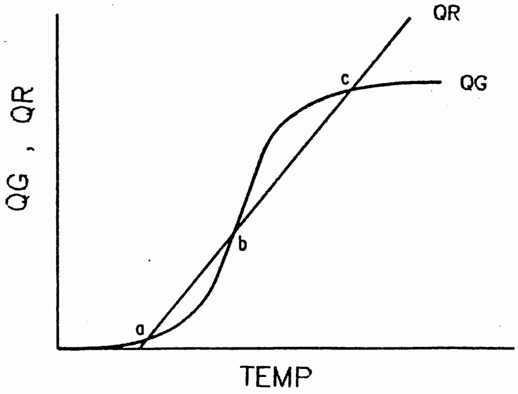
$$QR = \sum F_j \; C_{P,j} \; (T - T_o) \qquad (3.29)$$

It can be seen that the above equation is a linear function of T and thus, if QR is plotted against T, we get a straight line with a gradient.

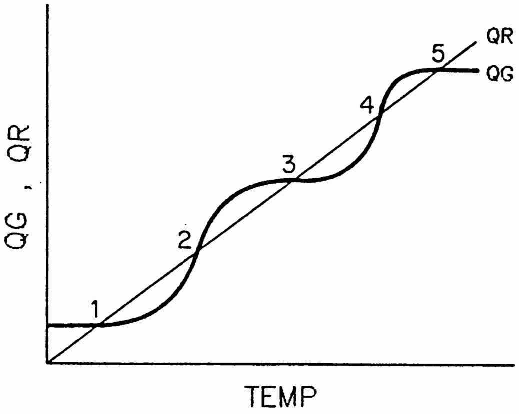
If a steady state is to occur in the system (i.e., a condition such that its temperature is neither rising nor falling), QG and QR must be equal. Steady states are thus represented by points of intersection of the heat generation curve with the heat removal line.

It is observed that for one irreversible exothermic reaction occurring in a CSTR there may be as many as three steady states as shown in Figure 2 (a) (Rase, 1977). The QG and QR curves in the figure intersect at three points indicating the existence of three possible steady states, one of which, point b is unstable. A slight change in temperature at point b will cause the system to move to one or the other steady steady states. For example, if the temperature increases slightly, QG becomes greater than QR, and the system heats up to the stable point c. It is stable because an increase in temperature will cause the removal rate to increase above the generation rate, and the system will return to c.

A decline in temperature at point b will force the



(a) Heat Generation and Heat Removal Curves for One Exothermic Reaction



(b) Heat Generation and Removal Curves with Series or Parallel reactions

Figure 2: Multiple Steady States in a CSTR

system to the other stable point a, for QR is greater than QG below b and the system will cool to point a.

The multiple steady states occur over a short range of inlet temperatures. Thus in order to avoid the multiple steady states, the inlet temperature to the reactor should be decreased or increased depending on the conversion level required.

When multiple reactions occur, more than three steady states are possible. Figure 2 (b) shows such a case when two reactions are occurring simultaneously (Fogler, 1986). Five steady states are possible in this case: three stable ones (points 1, 3, and 5) and two unstable ones (points 2, and 4)

Thus it is necessary, while designing a CSTR, to see if the steady state solution obtained is a stable one and also the stable solution desired.

Power Requirements for Mixing

An important consideration in the design of a CSTR is the power required to drive the impeller. To estimate the power required to rotate a given impeller at a given speed, empirical correlations of power (or power number) with the other variables of the system are needed. The number of baffles and the number of blades in the impeller are fixed. The variables that then enter the analysis are the important measurements of tank and impeller, the viscosity, μ, the density, ρ, and the speed, N (McCabe et al., 1985).

The power required is calculated from the power number, N_P, which is given by,

$$N_P = P\, g_c \,/\, N^3\, D_I{}^5\, \rho \qquad (3.17)$$

where

P - power required for mixing,

D_I - impeller diameter,

g_c - gravitational acceleration constant.

The power number in turn is calculated from the impeller Reynold's number given by,

$$(N_{Re})_I = D_I{}^2\, \rho\, N \,/\, \mu \qquad (3.18)$$

Power numbers are usually determined from the impeller Reynold's number using either the graphs available (Rase, 1977, McCabe et al., 1985) or typical manufacturers correlations. Manufacturers's data, which has been used in this work, are preferred for a turbine or propeller.

Reactors in Series and Parallel

Many times reactors are connected in series such that the exit stream from one reactor is the feed stream for the next reactor. When this occurs it is often possible to speed the calculations by defining the conversion in terms of location at a point downstream rather with respect to any one reactor. However, this definition can be used only if there are no side streams withdrawn and the feed stream enters only the first reactor in series. It is observed that the operation of CSTRs in parallel, assuming equal space time per reactor, gives the same conversion as a single reactor but increases the throughput or capacity proportional to the number of reactors.

This is not the case for multiple reactors in series. CSTRs operated in series approach plug flow and therefore higher conversion is achieved (Foutch and Johannes, 1987).

Recycle Considerations

It is sometimes desired to divide the reactor product stream and return a portion of it to the entrance of the reactor. In this case the recycle ratio, R, is defined as,

$$R = \frac{\text{volume of fluid returned to the reactor entrance}}{\text{volume leaving the system}}$$

For a stirred tank reactor, recycle has no effect on conversion, since we, essentially, are just mixing a mixed reactor.

CHAPTER IV

THE MODEL DESCRIPTION

Introduction

This model simulates a homogeneous continuous stirred tank reactor. A maximum of twenty reacting or product components and fifteen reactions is allowed. If needed, the introduction of more reactions and components is just a matter of changing the sizes of a few arrays. The program has been coded in such a way that it is easy to include models of other types of reactors such as batch, plug flow, or catalytic reactors. An effort was made to simplify the work of the user, but good preparation and organization are highly recommended. The general structure of this model consists of an input subroutine, a calculation routine and an output file. Appendix A contains the logic structures for the different subroutines in the program. The computer code which is written in FORTRAN is listed in Appendix H and a sample of the input and output data is shown in Appendix G.

Input Description

First the inlet and outlet stream numbers are specified. If more than one inlet or outlet stream is specified an error message will be prompted. The number of reactions and the number of components is entered next. It is necessary to fix the sequence number of the reactions and the components beforehand. Each of the components has a component identification number (I.D. number) and the list of the different component I.D. numbers is given in Table I. The sequence number of the components is different from that of their I.D. numbers. The user is next asked to specify the component I.D. numbers and the inlet flow rates of the various components. The mode of operation is entered next. Both isothermal and adiabatic operations are available to the user. The inlet temperature and pressure are then entered. The pressure drop is the next specification to be entered. In this case the user has a choice of specifying the outlet temperature or the pressure drop across the reactor. Then the kinetic input is asked for. The user has to specify whether each of the reactions is reversible or irreversible. The frequency factor and the activation energy for the irreversible reactions and the Gibb's free energy for the reversible reactions are entered. If the mode of operation is adiabatic the standard heats of the reactions at a reference temperature of 25°C will have to be entered. The stoichiometric coefficients and component powers in the rate expression are entered next. For inerts, the stoichiometric coefficient and order of the component are

TABLE I

COMPONENT I.D. NUMBERS

Component Name	Comp. I.D. Nos.	Symbol
Hydrogen	1	H2
Methane	2	CH4
Ethane	3	C2H6
Propane	4	C3H8
iso-butane	5	I-C4H10
n-Butane	6	N-C4H10
iso-Pentane	7	I-C5H12
n-Penatne	8	N-C5H12
neo-Pentane	9	NEO-C5
n-Hexane	10	N-C6H14
n-Heptane	11	N-C7H16
n-Octane	12	N-C8H18
n-Nonane	13	N-C9H20
n-Decane	14	N-C10H22
n-Undecane	15	N-C11H24
n-Dodecane	16	N-C12H26
n-Tridecane	17	N-C13H28
n-Tetradecane	18	N-C14H30
n-Pentadecane	19	N-C15H32
n-Hexadecane	20	N-C16H34
n-Heptadecane	21	N-C17H36
Ethylene	22	C2H4=
Propylene	23	C3H6=
1-Butene	24	1-C4H8
cis-2-Butene	25	C-2-C4H8
trans-2-Butene	26	T-2-C4H8
iso-Butene	27	I-C4H8
1,3 Butadiene	28	1,3-C4==
1-Pentene	29	1-C5H10
cis-2-Pentene	30	C-2-C5=
trans-2-Pentene	31	T-2-C5=
2-Methyl-1-Butene	32	2MT-1C4=
3-Methyl-1-Butene	33	3MT-1C4=
2-Methyl-2-Butene	34	2MT-2C4=
1-Hexene	35	C6H12=
Cyclopentane	36	CYC-C5
Methylcyclopentane	37	MTCYC-C5
Cyclohexane	38	CYC-C6
Methylcyclohexane	39	MTCYC-C6
Benzene	40	C6H6
Toluene	41	C7H8
o-Xylene	42	O-X
m-Xylene	43	M-X
p-Xylene	44	P-X
Ethylbenzene	45	EB
Nitrogen	46	N2

TABLE I (Continued)

Component Name	Comp. I.D. nos.	Symbol
Oxygen	47	O2
Carbon Monoxide	48	CO
Carbon Dioxide	49	CO2
Hydrogen Sulphide	50	H2S
Sulphur Dioxide	51	SO2
2-methyl-Pentane	52	2-MT-C5
3-methyl-Pentane	53	3-MT-C5
1-Heptene	54	1-C7H14=
Propadiene	55	C3H4==
1,2, Butadiene	56	1,2-C4==
Ethylcyclopentane	57	ETCYC-C5
Ethylcyclohexane	58	ETCYC-C6
Propylene oxide	59	C3H60
Propylene glycol	60	C3H8O2
Water	61	H20
Methanol	62	CH4O

both entered as zero. Once all the information about the kinetics is fully specified, the user has to specify that the type of fluid being handled is either a vapor or a liquid. Depending on this the user will have to specify the type of equation to use for physical property predictions. The user has a choice for gaseous operation among the Redlich-Kwong, Soave-Redlich-Kwong and the Peng-Robinson equations of state (Reid et al., 1987). For liquid operation the user has to specify the Hankinson Thomson method for density predictions (Reid et al., 1987). Since the power requirements for mixing are estimated by the program the user will have to specify the RPM of the stirrer to use.

The Convergence Criteria

Three types of convergence criteria are available to the user. The reactor volume can be fixed if the performance of an installed reactor is to be tested. In a few cases, to avoid overheating or freezing, the user might want to specify an upper or lower limit on the exit temperature as a convergence criterion. But usually, the user is interested in determining the rector size required to produce a desired yield of a certain component of interest. In this case, the sequence number of the component and outlet molar flow rate of the component can be specified to set the convergence criterion.

The initial guesses for the outlet molar flow rates, reactor volume, or outlet temperature will have to be given depending on the mode of operation and the convergence criterion chosen. Initial guesses can be very important for convergence to the proper solution in some cases.

Running a Series of Reactors

After the run is over the user will be given an option of making another run or exiting the program. If the user wants to make another run the type of run has to be specified, i.e, whether the reactor is to be run in series or a new run is to be made. If the reactor is to be run in series the user has to just specify the pressure drop across the next reactor, the convergence criterion in the next reactor, and the initial guesses.

Checking the Stability of the Steady State

For exothermic reactions there is a possibility of obtaining multiple steady states. The steady state obtained can be unstable. The model incorporates a method of checking for the stability of the steady state. This is done as follows,

Step I: First the run is made with the specified reactor volume and inlet temperature, following which the outlet conditions are viewed.

Step II: In order to check for the stability of this steady state, additional runs are made specifying the same reactor volume and the inlet temperature. However in this case a different outlet temperature is also specified for each run. Following this the QG and QR values are plotted against each of the temperatures. By viewing the plot the user can determine the stability of the steady state.

The values of QG and QR at the different outlet temperatures are obtained from a separate output file (HEAT.OUT) for the user.

Calculation Subroutines

Flow charts describing the following subroutines are included in Appendix A.

Subroutine STRFLOW:

This subroutine calculates the volumetric flow rate of the stream, Q, from the component molar flow rates, F_j, their molecular weights, and the calculated value of stream density as follows,

$$Q = \quad (F_j \; MW_j) \; / \; \rho \qquad (4.1)$$

where,

MW_j = molecular weight of component j, lbm/lbmole

ρ = density of stream, lbm/ft^3

Subroutine RATEC:

This subroutine calculates the rate constants of the reactions as a function of temperature, T, using the inputs of frequency factor and activation energy in the rate expressions.

Subroutine RATERN:

Using the stoichiometric coefficients and the order of each component with respect to each reaction, and using the calculated value of the rate constants from RATEC, this routine calculates the rate of various reactions. If there are reversible reactions the call for the subroutine to test the equilibrium criterion is given from this subroutine.

Subroutine RATECOMP:

Once the rate of all the reactions are determined, the outlet composition is easily computed considering the changes due to each reaction for each component.

This subroutine sums up the change of each component in all the reactions. This is done by multiplying the rates of the reactions by the respective stoichiometric coefficients of the components, then summing the calculated changes for each component.

Subroutine EQURN:

This subroutine uses the bisection method to solve for the rate of the reactions in equilibrium. Each time a value of the rate of the reaction is picked up, a call is then given to the subroutine EQURATE to see if the equilibrium criterion is satisfied. If it has been satisfied, then the value of the reaction rate is sent to subroutine RATERN, otherwise a new guess is made using the bisection method and the equilibrium criterion is tested till it is satisfied.

Subroutine EQURATE:

This subroutine sets up the equilibrium criterion for the reactions in equilibrium. In this routine the equilibrium constant at the temperature, T_o, is first calculated using the input Gibb's free energy value of the reaction at a reference temperature, T_o. Then Van Hoff's law along with the average heat of the reaction is used to determine the equilibrium constant at the specified temperature, T. Next using the system pressure, component flow rates and their stoichiometric coefficients, and the guess of the rate of the reaction from subroutine EQURN the equilibrium criterion is set up.

Subroutine TEMPDIF:

The change between the inlet and outlet temperature is a function of the rate of each reaction, the heat of the reaction, the molar flow rate of each component and its specific heat, and the reactor volume. The difference in temperatures is calculated by this subroutine. The values of QG (heat generated) and QR (heat added or removed) are generated from the calculations made in this subroutine.

The heat generated, QG, is given by,

$$QG = V \sum r_i \, (-\Delta H_i) \tag{4.2}$$

The heat added, QR, (for adiabatic operation) is given by,

$$QR = \sum F_j \, C_{P,j} \, (T - T_o) \tag{4.3}$$

For an exothermic reaction it is better to plot QG and QR at various outlet temperatures in order to know the stability of the steady state obtained by calculations.

Subroutine EQUATN:

This subroutine is the main calculation subroutine. The calls to the different subroutines mentioned earlier are given in the proper order from this subroutine. The function of this subroutine is setting up the equations to be solved. The subroutines STRRFLOW, RATEC, RATERN, RATECOMP and TEMPDIF are called in that order to set up these equations.

Subroutine NEWTON:

The calls to subroutine EQUATN, DER, and LINPAC are made from this subroutine. This subroutine uses Newton's method to solve for the n non-linear equations containing n unknowns generated by the subroutine EQUATN. In order to implement Newton's method, the Jacobian (the partial derivatives of each equation with respect to each variable) must be generated. This is done by the subroutine DER.

This subroutine then uses the values of the functions and the values of the partial derivatives of the function in order to develop a system of linear equations. The call is then made to LINPAC to solve the system of linear equations

Subroutine POWER:

In order to calculate the power required it was necessary to fix the type of agitator to use. For this work a six bladed turbine has been selected. This was mainly because it is used for a wide range of applications (Rase, 1977) and over a large range of reactor volumes.

The diameter of the tank is first selected depending on the required reactor volume for the process being studied. From this the diameter of the turbine is calculated. The ratios of impeller-to-tank-diameter recommended and generally used are,

Large tanks (over 200 gallons): 0.25-0.33
Small tanks (under 200 gallons): 0.33-0.5

Usually the upper limit in each case is used. After this, the impeller Reynold's number is calculated. The power number is calculated on the basis of the manufacturer's correlation. Finally the power required, P, (in hp) is calculated using the manufacturer's correlation (Rase, 1977),

$$P = 3.52E\text{-}03 * N_P\ (\rho/62.4)\ (N/60)^3\ (D_I/12)^5 + 0.5 \qquad (4.4)$$

Output Description

The subroutine OUTPUT uses all the input and the calculations done to give an output file. The type of operation and the conversion criteria are first listed. The reactions occurring in the reactor are then displayed with the component names shown as reactants and/or products. The order and stoichiometric coefficients of the components in the reactions are then listed. The inlet and outlet streams and their properties are listed next. Finally the reactor volume required and the power required for mixing are displayed.

CHAPTER V

DISCUSSION OF RESULTS

Since the model can be used for a homogeneous CSTR, two test cases are considered. The first case studied was the gaseous reaction of hydrodealkylation of toluene to produce benzene. The second case studied was a liquid phase reaction for production of propylene glycol from propylene oxide.

Process Description

Case I:

The hydrodealkylation of toluene to form benzene was the first test case considered. The thermal hydrodealkylation of toluene is found to be a low cost route to produce benzene. The feed to the process is toluene and hydrogen already in existence at most refineries. In this method, the toluene and hydrogen are heated to a high temperature where a chemical reaction takes place to produce benzene, methane and some other by-products. The benzene can be separated from these by-products and the unreacted toluene by a series of flash vessels and a distillation column.

Along with the major reaction of toluene with hydrogen, many side reactions occur.

Toluene + Hydrogen -----> Benzene + Methane (5.1)

Xylenes + Hydrogen -----> Toluene + Methane (5.2)

Ethyl benzene + Hydrogen ----> Benzene + Ethane (5.3)

2 Benzene = Diphenyl + Hydrogen (5.4)

The two major reactions considered in the simulation of the reactor are the following,

Toluene + Hydrogen -----> Benzene + Methane (5.5)

O-Xylene + Hydrogen -----> Toluene + Methane (5.6)

The second reaction usually lowers the conversion in the reactor.

<u>Pressure</u>: An operating pressure around 500 psia is chosen to keep the hydrogen partial pressure high enough to achieve high conversion.

<u>Temperature</u>: Pilot plant data (Feigelman et. al., Fowle and Pitts) suggest operating temperatures in the range of 1150-1350^{0}F. This is the range which has been mainly investigated. A maximum design temperature of 1500^{0}F is usually set with something in the neighborhood of 1400^{0}F being a normal operating limit (Rase,1977).

<u>Feed conditions</u>: The total amounts of by-products

formed is inversely proportional to the hydrogen-to-toluene ratio (Zimmerman and York, 1964). Higher values of hydrogen-to-toluene ratio also prevents coking in the reactor. Therefore a range of hydrogen-to-toluene ratio from 2-5 has been used. The feed to the reactor consists predominantly of hydrogen and toluene with a trace of o-xylene.

The rate data for the two reactions is given in Table II. The table also includes the heats of reactions for the two reactions. Both the reactions are exothermic.

Case 2:

The second case considered was the liquid phase reaction of the hydrolysis of propylene oxide to produce propylene glycol. The reaction is given below (Fogler, 1986),

Propylene Oxide + Water -----> Propylene Glycol

The input feed to the reactor consists of an equivolumetric mixture of propylene oxide and methanol along with water containing 0.1 wt% sulfuric acid. The sulfuric acid acts as a catalyst in the process. The volumetric flow rate of water is about 2.5 times the methanol-propylene oxide flow rate.

The molar feed rate to the reaction is as follows

Propylene oxide -- 43.03

Propylene glycol -- 0.0

TABLE II

RATE DATA FOR HYDRODEALKYLATION OF TOLUENE

Reaction 1: Toluene + Hydrogen ---> Benzene + Methane

$k = 2.58\ E{+}15\ EXP\ (-94100.0/RT)\ (ft^3)^{0.5}/(lbmole)^{0.5}\ hr$

Heat of reaction = -18032.92* Btu/lbmole

Reaction 2: O-Xylene + Hydrogen ---> Toluene + Methane

$k = 3.626\ E{+}15\ EXP\ (-96015.0/RT)\ (ft^3)^{0.5}/(lbmole)^{0.5}\ hr$

Heat of reaction = -18860.87* Btu/lbmole

---

* - heat of reaction at reference temperature of 25°C

Water -- 802.8

Methanol -- 71.87

Molar feed rates are in lbmole/hr.

The temperature of both streams is 58^{0}F prior to mixing, but there is an immediate rise of 17^{0}F in the temperature upon mixing of the two feedstreams caused by the heat of mixing. The entering temperature of feed has thus been taken as 75^{0}F for most of the runs.

Furusawa et al.,1969, state that under conditions similar to these, the reaction is first order in propylene oxide concentration.

Also, the frequency factor is 16.96×10^{12} hr^{-1}, and the activation energy is 32400.0 Btu/lbmole. The reaction is an irreversible exothermic reaction with heat of reaction of -36,400 Btu/lbmole.

Model Testing

Three convergence criteria and two operation modes are available to the user, for testing the performance of the model. Appendix B contains outputs of several runs testing the three convergence criteria (reactor volume, outlet temperature, and the production rate of a specified component) and the two operation modes (adiabatic and isothermal). The runs have been made under the following conditions.

Case I

Adiabatic operation

1) The production rate of benzene is 200 lbmole/hr
2) The specified outlet temperature is 1400°F
3) The specified reactor volume is 250 ft^3.
4) The specified reactor volume is 250 ft^3 and the hydrogen-to-toluene ratio is 4.
5) The specified reactor volume is 250 ft^3 and the hydrogen-to-toluene ratio is 5.

Isothermal operation

6) The specified reactor volume is 400 ft^3.
7) The production rate of benzene is 172 lbmole/hr

Case II

Adiabatic Operation

8) The specified reactor volume is 40 ft^3
9) The specified outlet temperature is 125°F
10) The outlet flow rate of propylene glycol is 4.3 lbmole/hr

Isothermal Operation

11) The production rate of propylene glycol is 30 lbmole/hr
12) The specified reactor volume is 120 ft^3

Checking the Stability of the Steady State

The model also includes a method for checking the stability of the steady state obtained for adiabatic operation in the reactor when an irreversible exothermic reaction is occurring in the reactor. In order to check this QG (heat generated) and QR (heat removed or added) are plotted against temperature in the reactor to see if the steady state solution obtained is a stable one and the one that is desired. This needs to be checked since there is a possibility of hitting a stable steady state with a low conversion or an unstable steady state along with the preferred stable steady state.

This is done in two steps. First a normal run is made specifying the reactor volume for the adiabatic operation. This gives a certain steady state solution. The next step involves carrying out several runs in which the same reactor volume and inlet temperature are specified and the outlet temperature is varied. The values of QG and QR for all the runs is obtained in a separate file HEAT.OUT along with the corresponding outlet temperatures. ORT in the output file is the outlet reactor temperature. A graph of QG and QR versus temperature is then drawn to check the stability of the steady state.

This procedure has been illustrated considering the two test cases.

Case I

Step I: First the run for reactor volume of 500 ft^3 and inlet temperature of 1200°F was made. The result shows that steady state is achieved at a temperature of 1431.90°F. Table III shows this result.

Step II: In order to check the stability of this steady state, several runs specifying reactor volume of 500 ft^3 and an inlet temperature of 1200°F for each were made. However in this case the outlet temperature was also specified in each run. The QG and QR values at different specified outlet temperatures are shown in Table IV. A plot of QG and QR versus temperature is shown in Figure 2. As can be seen from the plot the steady state solution obtained is a stable one.

Case II

Step I: When the run with reactor volume equal to 40 ft^3 was made a steady state was observed at a temperature of 151.30°F. Table V shows this result.

Step II: Several runs were made with reactor volume equal to 40 ft^3 and inlet temperature of 75°F. The QG and QR values obtained are given in Table VI. A plot of QG and QR versus temperature is seen in Figure 3. The plot shows that the steady state solution obtained is indeed a stable one.

TABLE III

OUTPUT TO FIND THE STEADY STATE FOR HYDRODEALKYLATION OF TOLUENE

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =     500.00  FT3


H2         +  C7H8        ->   CH4        +  C6H6


 RXN.   COMP. NAME   ORDER   STOICH.

   1    H2             0.50    -1.00
   1    CH4            0.00     1.00
   1    C6H6           0.00     1.00
   1    C7H8           1.00    -1.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.         1           2
   NAME           FEED 1      PROD. 1
 COMPONENT
 H2              450.000     229.013
 CH4               0.000     220.987
 C6H6              0.000     220.987
 C7H8            233.000      12.013

   TOTAL         683.000     683.000

 T,DEG F         1200.00     1431.90
 P,PSIA           495.00      490.00
 MOL WEIGHT      32.7614     32.7614
 D,LB/FT3         0.8879      0.7765
 L/F(MOLAR)       0.0000      0.0000


 VOLUMETRIC FLOW RATE =  28817.78  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.16  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =  500.00  FT3
```

TABLE IV

QG AND QR VALUES FOR THE PROCESS OF HYDRODEALKYLATION OF TOLUENE

```
ORT= 1200.00  QG= 0.175898E+07  QR=   0.000000
ORT= 1230.00  QG= 0.224941E+07  QR=    515537.
ORT= 1260.00  QG= 0.270871E+07  QR= 0.103107E+07
ORT= 1290.00  QG= 0.310220E+07  QR= 0.154661E+07
ORT= 1320.00  QG= 0.341728E+07  QR= 0.206215E+07
ORT= 1350.00  QG= 0.365863E+07  QR= 0.257769E+07
ORT= 1380.00  QG= 0.386341E+07  QR= 0.309322E+07
ORT= 1410.00  QG= 0.395726E+07  QR= 0.360876E+07
ORT= 1460.00  QG= 0.408728E+07  QR= 0.446799E+07
ORT= 1480.00  QG= 0.412185E+07  QR= 0.481168E+07
```

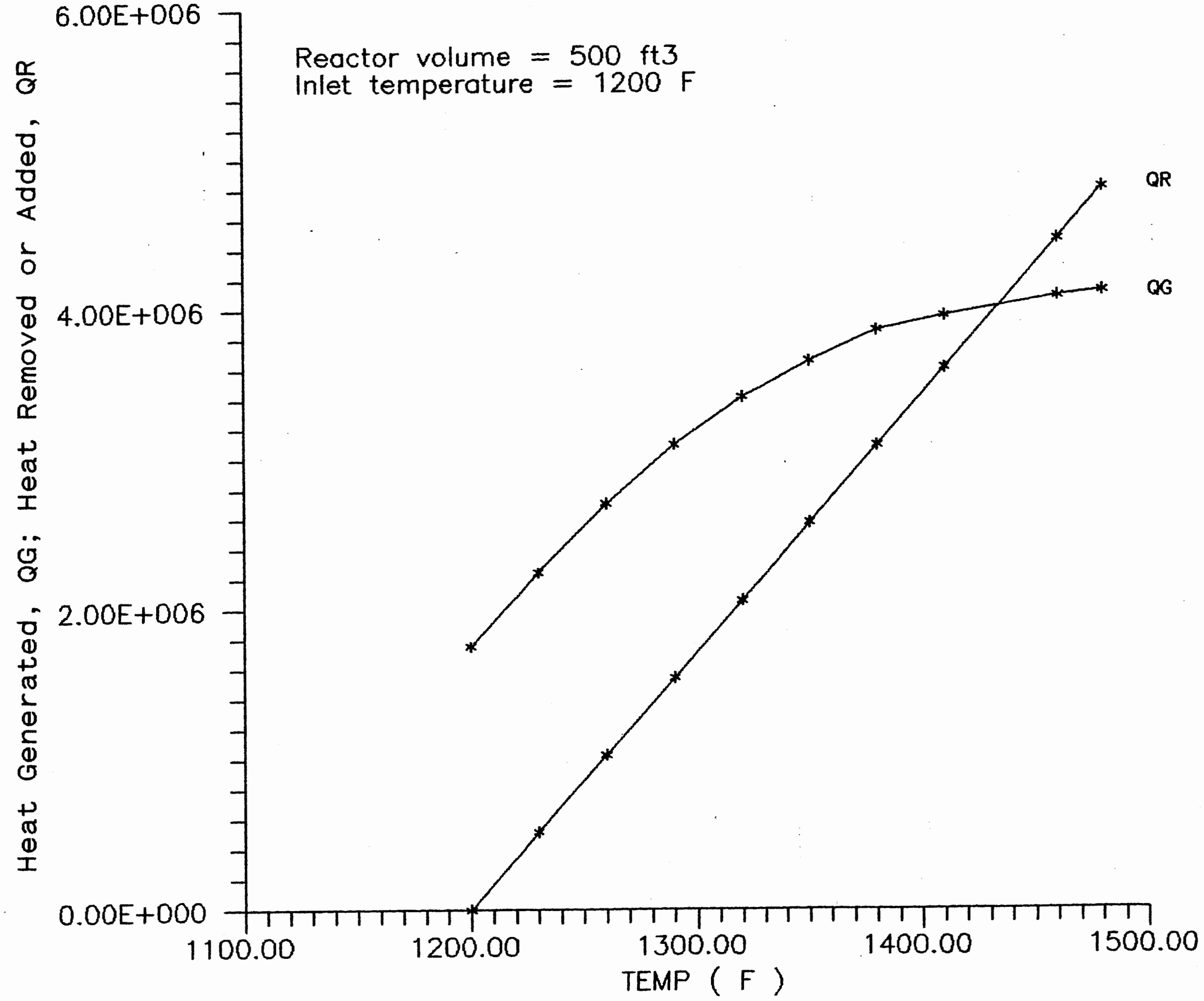


Figure 3: Heat Generation and Heat Removal Curve for Benzene from Toluene

TABLE V

OUTPUT TO FIND THE STEADY STATE FOR THE PROCESS OF PROPYLENE GLYCOL FROM PROPYLENE OXIDE

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =      40.00  FT3


  C3H6O     +  H2O        ->   C3H8O2

  METH        INERT

 RXN.   COMP. NAME   ORDER   STOICH.

   1    C3H6O         1.00    -1.00
   1    C3H8O2        0.00     1.00
   1    H2O           0.00    -1.00
   1    METH          0.00     0.00

UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.         1           2
   NAME           FEED 1      PROD. 1
 COMPONENT
 C3H6O            43.030        6.946
 C3H8O2            0.000       36.084
 H2O             802.800      766.716
 METH             71.870       71.870

   TOTAL         917.700      881.616

 T,DEG F          75.00       151.30
 P,PSIA           14.70        14.70
 MOL WEIGHT      20.9921      21.8514
 D,LB/FT3        60.1643      58.2159
 L/F(MOLAR)       1.0000       1.0000

 VOLUMETRIC FLOW RATE =    330.92  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.37  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =   40.00  FT3
```

TABLE VI

QG AND QR VALUES FOR THE PROCESS OF PROPYLENE GLYCOL FROM PROPYLENE OXIDE

```
ORT= 75.0000  QG=    166303.     QR=   0.000000
ORT= 85.0000  QG=    268543.     QR=     172144.
ORT= 95.0000  QG=    408942.     QR=     344287.
ORT= 105.000  QG=    583144.     QR=     516431.
ORT= 115.000  QG=    774597.     QR=     688574.
ORT= 125.000  QG=    960514.     QR=     860718.
ORT= 135.000  QG= 0.112744E+07   QR= 0.103286E+07
ORT= 145.000  QG= 0.125592E+07   QR= 0.120500E+07
ORT= 155.000  QG= 0.134902E+07   QR= 0.137715E+07
ORT= 165.000  QG= 0.141420E+07   QR= 0.154929E+07
```

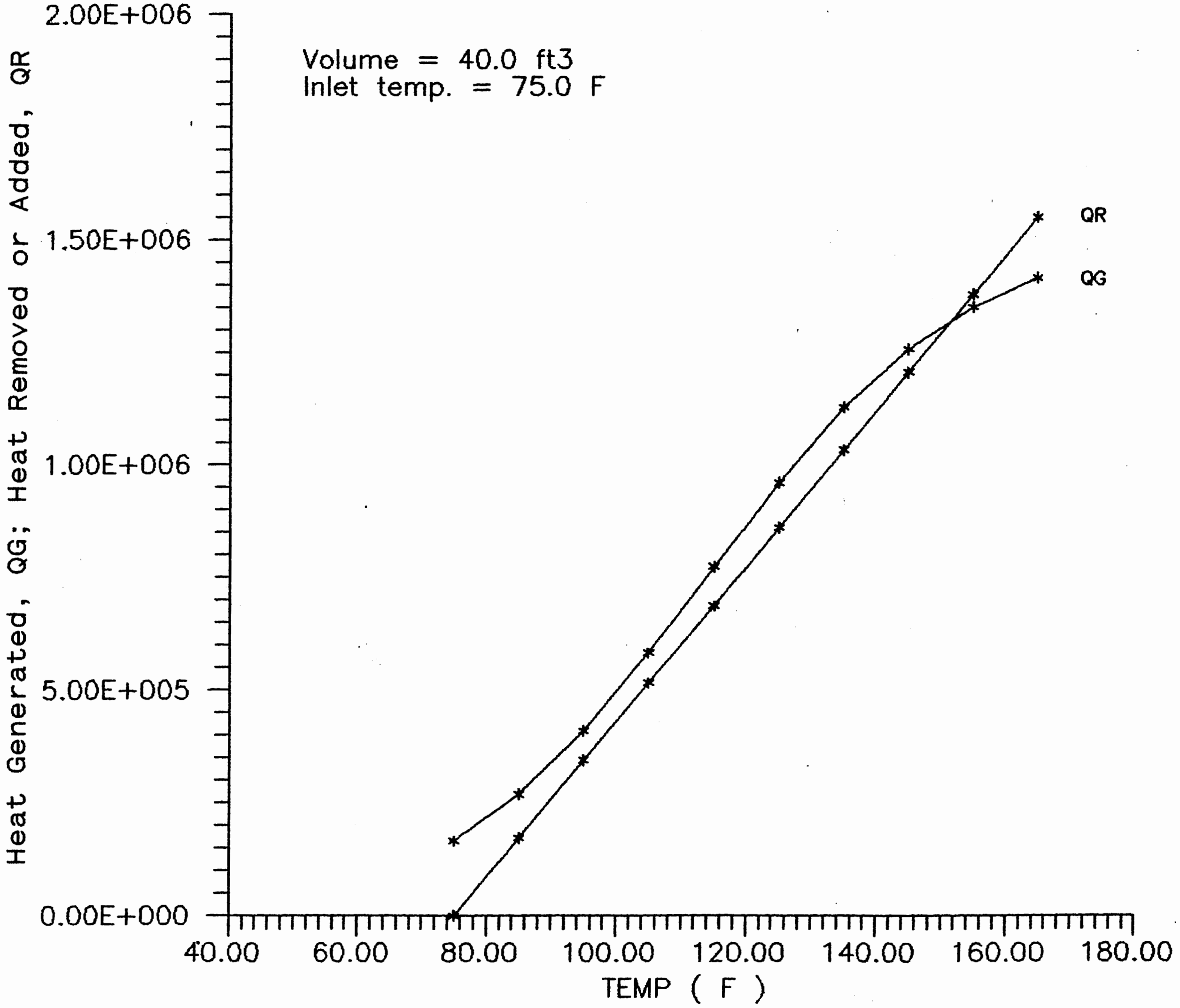


Figure 4: Heat Generation and Removal Curves for Propylene Glycol

Effect of Using Reactors in Series

Two identical CSTRs are simulated in series, and their performance is tested against a single reactor twice as large as shown in Figure 4.

Case I

The output for the first case can be seen in Tables VII-VIII. Using an inlet temperature and pressure of 1200°F and 495 psia, respectively, it is seen that when one reactor of volume equal to 250 ft^3 is used benzene production of 206.39 lbmole/hr is obtained. Whereas when two equal reactors of 125 ft^3 are used a benzene production of 219.68 lbmole/hr is obtained.

An increase in the toluene conversion in the reactor is also observed. This is chiefly because a train of CSTRs in series approach plug flow reactor. More conversion is observed when the number of reactors in series is increased.

Case II

The output for this case has been included in Tables IX-X. In this case two isothermal reactors were simulated in series against one reactor twice as large. It is seen that when one reactor of volume equal to 120 ft^3 is used a propylene glycol production rate of 11.36 lbmole/hr is obtained. Whereas, when two reactors of volume 60 ft^3 are

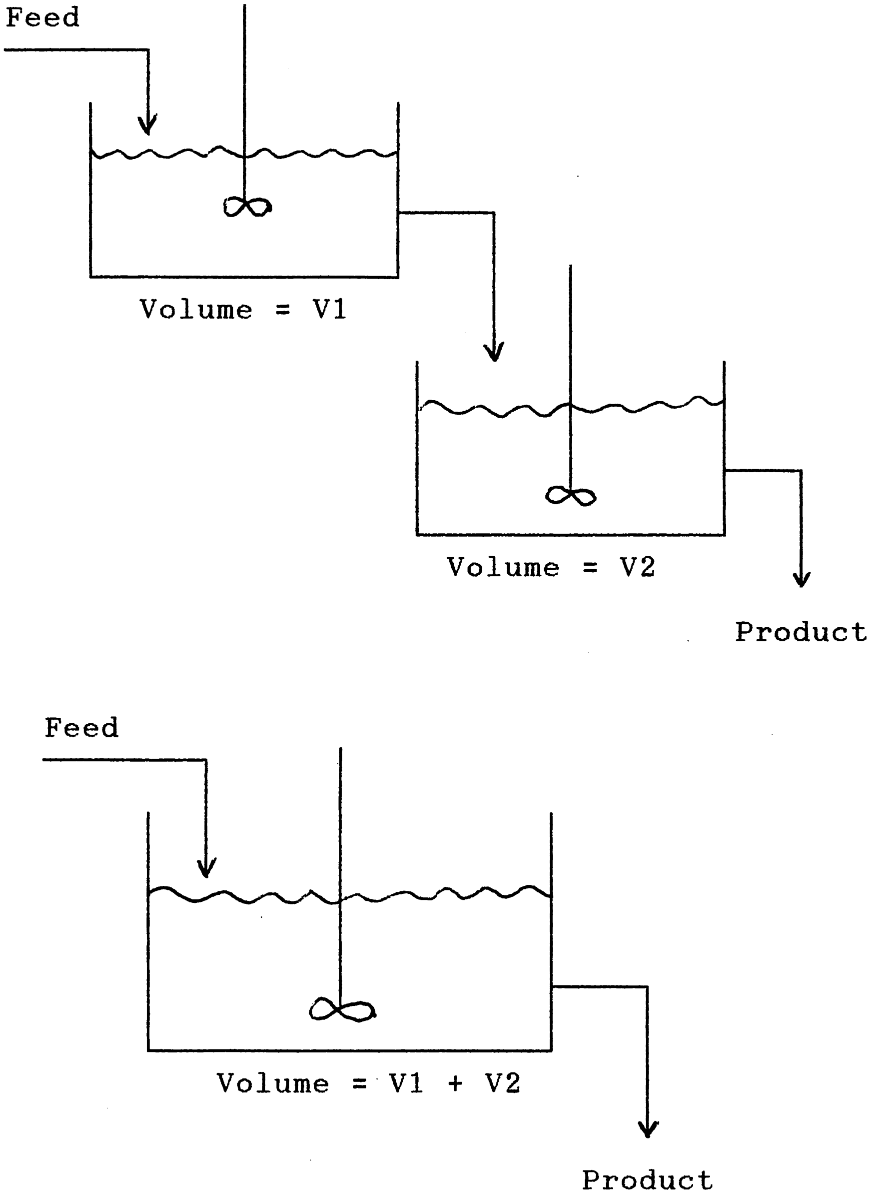


Figure 5: Comparison of Reactors in Series

TABLE VII

OUTPUT USING ONE LARGE REACTOR FOR THE CASE OF HYDRODEALKYLATION OF TOLUENE

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =      250.00   FT3


H2          +  C7H8         ->    CH4         +  C6H6


 RXN.    COMP. NAME    ORDER    STOICH.

   1     H2             0.50     -1.00
   1     CH4            0.00      1.00
   1     C6H6           0.00      1.00
   1     C7H8           1.00     -1.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.          1           2
   NAME            FEED 1      PROD. 1
 COMPONENT
 H2               450.000      243.610
 CH4                0.000      206.390
 C6H6               0.000      206.390
 C7H8             233.000       26.610

   TOTAL          683.000      683.000

 T,DEG F          1200.00      1416.58
 P,PSIA            495.00       490.00
 MOL WEIGHT       32.7614      32.7614
 D,LB/FT3          0.8879       0.7826
 L/F(MOLAR)        0.0000       0.0000


 VOLUMETRIC FLOW RATE =  28590.19   FT3/HR


 POWER REQUIRED FOR MIXING   =  1.03  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =  250.00   FT3
```

TABLE VIII

OUTPUT USING TWO REACTORS IN SERIES FOR THE CASE OF HYDRODEALKYLATION OF TOLUENE

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =     125.00  FT3


H2         +  C7H8       ->   CH4        +  C6H6


 RXN.   COMP. NAME   ORDER   STOICH.

   1    H2            0.50    -1.00
   1    CH4           0.00     1.00
   1    C6H6          0.00     1.00
   1    C7H8          1.00    -1.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.         1           2
   NAME           FEED 1      PROD. 1
 COMPONENT
 H2              450.000     289.826
 CH4               0.000     160.174
 C6H6              0.000     160.174
 C7H8            233.000      72.826

   TOTAL         683.000     683.000

 T,DEG F         1200.00     1368.08
 P,PSIA           495.00      492.50
 MOL WEIGHT      32.7614     32.7614
 D,LB/FT3         0.8879      0.8065
 L/F(MOLAR)       0.0000      0.0000


 VOLUMETRIC FLOW RATE =  27746.08  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.01  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )

 THE REACTOR VOLUME =  125.00  FT3
```

TABLE VIII (Continued)

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =     125.00  FT3


H2         +  C7H8       ->   CH4        +  C6H6


 RXN.    COMP. NAME    ORDER    STOICH.

   1     H2             0.50     -1.00
   1     CH4            0.00      1.00
   1     C6H6           0.00      1.00
   1     C7H8           1.00     -1.00


UNIT OPERATION NO.  2  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.         2           3
   NAME           FEED 2      PROD. 2
 COMPONENT
 H2              289.826     230.356
 CH4             160.174     219.644
 C6H6            160.174     219.644
 C7H8             72.826      13.356

   TOTAL         683.000     683.000

 T,DEG F         1368.08     1429.20
 P,PSIA           492.50      490.00
 MOL WEIGHT      32.7614     32.7614
 D,LB/FT3         0.8122      0.7775
 L/F(MOLAR)       0.0000      0.0000


 VOLUMETRIC FLOW RATE =  28777.93  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.01  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =  125.00  FT3
```

TABLE IX

OUTPUT USING ONE LARGE REACTOR FOR THE CASE OF PROPYLENE GLYCOL FROM PROPYLENE OXIDE

```
THE OPERATION IN THE REACTOR IS ISOTHERMAL

THE SPECIFIED REACTOR VOLUME =     120.00  FT3


  C3H6O     +  H2O        ->   C3H8O2

  METH        INERT

 RXN.   COMP. NAME   ORDER   STOICH.

   1    C3H6O         1.00    -1.00
   1    C3H8O2        0.00     1.00
   1    H2O           0.00    -1.00
   1    METH          0.00     0.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.        1           2
   NAME           FEED 1      PROD. 1
 COMPONENT
 C3H6O            43.030      31.694
 C3H8O2            0.000      11.336
 H2O             802.800     791.464
 METH             71.870      71.870

   TOTAL         917.700     906.364

 T,DEG F           75.00       75.00
 P,PSIA            14.70       14.70
 MOL WEIGHT      20.9921     21.2547
 D,LB/FT3        60.1643     60.3984
 L/F(MOLAR)       1.0000      1.0000


 VOLUMETRIC FLOW RATE =    319.34  FT3/HR

 POWER REQUIRED FOR MIXING   =  2.17  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )

 THE REACTOR VOLUME =  120.00  FT3
```

TABLE X

OUTPUT USING TWO REACTORS IN SERIES FOR THE CASE OF PROPYLENE GLYCOL FROM PROPYLENE OXIDE

```
THE OPERATION IN THE REACTOR IS ISOTHERMAL

THE SPECIFIED REACTOR VOLUME =      60.00  FT3


  C3H6O     +  H2O        ->   C3H8O2

  METH       INERT

 RXN.   COMP. NAME   ORDER   STOICH.

   1    C3H6O         1.00    -1.00
   1    C3H8O2        0.00     1.00
   1    H2O           0.00    -1.00
   1    METH          0.00     0.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.        1           2
   NAME           FEED 1     PROD. 1
 COMPONENT
 C3H6O            43.030      36.512
 C3H8O2            0.000       6.518
 H2O             802.800     796.282
 METH             71.870      71.870

   TOTAL         917.700     911.182

 T,DEG F           75.00       75.00
 P,PSIA            14.70       14.70
 MOL WEIGHT      20.9921     21.1423
 D,LB/FT3        60.1643     60.2948
 L/F(MOLAR)       1.0000      1.0000


 VOLUMETRIC FLOW RATE =    319.89  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.24   HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )
```

TABLE X (Continued)

```
THE OPERATION IN THE REACTOR IS ISOTHERMAL

THE SPECIFIED REACTOR VOLUME =      60.00  FT3


  C3H6O      + H2O         ->   C3H8O2

  METH        INERT

 RXN.    COMP. NAME   ORDER   STOICH.

   1     C3H6O         1.00    -1.00
   1     C3H8O2        0.00     1.00
   1     H2O           0.00    -1.00
   1     METH          0.00     0.00


UNIT OPERATION NO.  2  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.         2           3
   NAME           FEED 2      PROD. 2
 COMPONENT
 C3H6O            36.512       30.972
 C3H8O2            6.518       12.058
 H2O             796.282      790.742
 METH             71.870       71.870

   TOTAL         911.182      905.642

 T,DEG F           75.00        75.00
 P,PSIA            14.70        14.70
 MOL WEIGHT      21.1423      21.2717
 D,LB/FT3        60.3045      60.4139
 L/F(MOLAR)       1.0000       1.0000


 VOLUMETRIC FLOW RATE =    319.26  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.24  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =   60.00  FT3
```

---

used a propylene glycol production rate of 12.06 lbmole/hr is obtained. A higher conversion of propylene oxide is also observed.

Effect of using Reactors in Parallel

Two identical C.S.T.R's in parallel are simulated against a single reactor twice as large as shown in Figure 5. Results for both the cases considered are shown in Tables XI-XII. It is observed from these results that using reactors in parallel does not affect the production rate of the desired components nor the conversion in the reactor.

Verification of some Reactor Design Principles

Referring to the outputs for the runs described above:

i) The reaction of toluene with hydrogen, being exothermic in nature, indicates that an adiabatic operation of the reactor results in a smaller volume than the isothermal case. Thus when the operation in the reactor is adiabatic, a reactor volume of 347.81 ft^3 is necessary to meet a benzene production rate of 200 ft^3. Whereas when the operation in the reactor is switched to isothermal, a much larger reactor is needed to meet a benzene production of 172 lbmole/hr for the same inlet temperature.

ii) When the inlet temperature of the feed is 1200^0F a benzene production rate of 192.45 lbmole/hr is

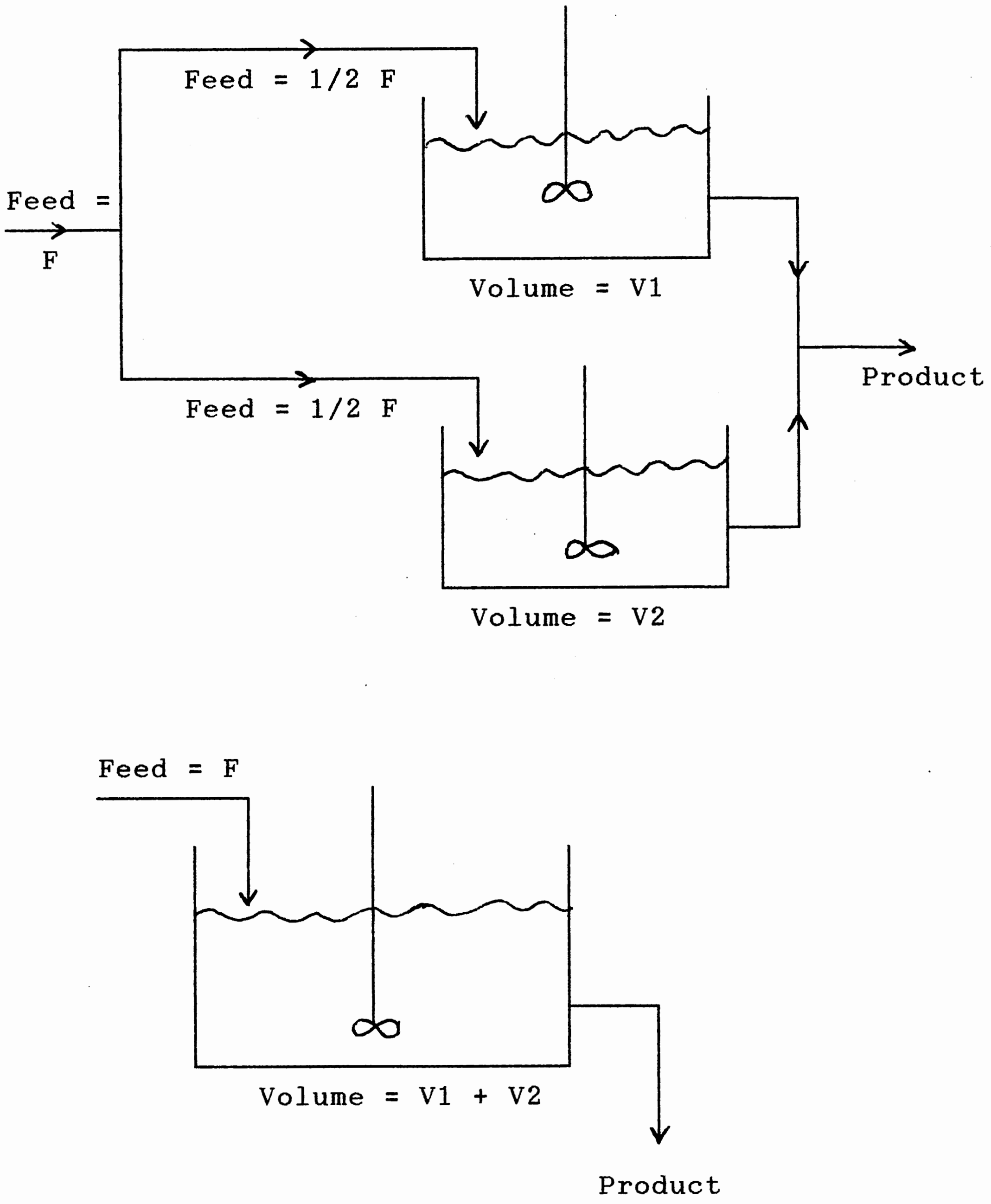


Figure 6: Comparison of Reactors in Parallel

TABLE XI

OUTPUT USING ONE SINGLE REACTOR

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =      250.00  FT3


H2         +  C7H8        ->   CH4        +  C6H6


 RXN.    COMP. NAME   ORDER   STOICH.

   1     H2            0.50    -1.00
   1     CH4           0.00     1.00
   1     C6H6          0.00     1.00
   1     C7H8          1.00    -1.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.          1           2
   NAME            FEED 1     PROD. 1
 COMPONENT
 H2               450.000     243.610
 CH4                0.000     206.390
 C6H6               0.000     206.390
 C7H8             233.000      26.610

   TOTAL          683.000     683.000

 T,DEG F          1200.00     1416.58
 P,PSIA            495.00      490.00
 MOL WEIGHT       32.7614     32.7614
 D,LB/FT3          0.8879      0.7826
 L/F(MOLAR)        0.0000      0.0000


 VOLUMETRIC FLOW RATE =  28590.19  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.03  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =  250.00  FT3
```

TABLE XII

OUTPUT USING TWO REACTORS IN PARALLEL

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =      125.00   FT3


H2         +  C7H8        ->    CH4         +  C6H6


 RXN.    COMP. NAME    ORDER    STOICH.

   1     H2              0.50    -1.00
   1     CH4             0.00     1.00
   1     C6H6            0.00     1.00
   1     C7H8            1.00    -1.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>       PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.          1           3
   NAME             FEED 1      PROD. 1
 COMPONENT
 H2                225.000     121.806
 CH4                 0.000     103.194
 C6H6                0.000     103.194
 C7H8              116.500      13.306

   TOTAL           341.500     341.500

 T,DEG F           1200.00     1416.58
 P,PSIA             495.00      490.00
 MOL WEIGHT        32.7614     32.7614
 D,LB/FT3           0.8879      0.7826
 L/F(MOLAR)         0.0000      0.0000


 VOLUMETRIC FLOW RATE =  14295.45   FT3/HR


 POWER REQUIRED FOR MIXING    =  1.01   HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =  125.00  FT3
```

TABLE XII (Continued)

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =     125.00   FT3


H2        +  C7H8       ->   CH4       +  C6H6


 RXN.   COMP. NAME   ORDER   STOICH.

   1    H2            0.50    -1.00
   1    CH4           0.00     1.00
   1    C6H6          0.00     1.00
   1    C7H8          1.00    -1.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.        2           4
   NAME           FEED 1      PROD. 1
 COMPONENT
 H2              225.000     121.806
 CH4               0.000     103.194
 C6H6              0.000     103.194
 C7H8            116.500      13.306

   TOTAL         341.500     341.500

 T,DEG F         1200.00     1416.58
 P,PSIA           495.00      490.00
 MOL WEIGHT      32.7614     32.7614
 D,LB/FT3         0.8879      0.7826
 L/F(MOLAR)       0.0000      0.0000


 VOLUMETRIC FLOW RATE =  14295.45  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.01  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =  125.00  FT3
```

observed whereas when the temperature is increased to 1250°F a production rate of 204.13 lbmole/hr is observed. Thus increasing the feed temperature, for exothermic reactions, increases the yield of benzene as well as the conversion of toluene. This is because the rate of the reaction increases with increase in temperature.

iii) Using two reactors in series instead of one large reactor, double in size, increases the conversion in the reactor (for both adiabatic and isothermal cases). However if two reactors in parallel are used the same conversion is observed all the other conditions being the same.

iv) Under adiabatic operation and with the volume equal to 250 ft^3 the reactor exit temperature is 1422°F. However, when an upper limit of 1400°F is set on the exit temperature, less production is obtained since the reactor volume cannot reach the full 250 ft^3. The same effect is observed in the second case studied too.

v) The power required for mixing gases is less comparative to that for liquids.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

The purpose behind this work was to simulate a homogeneous continuous stirred tank reactor. The computer code of the model is given in Appendix H. Based on the structure and the performance of this model, several conclusions are drawn.

1. Despite the enormous number of calculations involved simulation of a CSTR can be performed with little CPU time, i.e, it takes about 5 seconds on an IBM 386/87 clone if the reactor volume is 40 ft^3 in the case of production of propylene glycol.

2. For exothermic reactions, the steady state can be checked for stability easily by plotting heat generated and heat removed or added against temperature. In case of exothermic reaction, multiple steady states can occur for given process conditions. In this case by just viewing the above plot one can get an idea of the process conditions that can give a stable steady state.

3. It is observed that initial guesses can be very important for convergence of solution, for adiabatic cases. In some cases divergence was observed whereas in some cases more time was required for convergence of the solution.

For this reason, it is useful that the guess be as close to the solution as possible. An idea of a good guess can be obtained by running the isothermal case first at different temperatures.

4. It was observed that increasing the hydrogen-to-toluene ratio, keeping the reactor volume constant, decreases the yield of benzene for the case of hydrodealkylation of toluene.

5. The Rowlinson-Bondi correlation was tried for prediction of specific heat of liquids for alcohols and water. However large errors were observed in the predictions (about 50-60%).

Since several assumptions are made within this CSTR model calculation, several recommendations removing some of these constraints will serve to improve parts of this work.

1. The maximum number of reactions and components allowed can be increased, if needed, by simply changing the size of a few arrays in the calculation routine of the reactor.

2. The kinetic parts of the calculations have been coded in such a way that it can be used when modelling other types of reactors such as plug flow or fluidized bed reactors. In this case, the kinetic parts should be used along with the material and energy balance equations for that particular reactor.

3. Ideality is assumed, for both gases and liquids, only when the extent of the reversible reaction is

calculated. This assumption can be avoided if both the forward and reverse rate constants in the reversible reaction are known. In that case, such a reaction should be modelled as two irreversible reactions to avoid the assumption.

4. A heterogeneous reactor model can be introduced by using a cubic EOS for both gas and liquid phases, or the split EOS approach if the activity coefficient correlations are available.

5. The interaction parameter has been excluded from the liquid viscosity predictions. This can be included in the model prediction, however, this requires either some experimental data to establish the value of an interaction parameter specific for each binary pair in the mixture or implementation of a group contribution technique.

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APPENDICES

APPENDIX A

LOGIC STRUCTURE OF THE SUBROUTINES

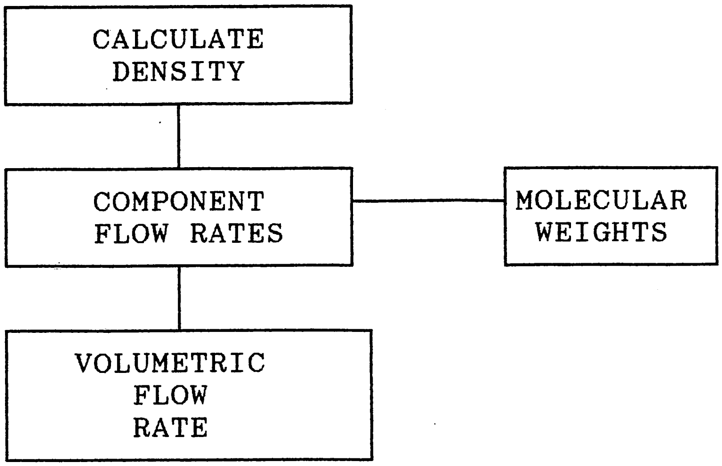

Figure 7: Logic Structure for STRFLO

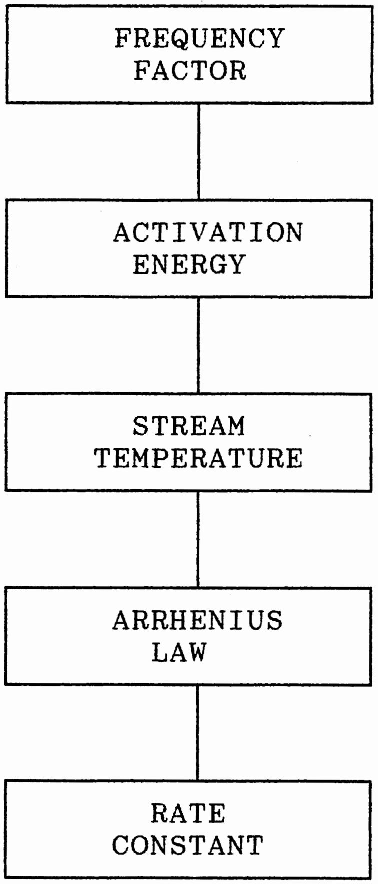

Figure 8: Logic Structure for RATEC

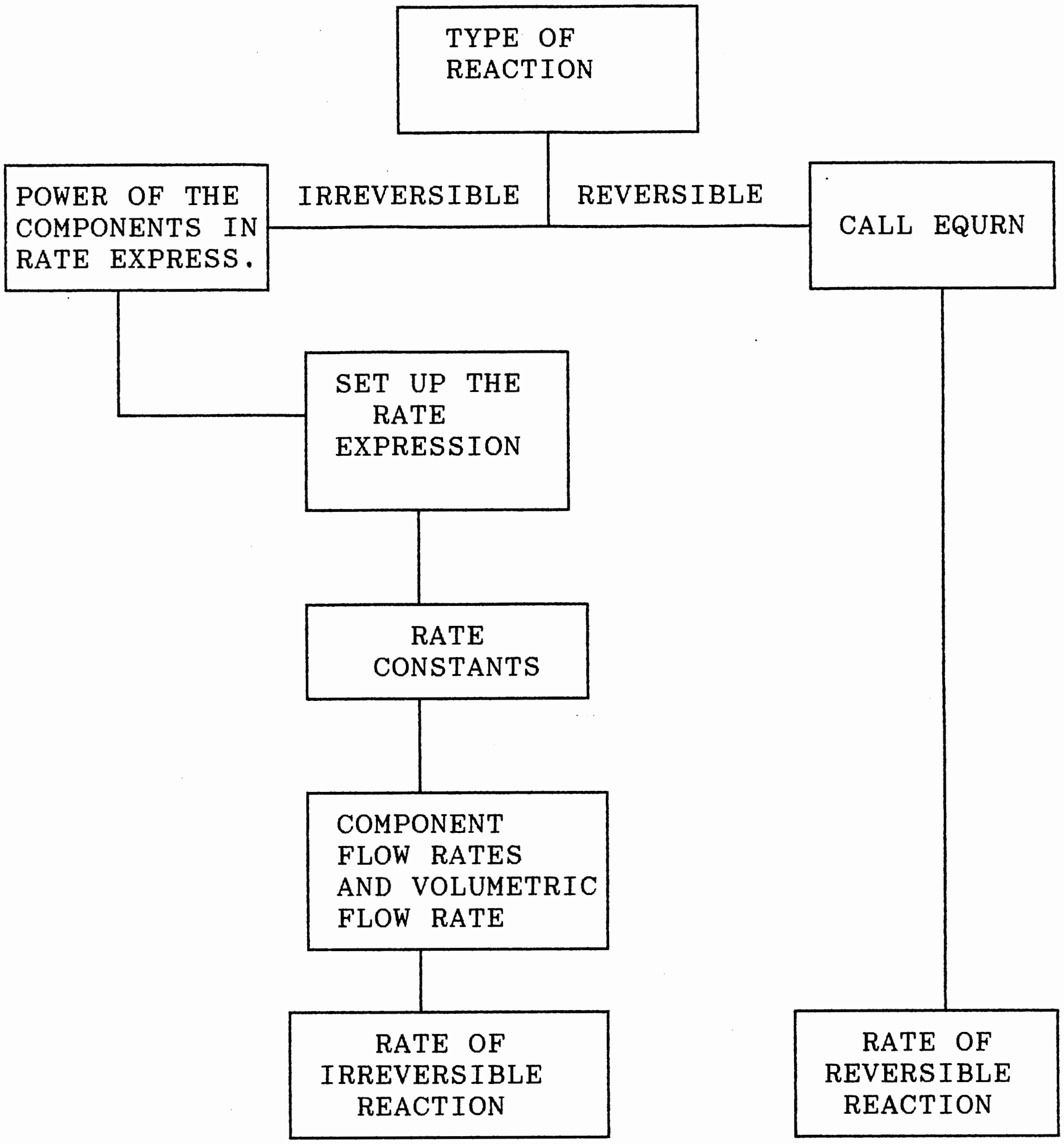

Figure 9: Logic Structure for RATERN

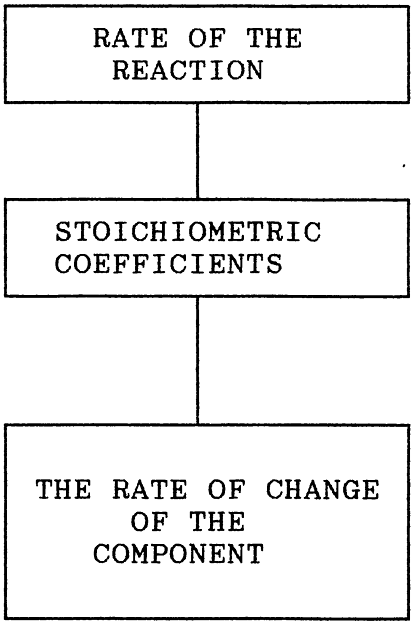

Figure 10: Logic Structure for RATECOMP

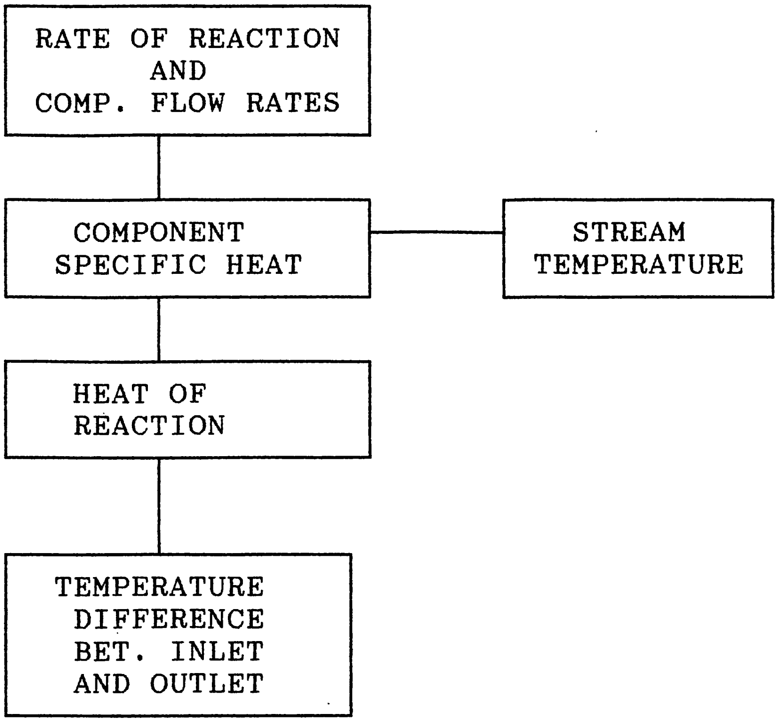

Figure 11: Logic Structure for TEMPDIF

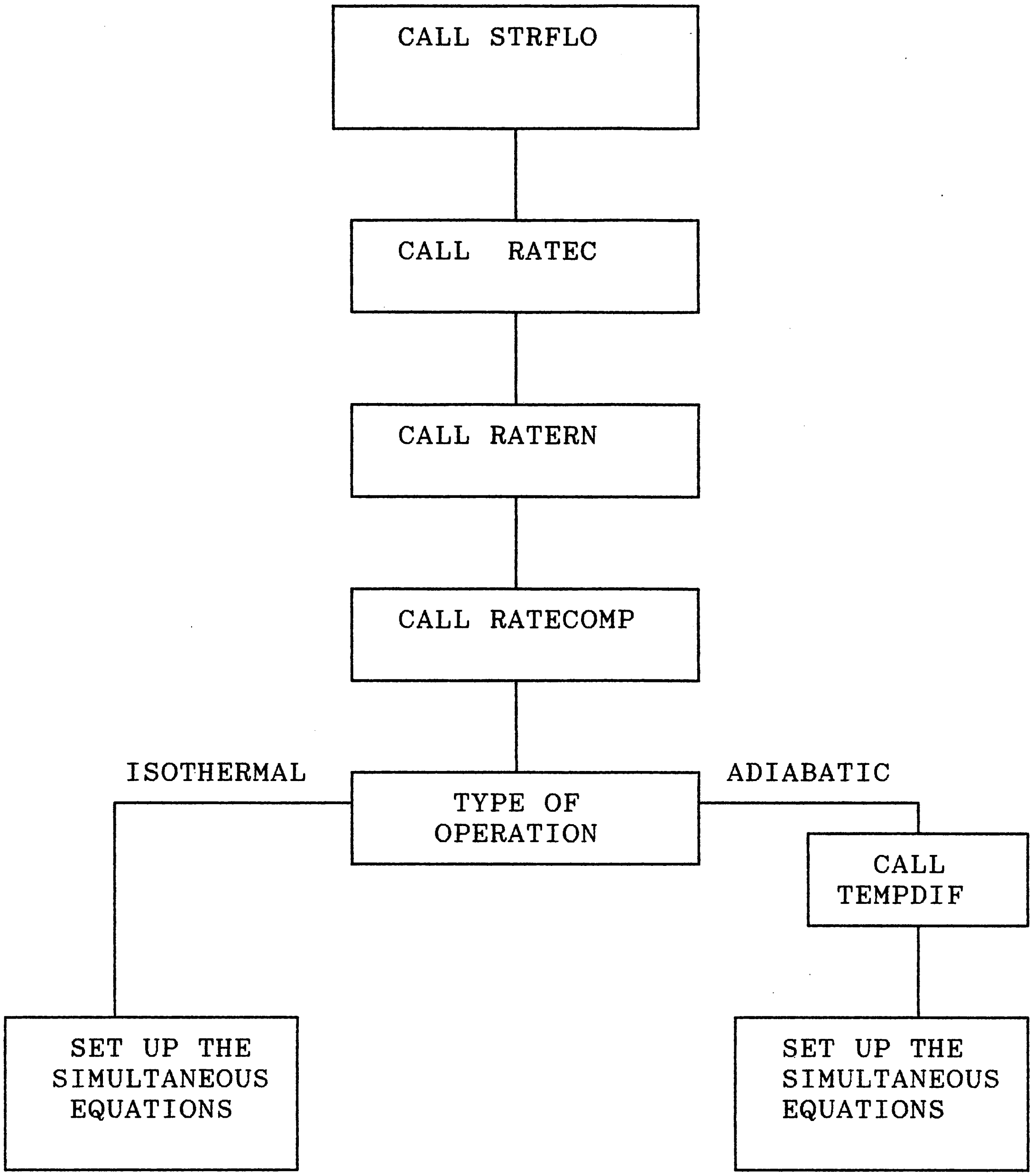

Figure 12: Logic Structure for EQUATN

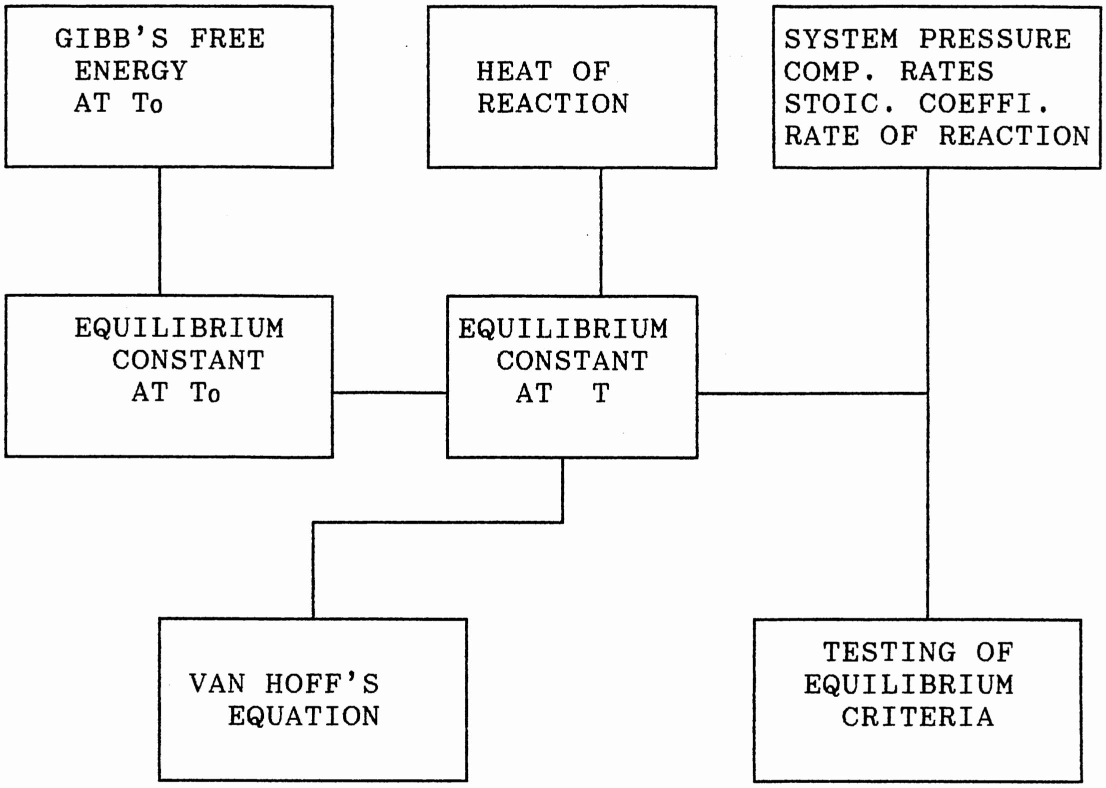

Figure 13: Logic Structure for EQURN

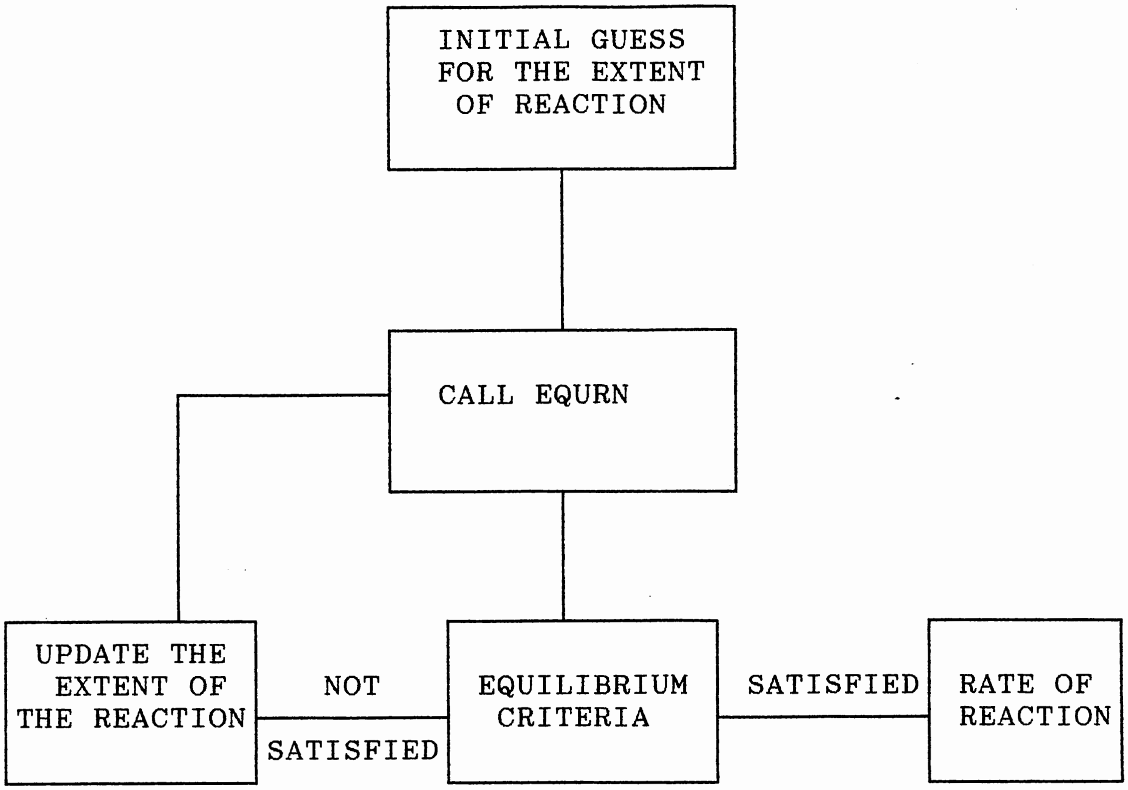

Figure 14: Logic Structure for EQURATE

APPENDIX B

SIMULATION RESULTS

TABLE XIII

TYPICAL OUTPUTS TESTING THE CONVERGENCE CRITERIA AND OPERATION MODES FOR HYDRODEALKYLATION OF TOLUENE

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE PROD. RATE OF COMP.#  3  IS  200.00  LBMOLES/HR

 H2        +  C7H8       ->  CH4       +  C6H6

 H2        +  O-X        ->  CH4       +  C7H8

  RXN.   COMP. NAME   ORDER   STOICH.
    1    H2            0.50    -1.00
    1    CH4           0.00     1.00
    1    C6H6          0.00     1.00
    1    C7H8          1.00    -1.00
    1    O-X           0.00     0.00
    2    H2            0.50    -1.00
    2    CH4           0.00     1.00
    2    C6H6          0.00     0.00
    2    C7H8          0.00     1.00
    2    O-X           1.00    -1.00
 UNIT OPERATION NO.  1  IS A REAC UNIT
         FEEDS>>>>>>>>      PRODUCTS>>>>
 STREAM FLOW RATES ARE LB-MOLES/HR
  STREAM NO.          1           2
    NAME            FEED 1      PROD. 1
  COMPONENT
  H2               450.000     237.692
  CH4               18.700     231.008
  C6H6               0.000     200.000
  C7H8             203.300      15.608
  O-X               12.700       0.392

    TOTAL          684.700     684.700

  T,DEG F          1200.00     1430.88
  P,PSIA            495.00      490.00
  MOL WEIGHT       31.0907     31.0907
  D,LB/FT3          0.8408      0.7372
  L/F(MOLAR)        0.0000      0.0000

  VOLUMETRIC FLOW RATE =  28878.34  FT3/HR

  POWER REQUIRED FOR MIXING   =  1.15  HP
  (ASSUMING SIX-BLADE TURBINE,
   AND FOUR BAFFLES IN REAC. )

  THE REACTOR VOLUME =  347.81  FT3
```

TABLE XIII (Continued)

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED OUTLET TEMPERATURE =     1400.00   DEG F

H2          +  C7H8        ->   CH4         +  C6H6

H2          +  O-X         ->   CH4         +  C7H8

 RXN.   COMP. NAME   ORDER    STOICH.
   1    H2            0.50     -1.00
   1    CH4           0.00      1.00
   1    C6H6          0.00      1.00
   1    C7H8          1.00     -1.00
   1    O-X           0.00      0.00
   2    H2            0.50     -1.00
   2    CH4           0.00      1.00
   2    C6H6          0.00      0.00
   2    C7H8          0.00      1.00
   2    O-X           1.00     -1.00
UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>       PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.          1           2
   NAME            FEED 1      PROD. 1
 COMPONENT
 H2               450.000     266.132
 CH4               18.700     202.568
 C6H6               0.000     172.321
 C7H8             203.300      42.526
 O-X               12.700       1.153

   TOTAL          684.700     684.700

 T,DEG F          1200.00     1400.00
 P,PSIA            495.00      490.00
 MOL WEIGHT       31.0907     31.0907
 D,LB/FT3          0.8408      0.7542
 L/F(MOLAR)        0.0000      0.0000

 VOLUMETRIC FLOW RATE =  28225.26  FT3/HR

 POWER REQUIRED FOR MIXING   =  1.02  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )

 THE REACTOR VOLUME =  156.68  FT3
```

TABLE XIII (Continued)

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =     250.00  FT3

H2         +  C7H8        ->   CH4        +  C6H6

H2         +  O-X         ->   CH4        +  C7H8

 RXN.   COMP. NAME   ORDER   STOICH.
   1    H2            0.50    -1.00
   1    CH4           0.00     1.00
   1    C6H6          0.00     1.00
   1    C7H8          1.00    -1.00
   1    O-X           0.00     0.00
   2    H2            0.50    -1.00
   2    CH4           0.00     1.00
   2    C6H6          0.00     0.00
   2    C7H8          0.00     1.00
   2    O-X           1.00    -1.00
UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.          1           2
   NAME            FEED 1      PROD. 1
 COMPONENT
 H2               450.000     245.438
 CH4               18.700     223.262
 C6H6               0.000     192.450
 C7H8             203.300      22.961
 O-X               12.700       0.589

   TOTAL          684.700     684.700

 T,DEG F          1200.00     1422.47
 P,PSIA            495.00      490.00
 MOL WEIGHT       31.0907     31.0907
 D,LB/FT3          0.8408      0.7403
 L/F(MOLAR)        0.0000      0.0000

 VOLUMETRIC FLOW RATE =  28754.43  FT3/HR

 POWER REQUIRED FOR MIXING   =  1.05  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )

 THE REACTOR VOLUME =  250.00  FT3
```

TABLE XIII (Continued)

```
THE OPERATION IN THE REACTOR IS ISOTHERMAL

THE SPECIFIED REACTOR VOLUME =     400.00  FT3

H2          +  C7H8        ->   CH4        +  C6H6

H2          +  O-X         ->   CH4        +  C7H8

 RXN.   COMP. NAME   ORDER    STOICH.
   1    H2            0.50     -1.00
   1    CH4           0.00      1.00
   1    C6H6          0.00      1.00
   1    C7H8          1.00     -1.00
   1    O-X           0.00      0.00
   2    H2            0.50     -1.00
   2    CH4           0.00      1.00
   2    C6H6          0.00      0.00
   2    C7H8          0.00      1.00
   2    O-X           1.00     -1.00
UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.         1           2
   NAME           FEED 1      PROD. 1
 COMPONENT
 H2              450.000     365.301
 CH4              18.700     103.399
 C6H6              0.000      77.036
 C7H8            203.300     133.928
 O-X              12.700       5.036

   TOTAL         684.700     684.700

 T,DEG F         1200.00     1200.00
 P,PSIA           495.00      490.00
 MOL WEIGHT      31.0907     31.0907
 D,LB/FT3         0.8408      0.8353
 L/F(MOLAR)       0.0000      0.0000

 VOLUMETRIC FLOW RATE =  25491.30  FT3/HR

 POWER REQUIRED FOR MIXING   =  1.17  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )

 THE REACTOR VOLUME =  400.00  FT3
```

TABLE XIII (Continued)

```
THE OPERATION IN THE REACTOR IS ISOTHERMAL

THE PROD. RATE OF COMP.#  3  IS  172.00  LBMOLES/HR

 H2         +  C7H8       ->   CH4        +  C6H6

 H2         +  O-X        ->   CH4        +  C7H8

  RXN.   COMP. NAME   ORDER   STOICH.
    1    H2            0.50    -1.00
    1    CH4           0.00     1.00
    1    C6H6          0.00     1.00
    1    C7H8          1.00    -1.00
    1    O-X           0.00     0.00
    2    H2            0.50    -1.00
    2    CH4           0.00     1.00
    2    C6H6          0.00     0.00
    2    C7H8          0.00     1.00
    2    O-X           1.00    -1.00
 UNIT OPERATION NO.  1  IS A REAC UNIT

         FEEDS>>>>>>>>      PRODUCTS>>>>
 STREAM FLOW RATES ARE LB-MOLES/HR
  STREAM NO.         1           2
    NAME           FEED 1      PROD. 1
  COMPONENT
  H2              450.000     266.394
  CH4              18.700     202.306
  C6H6              0.000     172.000
  C7H8            203.300      42.906
  O-X              12.700       1.094

    TOTAL         684.700     684.700

  T,DEG F         1200.00     1200.00
  P,PSIA           495.00      490.00
  MOL WEIGHT      31.0907     31.0907
  D,LB/FT3         0.8408      0.8381
  L/F(MOLAR)       0.0000      0.0000

  VOLUMETRIC FLOW RATE =  25402.06  FT3/HR

  POWER REQUIRED FOR MIXING   =  5.39  HP
  (ASSUMING SIX-BLADE TURBINE,
   AND FOUR BAFFLES IN REAC. )

  THE REACTOR VOLUME = 3247.67  FT3
```

TABLE XIV

OUTPUT USING HYDROGEN-TO-TOLUENE RATIO OF 4

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =     250.00  FT3

H2        + C7H8       ->   CH4       + C6H6

H2        + O-X        ->   CH4       + C7H8

 RXN.   COMP. NAME  ORDER   STOICH.
   1    H2           0.50    -1.00
   1    CH4          0.00     1.00
   1    C6H6         0.00     1.00
   1    C7H8         1.00    -1.00
   1    O-X          0.00     0.00
   2    H2           0.50    -1.00
   2    CH4          0.00     1.00
   2    C6H6         0.00     0.00
   2    C7H8         0.00     1.00
   2    O-X          1.00    -1.00
UNIT OPERATION NO.  1  IS A REAC UNIT
        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.        1           2
   NAME           FEED 1      PROD. 1
 COMPONENT
 H2              800.000     622.189
 CH4              18.700     196.511
 C6H6              0.000     166.432
 C7H8            203.300      48.246
 O-X              12.700       1.321

   TOTAL        1034.700    1034.700

 T,DEG F         1200.00     1368.13
 P,PSIA           495.00      490.00
 MOL WEIGHT      21.2558     21.2558
 D,LB/FT3         0.5732      0.5223
 L/F(MOLAR)       0.0000      0.0000

 VOLUMETRIC FLOW RATE =  42105.96  FT3/HR

 POWER REQUIRED FOR MIXING   =  1.04  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )

 THE REACTOR VOLUME =  250.00  FT3
```

TABLE XV

OUTPUT USING HYDROGEN-TO-TOLUENE
RATIO OF 5

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =     250.00  FT3

H2        +  C7H8       ->   CH4       +  C6H6

H2        +  O-X        ->   CH4       +  C7H8

 RXN.   COMP. NAME   ORDER   STOICH.
   1    H2            0.50    -1.00
   1    CH4           0.00     1.00
   1    C6H6          0.00     1.00
   1    C7H8          1.00    -1.00
   1    O-X           0.00     0.00
   2    H2            0.50    -1.00
   2    CH4           0.00     1.00
   2    C6H6          0.00     0.00
   2    C7H8          0.00     1.00
   2    O-X           1.00    -1.00
UNIT OPERATION NO.  1  IS A REAC UNIT
        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.        1           2
   NAME           FEED 1      PROD. 1
 COMPONENT
 H2             1000.000     852.683
 CH4              18.700     166.017
 C6H6              0.000     136.923
 C7H8            203.300      76.771
 O-X              12.700       2.306

   TOTAL        1234.700    1234.700

 T,DEG F         1200.00     1329.65
 P,PSIA           495.00      490.00
 MOL WEIGHT      18.1393     18.1393
 D,LB/FT3         0.4890      0.4546
 L/F(MOLAR)       0.0000      0.0000

 VOLUMETRIC FLOW RATE =  49267.27  FT3/HR

 POWER REQUIRED FOR MIXING    =  1.03  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )

 THE REACTOR VOLUME =  250.00  FT3
```

TABLE XVI

OUTPUTS TESTING THE CONVERGENCE CRITERIA AND OPERATION MODES FOR THE CASE OF PROPYLENE GLYCOL FROM PROPYLENE OXIDE

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =      40.00  FT3


  C3H6O     +  H2O        ->   C3H8O2

  METH       INERT

 RXN.   COMP. NAME   ORDER   STOICH.

   1    C3H6O         1.00    -1.00
   1    C3H8O2        0.00     1.00
   1    H2O           0.00    -1.00
   1    METH          0.00     0.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.        1           2
   NAME           FEED 1      PROD. 1
 COMPONENT
 C3H6O            43.030        6.946
 C3H8O2            0.000       36.084
 H2O             802.800      766.716
 METH             71.870       71.870

   TOTAL         917.700      881.616

 T,DEG F           75.00       151.30
 P,PSIA            14.70        14.70
 MOL WEIGHT      20.9921      21.8514
 D,LB/FT3        60.1643      58.2159
 L/F(MOLAR)       1.0000       1.0000

 VOLUMETRIC FLOW RATE =    330.92  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.37  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =   40.00  FT3
```

TABLE XVI (Continued)

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED OUTLET TEMPERATURE =      125.00  DEG F

  C3H6O      +  H2O         ->   C3H8O2

  METH       INERT

 RXN.   COMP. NAME   ORDER   STOICH.

   1    C3H6O         1.00    -1.00
   1    C3H8O2        0.00     1.00
   1    H2O           0.00    -1.00
   1    METH          0.00     0.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.        1           2
   NAME          FEED 1     PROD. 1
 COMPONENT
 C3H6O            43.030      19.384
 C3H8O2            0.000      23.646
 H2O             802.800     779.154
 METH             71.870      71.870

   TOTAL         917.700     894.054

 T,DEG F           75.00      125.00
 P,PSIA            14.70       14.70
 MOL WEIGHT      20.9921     21.5474
 D,LB/FT3        60.1643     58.9330
 L/F(MOLAR)       1.0000      1.0000


 VOLUMETRIC FLOW RATE =    326.89  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.37   HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =   30.87  FT3
```

TABLE XVI (Continued)

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE PROD. RATE OF COMP.#  2  IS   38.73  LBMOLES/HR

   C3H6O     +  H2O        ->   C3H8O2

   METH        INERT

  RXN.   COMP. NAME   ORDER   STOICH.

    1    C3H6O         1.00    -1.00
    1    C3H8O2        0.00     1.00
    1    H2O           0.00    -1.00
    1    METH          0.00     0.00


 UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
 STREAM FLOW RATES ARE LB-MOLES/HR
  STREAM NO.        1           2
    NAME          FEED 1      PROD. 1
  COMPONENT
  C3H6O           43.030       4.300
  C3H8O2           0.000      38.730
  H2O            802.800     764.070
  METH            71.870      71.870

    TOTAL        917.700     878.970

  T,DEG F          75.00      156.90
  P,PSIA           14.70       14.70
  MOL WEIGHT     20.9921     21.9172
  D,LB/FT3       60.1643     58.0730
  L/F(MOLAR)      1.0000      1.0000


  VOLUMETRIC FLOW RATE =    331.73  FT3/HR


  POWER REQUIRED FOR MIXING    =  1.66  HP
  (ASSUMING SIX-BLADE TURBINE,
   AND FOUR BAFFLES IN REAC. )


  THE REACTOR VOLUME =   54.56  FT3
```

TABLE XVI (Continued)

```
THE OPERATION IN THE REACTOR IS ISOTHERMAL

THE SPECIFIED REACTOR VOLUME =     120.00  FT3

  C3H6O     +  H2O        ->   C3H8O2

  METH       INERT

 RXN.   COMP. NAME   ORDER   STOICH.

   1    C3H6O         1.00    -1.00
   1    C3H8O2        0.00     1.00
   1    H2O           0.00    -1.00
   1    METH          0.00     0.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.        1           2
   NAME           FEED 1     PROD. 1
 COMPONENT
 C3H6O            43.030      31.694
 C3H8O2            0.000      11.336
 H2O             802.800     791.464
 METH             71.870      71.870

   TOTAL         917.700     906.364

 T,DEG F           75.00       75.00
 P,PSIA            14.70       14.70
 MOL WEIGHT      20.9921     21.2547
 D,LB/FT3        60.1643     60.3984
 L/F(MOLAR)       1.0000      1.0000


 VOLUMETRIC FLOW RATE =    319.34  FT3/HR


 POWER REQUIRED FOR MIXING   =  2.17  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =  120.00  FT3
```

TABLE XVI (Continued)

```
THE OPERATION IN THE REACTOR IS ISOTHERMAL

THE PROD. RATE OF COMP.#  2  IS   30.00  LBMOLES/HR

   C3H6O     +  H2O        ->   C3H8O2

   METH         INERT

  RXN.    COMP. NAME   ORDER   STOICH.

    1     C3H6O         1.00    -1.00
    1     C3H8O2        0.00     1.00
    1     H2O           0.00    -1.00
    1     METH          0.00     0.00


 UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
 STREAM FLOW RATES ARE LB-MOLES/HR
  STREAM NO.         1           2
    NAME           FEED 1      PROD. 1
  COMPONENT
  C3H6O            43.030      13.030
  C3H8O2            0.000      30.000
  H2O             802.800     772.800
  METH             71.870      71.870

    TOTAL         917.700     887.700

  T,DEG F           75.00       75.00
  P,PSIA            14.70       14.70
  MOL WEIGHT      20.9921     21.7016
  D,LB/FT3        60.1643     60.8002
  L/F(MOLAR)       1.0000      1.0000


  VOLUMETRIC FLOW RATE =    317.23  FT3/HR


  POWER REQUIRED FOR MIXING   = 12.37  HP
  (ASSUMING SIX-BLADE TURBINE,
   AND FOUR BAFFLES IN REAC. )


  THE REACTOR VOLUME =  767.37  FT3
```

APPENDIX C

CALCULATION OF LIQUID HEAT CAPACITY

Constant Pressure Liquid Heat Capacity:

The constant pressure liquid heat capacity is calculated from the constant pressure ideal gas heat capacity by the Rowlinson-Bondi correlation (Reid et al., 1987) as follows,

$$C_{\sigma L} = R * \left(\frac{(C_{pL} - C_{p}^{o})}{R} - \frac{(C_{pL} - C_{\sigma L})}{R} \right) + C_{p}^{0}$$

where,

$$(C_{pL} - C_{p}^{o}) / R = 1.45 + 0.45/(1-0.803) + (0.25)(0.202) \\ (17.11 + (25.2)(1-0.803)^{1/3} / 0.803 + \\ 1.742/(1-0.803))$$

$$(C_{pL} - C_{\sigma L}) / R = \mathrm{Exp}\,(20.1\, T_r - 17.9)$$

C_{pL} - represents the change in enthalpy with temperature at constant pressure.

C_{p}^{o} - the ideal gas heat capacity.

$C_{\sigma L}$ - represents the variation in enthalpy of a saturated liquid with temperature.

T_r - reduced temperature.

Constant Pressure Heat Capacity for Alcohols and Water:

The liquid heat capacity for alcohols and water has been calculated from the correlations presented by Miller et.al (1976) as follows,

$$C_p / R = A + B T + C T^2$$

A, B, and C are constants to calculate the liquid heat capacity and are characteristic of the pure fluid.

APPENDIX D

CALCULATION OF GAS AND LIQUID VISCOSITY

Estimation of the gas viscosity:

The viscosity of the gases has been calculated using the Method of Chung et al. (Reid et al., 1987),

$$\mu = 40.785 \ (F_c \ (MW \ T)^{1/2} \ ) \ / \ (V_c^{2/3} \quad {}_v) \qquad (D.1)$$

where,

$$F_c = 1 - 0.2756 \ w + 0.059035 \ \mu_r \qquad (D.2)$$

$$\mu_r = 131.3 \ (\ m \ ) \ / \ (V_c T_c)^{1/2} \qquad (D.3)$$

$$\sigma_v = [A(T^*)^{-B}] + C[\exp(-D \ T^*)] + E[\exp(-F \ T^*)] \qquad (D.4)$$

where,

A=1.16145 B=0.14874 C=0.52487 D=0.77320 E=2.16178

F=2.43787

For a mixture the Method of Wilke (Reid et al., 1987) has been used. According to this method,

$$\mu_m = \quad (y_i \ \mu_i)/ \ (\quad y_j \ \text{ø}_{ij}) \qquad (D.5)$$

where according to the Herning and Zipperer approximation (Reid et al., 1987),

$$\text{ø}_{ij} = (\ MW_j \ / \ MW_i \ )^{1/2} \qquad (D.6)$$

Estimation of the Liquid Viscosity:

The liquid viscosity is calculated using the constants published by Van Velzen et al. (1972), Yaws et al. (1976), and Duhne et al. (1979) and given by Reid et al. (1987)

using three types of equations applicable to different hydrocarbons. The equations are,

$$\mu = A\ T^{B} \tag{D.7}$$

$$\mu = \exp\ (\ A + B/T\ ) \tag{D.8}$$

$$\mu = \exp\ (\ A + B/T + C\ T + D\ T^{2}\ ) \tag{D.9}$$

Reid et al. (1987) have also given a list of the type of equation to use for different hydrocarbons. A, B, C, and D are constants characteristic of the pure fluid.

For a mixture

$$\mu_m = \exp\ (\ \Sigma\ x_i\ \ln \mu_i\ ) \tag{D.10}$$

APPENDIX E

GENENERALISED TWO CONSTANT CUBIC EOS

Generalised Two-Constant Cubic EOS Predictions:

$$Z^3 - (1 + B - u\ B)\ Z^2 + (A + w\ B^2 - u\ B - u\ B^2\ )\ Z - A\ B - w\ B^2 - w\ B^3 = 0.0 \qquad (E.1)$$

$$A = \sum_i \sum_j x_i\ x_j\ (\ a_i\ a_j\ )^{0.5}\ (\ 1 - C_{ij}\ ) \qquad (E.2)$$

$$B = \sum_i \sum_j x_i\ x_j\ (\ b_i + b_j\ )^{0.5}\ (\ 1 + D_{ij}\ ) \qquad (E.3)$$

$$a_i = omga\ P_{r,i}\ \alpha_i\ /\ T_{r,i} \qquad (E.4)$$

$$b_i = omgb\ P_{r,i}\ /\ T_{r,i} \qquad (E.5)$$

$$\alpha_i = [\ 1 + F_{a,i}\ (\ 1 - T_{r,i}\ )^{0.5}\ ]^2 \qquad (E.6)$$

For the RK equation:

$$F_{a,i} = (\ (1\ /\ (\ T_{r,i}\ )^{0.25}) - 1.0)\ /\ (1. - (T_{r,i})^{0.5}) \qquad (E.7)$$

For the SRK equation:

$$F_{a,i} = 0.48 + 1.574\ w_i - 0.176\ w_i^2 \qquad (E.8)$$

For the PR Equation:

$$F_{a,i} = 0.37646 + 1.54226\ w_i - 0.26992\ w_i^2 \qquad (E.9)$$

TABLE XVII

CONSTANTS FOR THE CUBIC EOS

Constants	R K	SRK	PR
u	1	1	2
w	0	0	-1
omga	0.42747	0.42747	0.457235
omgb	0.08664	0.08664	0.077796

APPENDIX F

HANKINSON THOMSON METHOD PREDICTIONS

Hankinson-Thomson Method for liquids:

The Hankinson and Thomson method is used for prediction of the liquid density. Hankinson and Thomson (Reid et al., 1987) present the following correlation for densities of liquids

$$V_s \;/\; V^* = V_R^o \; [1 - w \; V_R^\delta]$$

$$V_R^o = 1 + a\;(1 - T_r)^{1/3} + b\;(1 - T_r)^{2/3} + c\;(1 - T_r) + d\;(1 - T_r)^{4/3} \qquad 0.25 < T_r < 0.95$$

$$V_R^\delta = [e + f\;T_r + g\;T_r^2 + h\;T_r^3] \;/\; (T_r - 1.00001) \qquad 0.25 < T_r < 1.0$$

$a=-1.52816 \quad b=1.43907 \quad c=-0.81446 \quad d=0.190454$

$e=-0.296123 \quad f=0.386914 \quad g=-0.0427258 \quad h=-0.0480645$

If a value of V^* is not available it can be estimated by:

$$V^* = (R\;T_c \;/\; P_c)\;(a + b\;w + c\;w^2)$$

For a mixture,

$$T_{c,m} = \sum_i \sum_j x_i \; x_j \; V^*_{ij} \; T_{c,ij} \;\;/\;\; V_m^*$$

$$V_m^* = (1/4)\;[\;\Sigma\; x_i \; V_i^* + 3\;(\;\Sigma\; x_i \; V_i^*2/3\;)\;(\;\Sigma\; x_i \; V_i^{*1/3}\;)$$

$$V_{ij}^* \; T_{c,ij} = (\; V_i^* \; T_{c,i} \; V_j^* \; T_{c,j}\;)^{1/2}$$

$$w_m = \Sigma\; x_i \; w_i$$

APPENDIX G

PROGRAM INPUT AND OUTPUT

PROGRAM INPUT:

(For the case of hydrodealkylation of toluene, one irreversible reaction and adiabatic operation in the reactor)

```
ENTER THE STREAM ID NO TO REACTOR UNIT
1

ENTER PRODUCT STREAM ID NO FROM REACTOR
2

ENTER NO. OF COMPONENTS
4

ENTER NO. OF REACTIONS
1

ENTER COMP. ID NO OF COMP #   1
1

ENTER INLET FLOW RATE OF COMP #   1IN LB-MOLS/HR
450.0

ENTER COMP. ID NO OF COMP #   2
2

ENTER INLET FLOW RATE OF COMP #   2IN LB-MOLS/HR
0.0

ENTER COMP. ID NO OF COMP #   3
40

ENTER INLET FLOW RATE OF COMP #   3IN LB-MOLS/HR
0.0

ENTER COMP. ID NO OF COMP #   4
41

ENTER INLET FLOW RATE OF COMP #   4IN LB-MOLS/HR
233.0

ENTER TYPE OF OPERATION
 ENTER    0     FOR ISOTHERMAL
 ENTER    1     FOR ADIABATIC

1
```

```
IS REACTION   1IN EQUILIBRIUM
 ENTER    1:NO     2:YES

******* WARNING ********

    IT IS BETTER TO SIMULATE A REVERSIBLE REACTION AS
TWO IRREVERSIBLE REACTIONS IF THE FORWARD AND REVERSE
REACTION RATE EQUATIONS ARE KNOWN SINCE IDEALITY HAS BEEN
ASSUMED FOR FORMULATING THE EQUILIBRIUM CRITERION FOR
REVERSIBLE REACTIONS.

*************************
1

ENTER THE FREQUENCY FACTOR OF REACTION  1
2.58E+15

ENTER THE ACTIVATION ENERGY OF REACTION  1
98100.0

ENTER THE HEAT OF REACTION  1
-18032.92

ENTER ORDER OF COMPONENT #   1IN REACTION   1
0.5

ENTER THE STOICHIOMETRIC COEFF. OF COMP #   1
 IN REACTION   1
-1.0

ENTER ORDER OF COMPONENT #   2IN REACTION   1
0.0

ENTER THE STOICHIOMETRIC COEFF. OF COMP #   2
 IN REACTION   1
1.0

ENTER ORDER OF COMPONENT #   3IN REACTION   1
0.0

ENTER THE STOICHIOMETRIC COEFF. OF COMP #   3
 IN REACTION   1
1.0

ENTER ORDER OF COMPONENT #   4IN REACTION   1
1.0

ENTER THE STOICHIOMETRIC COEFF. OF COMP #   4
 IN REACTION   1
-1.0
```

```
ENTER THE TYPE OF EQN. TO USE
      1   RK
      2   SRK
      3   PR
      4   HBT

USE 1,2, OR 3 FOR GASES
AND 4 FOR LIQUIDS

2

ENTER THE TYPE OF FLUID
      1    LIQUID
      2    GASES
2

ENTER THE INLET TEMP IN DEG F
1200.0

ENTER THE INLET PRESSURE IN PSIA
495.0

ENTER THE OUTLET PR. OPTION
ENTER 1 IF PR. DROP IS TO BE SPECIFIED
ENTER 0 IF OUTLET PR. IS TO BE SPECIFIED

0

ENTER OUTLET PR. FROM REACTOR IN PSIA
490.0

ENTER THE RPM FOR STIRRER
100.0

ENTER THE CONVERSION CRITERIA
      0 FOR REACTOR VOLUME
      1 FOR OUTLET TEMP
      2 FOR PRODUCTION RATE

0

ENTER THE DESIRED REACTOR VOLUME IN FT3
500.0

DO YOU WANT TO SPECIFY TEMP ALSO
       0  YES
       1  NO

1

ENTER GUESS FOR FLOW RATE OF COMP. NO    1
250.0
```

```
ENTER GUESS FOR FLOW RATE OF COMP. NO    2
200.0

ENTER GUESS FOR FLOW RATE OF COMP. NO    3
200.0

ENTER GUESS FOR FLOW RATE OF COMP. NO    4
33.0

ENTER GUESS FOR THE OUTLET TEMPERATURE IN DEG F
1420.0
```

PROGRAM OUTPUT:

The output from the program will be saved in a file known as CSTR.OUT. A sample output is given in Table XVIII. The values of heat generated, QG, and the heat removed or added, QR, are saved in a separate file known as HEAT.OUT. A sample output of this file is given in Table XIX.

TABLE XVIII

A SAMPLE OUTPUT FOR THE CASE OF HYDRODEALKYLATION OF TOLUENE

```
THE OPERATION IN THE REACTOR IS ADIABATIC

THE SPECIFIED REACTOR VOLUME =     500.00  FT3


H2         +  C7H8       ->   CH4        +  C6H6


 RXN.    COMP. NAME   ORDER   STOICH.

   1     H2             0.50    -1.00
   1     CH4            0.00     1.00
   1     C6H6           0.00     1.00
   1     C7H8           1.00    -1.00


UNIT OPERATION NO.  1  IS A REAC UNIT

        FEEDS>>>>>>>>      PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLES/HR
 STREAM NO.          1           2
   NAME            FEED 1      PROD. 1
 COMPONENT
 H2               450.000     229.013
 CH4                0.000     220.987
 C6H6               0.000     220.987
 C7H8             233.000      12.013

   TOTAL          683.000     683.000

 T,DEG F          1200.00     1431.90
 P,PSIA            495.00      490.00
 MOL WEIGHT       32.7614     32.7614
 D,LB/FT3          0.8879      0.7765
 L/F(MOLAR)        0.0000      0.0000


 VOLUMETRIC FLOW RATE =  28817.78  FT3/HR


 POWER REQUIRED FOR MIXING   =  1.16  HP
 (ASSUMING SIX-BLADE TURBINE,
  AND FOUR BAFFLES IN REAC. )


 THE REACTOR VOLUME =  500.00  FT3
```

TABLE XIX

A SAMPLE OUTPUT OF QG AND QR VALUES FOR THE CASE OF HYDRODEALKYLATION OF TOLUENE

```
ORT= 1200.00  QG= 0.175898E+07  QR=   0.000000
ORT= 1230.00  QG= 0.224941E+07  QR=    515537.
ORT= 1260.00  QG= 0.270871E+07  QR= 0.103107E+07
ORT= 1290.00  QG= 0.310220E+07  QR= 0.154661E+07
ORT= 1320.00  QG= 0.341728E+07  QR= 0.206215E+07
ORT= 1350.00  QG= 0.365863E+07  QR= 0.257769E+07
ORT= 1380.00  QG= 0.386341E+07  QR= 0.309322E+07
ORT= 1410.00  QG= 0.395726E+07  QR= 0.360876E+07
ORT= 1460.00  QG= 0.408728E+07  QR= 0.446799E+07
ORT= 1480.00  QG= 0.412185E+07  QR= 0.481168E+07
```

APPENDIX H

THE COMPUTER CODE OF THE MODEL

```
C$DEBUG
C
C     ****************************************************
C
C          This program simulates a homogeneous continuous
C     stirred tank reactor.  A maximum of twenty reacting
C     or product components and fifteen reactions are
C     allowed.
C
C                                   Shriniwas S. Talwalkar
C     ****************************************************
      DIMENSION X(20),FX(20),Y(20)
      CHARACTER*4 CNAME1(20),CNAME2(20)
      COMMON/VAR11/NCP
      COMMON/VAR12/F(20)
      COMMON/RT2/TOP
      COMMON/RT4/ISN
      COMMON/AL1/IEOS,IPROP
      COMMON/AL2/IFD(20)
      COMMON/AL3/TC(20),PC(20),OMG(20),TB(20),WT(20),
     1           ZRA(20)
      COMMON/AL5/CNAME1,CNAME2
      COMMON/AL4/CPA(20),CPB(20),CPC(20),CPD(20),CPE(20),
     1           CPF(20)
      COMMON/EN/CPVAPA(20),CPVAPB(20),CPVAPC(20),CPVAPD(20)
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
      COMMON/HI/EQNO(20),A(20),B(20),C(20),D(20)
      COMMON/VAR/TIN
      COMMON/VAD/PIN,OPR
      COMMON/UO1/ICC,CSN,PFR,VR,ORT,MD1,PL,RS
      COMMON/FIX1/FO(20)
      COMMON/OL2/QGE,QRE
      COMMON/OT1/IST
      COMMON/OV/DM(20)
      COMMON/ST1/RPM
      OPEN(14,FILE='CSTR.OUT',STATUS='UNKNOWN')
      OPEN(11,FILE='DATA.DAT',STATUS='UNKNOWN')
      OPEN(3,FILE='HEAT.OUT',STATUS='UNKNOWN')
      OPEN(12,FILE='R.OUT',STATUS='UNKNOWN')
      CALL INPUT
      MAT=0
      RVF=0.0
      MD1=ISN-1
C
C     Transfer the inlet flow rates of components from
C     array FO to F.
C
      DO 10 I=1,NCP
      FO(I)=F(I)
 10   CONTINUE
 92   CONTINUE
      IF(MAT.EQ.1) GO TO 93
```

```
C
C     Enter inlet conditions.
C
      WRITE(6,7)
  7   FORMAT('ENTER THE INLET TEMP IN DEG F')
      READ(5,*) TIN
      WRITE(6,8)
  8   FORMAT('ENTER THE INLET PRESSURE IN PSIA')
      READ(5,*) PIN
 93   WRITE(6,94)
 94   FORMAT('ENTER THE OUTLET PR. OPTION',
     1 / 'ENTER 1 IF PR. DROP IS TO BE SPECIFIED',
     2 / 'ENTER 0 IF OUTLET PR. IS TO BE SPECIFIED'/)
      READ(5,*) OPO
      IF(OPO)93,95,96
 95   WRITE(6,97)
 97   FORMAT('ENTER OUTLET PR. FROM REACTOR IN PSIA')
      READ(5,*) OPR
      GO TO 99
 96   WRITE(6,98)
 98   FORMAT('ENTER PR. DROP ACROSS REACTOR')
      READ(5,*) PRD
      OPR=PIN-PRD
 99   WRITE(6,131)
 131  FORMAT('ENTER THE RPM FOR STIRRER')
      READ(5,*) RPM
      N=NCP
      IF(TOP.EQ.1) N=N+1
C
C     Input for the conversion criterion
C
 71   WRITE(6,16)
 16   FORMAT('ENTER THE CONVERSION CRITERIA',
     1 / '      0 FOR REACTOR VOLUME  ',
     2 / '      1 FOR OUTLET TEMP  ',
     3 / '      2 FOR PRODUCTION RATE '/)
      READ(5,*) ICC
      IF(ICC)71,17,19
 17   WRITE(6,18)
 18   FORMAT('ENTER THE DESIRED REACTOR VOLUME IN FT3')
      READ(5,*) VR
      WRITE(6,301)
 301  FORMAT('DO YOU WANT TO SPECIFY TEMP ALSO',
     1 / '       0  YES              ',
     2 / '       1  NO               '/)
      READ(5,*) IST
      IF(IST.EQ.0) THEN
      N=N-1
      WRITE(6,302)
 302  FORMAT('ENTER THE TEMP IN F')
      READ(5,*) ORT
      END IF
      GO TO 27
```

```
 19   IF(ICC.GT.2)GO TO 71
      IF(ICC.EQ.2)GO TO 23
      WRITE(6,21)
 21   FORMAT('ENTER THE OUTLET REACTOR TEMP IN F')
      READ(5,*) ORT
      GO TO 27
 23   WRITE(6,22)
 22   FORMAT('ENTER THE COMPONENT SEQUENCE NO.')
      READ(5,*) CSN
      WRITE(6,24)
 24   FORMAT('ENTER THE DESIRED PRODUCTION RATE')
      READ(5,*) PFR
C
C    Store the guesses in the X array.
C
27   DO 20 I=1,NCP
      IF(ICC.EQ.2.AND.I.EQ.CSN) GO TO 191
      WRITE(6,30) I
 30   FORMAT('ENTER GUESS FOR F(I) OF COMP. NO ',I4)
      READ(5,*) X(I)
 191  CONTINUE
 20   CONTINUE
      ERLIM=1.E-2
      IF(TOP.EQ.0) GO TO 31
      IF(ICC.EQ.0) GO TO 35
      IF(ICC.EQ.1) GO TO 33
      IF(ICC.EQ.2) GO TO 34
 35   RV=VR
      IF(IST.EQ.0) GO TO 78
      WRITE(6,72)
 72   FORMAT('ENTER GUESS FOR THE REACTOR TEMP')
      READ(5,*) X(N)
      GO TO 78
 33   WRITE(6,70)
      READ(5,*) X(N)
      GO TO 161
 34   WRITE(6,70)
      READ(5,*) RV
      X(CSN)=RV
      WRITE(6,72)
      READ(5,*) X(N)
      GO TO 78
 31   IF(ICC.EQ.0) GO TO 75
      WRITE(6,70)
 70   FORMAT('ENTER THE GUESS FOR REACTOR VOLUME')
      READ(5,*) RV
      X(CSN)=RV
      GO TO 78
 75   RV=VR
      GO TO 78
 161  RV=X(N)
 78   CALL NEWTON(RV,N,X,FX,ERLIM)
      WRITE(3,*) 'AT ORT=',ORT,'QGE=',QGE,'QRE=',QRE
```

```
      WRITE(12,*) 'OVER'
C
C     Option of making another run
C
      WRITE(6,91)
 91   FORMAT('DO YOU WANT TO MAKE ANOTHER RUN',
     1 / '      0   YES   ',
     2 / '      1   NO   '/)
      READ(5,*) MRUN
      RVF=RVF+RV
      IF(ICC.EQ.1) THEN
      RS=X(N)
      GO TO 163
      END IF
      IF(ICC.EQ.2) THEN
      RS=X(CSN)
      GO TO 163
      END IF
      RS=RV
 163  IF(MRUN.EQ.1) THEN
      MD1=MD1+1
      IF(TYRUN.EQ.1) MD1=ISN
      GO TO 202
      END IF
C
C     Option of running the next reactor in series
C
      WRITE(6,201)
 201  FORMAT('ENTER THE TYPE OF RUN',
     1 / '    0   IF THE REACTOR IS TO BE IN SERIES',
     2 / '    1   IF A NEW RUN IS TO BE MADE'/)
      READ(5,) TYRUN
      IF(TYRUN.EQ.0) GO TO 203
      MD1=ISN
      CALL OUTPUT(X)
      MAT=2
      GO TO 92
C
C     The outlet stream properties are converted into
C     input to the next reactor in series.
C
 203  MD1=MD1+1
      CALL OUTPUT(X)
      DO 111 I=1,NCP
      FO(I)=X(I)
 111  CONTINUE
      PIN=OPR
      IF(ICC.EQ.1) THEN
      TIN=ORT
      GO TO 162
      END IF
      IF(TOP.EQ.1) TIN=X(N)
 162  MAT=1
```

```
      GO TO 92
 202  CALL OUTPUT(X)
      STOP
      END

C
C
C     Input Subroutine
C
      SUBROUTINE INPUT
      CHARACTER*4 CI(2)
      DOUBLE PRECISION CINP(28)
      CHARACTER*4 CNAME1(20),CNAME2(20)
      COMMON/VAR11/NCP
      COMMON/VAR12/F(20)
      COMMON/VAR18/NRX
      COMMON/VAR19/KRX(15)
      COMMON/VAR22/AO(15),AE(15)
      COMMON/VAR31/OCP(20,15)
      COMMON/VAR51/STOC(20,15)
      COMMON/RT1/HR(15)
      COMMON/RT2/TOP
      COMMON/RT4/ISN
      COMMON/EMP1/GFE(15)
      COMMON/AL1/IEOS,IPROP
      COMMON/AL2/IFD(20)
      COMMON/AL3/TC(20),PC(20),OMG(20),TB(20),WT(20),
     1             ZRA(20)
      COMMON/AL5/CNAME1,CNAME2
      COMMON/AL4/CPA(20),CPB(20),CPC(20),CPD(20),CPE(20),
     1           CPF(20)
      COMMON/EN/CPVAPA(20),CPVAPB(20),CPVAPC(20),CPVAPD(20)
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
      COMMON/HI/EQNO(20),A(20),B(20),C(20),D(20)
      COMMON/OT1/IST
      COMMON/OV/DM(20)
      COMMON/ST1/RPM
      WRITE(6,1)
  1   FORMAT('ENTER THE STREAM ID NO TO REACTOR UNIT',I3)
      READ(5,*) ISN
      WRITE(6,2)
  2   FORMAT('ENTER PRODUCT STREAM ID NO FROM REACTOR',I3)
      READ(5,*) NSN
      WRITE(6,3)
  3   FORMAT('ENTER NO. OF COMPONENTS')
      READ(5,*) NCP
      WRITE(6,4)
  4   FORMAT('ENTER NO. OF REACTIONS')
      READ(5,*) NRX
      DO 10 J=1,NCP
      WRITE(6,5) J
  5   FORMAT('ENTER COMP. ID NO OF COMP #',I3)
      READ(5,*) IFD(J)
```

```
      WRITE(6,6) J
 6    FORMAT('ENTER FLOW RATE OF COMP #',I3,'IN LB-
     1        MOLS/HR')
      READ(5,*) F(J)
10    CONTINUE
      WRITE(6,9)
 9    FORMAT('ENTER TYPE OF OPERATION',
     1 / ' ENTER   0    FOR ISOTHERMAL ',
     2 / ' ENTER   1    FOR ADIABATIC  '/)
      READ(5,*) TOP
      DO 30 I=1,NRX
      WRITE(6,28) I
28    FORMAT('IS REACTION ',I3,'IN EQUILIBRIUM',
     1 / ' ENTER    1:NO     2:YES    '/)
      READ(5,*) KRX(I)
      IF(KRX(I).EQ.2)GO TO 40
      WRITE(6,29) I
29    FORMAT('ENTER THE FREQUENCY FACTOR OF REACTION',I3)
      READ(5,*) AO(I)
      WRITE(6,31) I
31    FORMAT('ENTER THE ACTIVATION ENERGY OF REACTION',I3)
      READ(5,*) AE(I)
      WRITE(6,32) I
32    FORMAT('ENTER THE HEAT OF REACTION',I3)
      READ(5,*) HR(I)
      GO TO 50
40    WRITE(6,33) I
33    FORMAT('ENTER THE GIBBS FREE ENERGY FOR REACTION',I3)
      READ(5,*) GFE(I)
      WRITE(6,34) I
34    FORMAT('ENTER THE HEAT OF REACTION',I3)
      READ(5,*) HR(I)
50    CONTINUE
30    CONTINUE
      DO 70 J=1,NRX
       DO 60 I=1,NCP
      IF(KRX(J).EQ.2)GO TO 36
      WRITE(6,35) I,J
35    FORMAT('ENTER ORDER OF COMPONENT #',I4,'IN
     1        REACTION',I4)
      READ(5,*) OCP(I,J)
36    WRITE(6,37) I,J
37    FORMAT('ENTER THE STOICHIOMETRIC COEFF. OF COMP
     1       #',I4, ' IN REACTION',I4)
      READ(5,*) STOC(I,J)
60     CONTINUE
70    CONTINUE
      WRITE(6,13)
13    FORMAT('ENTER THE TYPE OF EQN. TO USE',
     1 / '      1   RK    ',
     2 / '      2   SRK   ',
     3 / '      3   PR    ',
     4 / '      4   HBT   '/)
```

```
      READ(5,*) IEOS
      WRITE(6,12)
 12   FORMAT('ENTER THE TYPE OF FLUID',
     1 / '      1    LIQUID',
     2 / '      2    VAPOR'/)
      READ(5,*) IPROP
C
C     Read component properties from the data file
C
      IFD(NCP+1)=62
      DO 201 I=1,62
      READ(11,100) CI(1),CI(2),(CINP(K),K=1,28)
 100  FORMAT(/1X,2A4,1X,3F8.4/1X,5F8.4,1X/1X,3F8.4,1X/1X,
     1       4E10.3,1X/1X,3F10.5,1X/1X,3F10.5,
     2       1X/1X,4E10.3,1X/1X,3F10.5,1X/)
      DO 202 J=1,NCP+1
      IF(I.EQ.IFD(J)) THEN
      CNAME1(J)=CI(1)
      CNAME2(J)=CI(2)
      TC(J)=CINP(1)
      PC(J)=CINP(2)
      OMG(J)=CINP(3)
      TB(J)=CINP(4)
      WT(J)=CINP(5)
      ZRA(J)=CINP(6)
      VC(J)=CINP(7)
      CPLA(J)=CINP(8)
      CPLB(J)=CINP(9)
      CPLC(J)=CINP(10)
      EQNO(J)=CINP(11)
      A(J)=CINP(12)
      B(J)=CINP(13)
      C(J)=CINP(14)
      D(J)=CINP(15)
      CPA(J)=CINP(16)
      CPB(J)=CINP(17)
      CPC(J)=CINP(18)
      CPD(J)=CINP(19)
      CPE(J)=CINP(20)
      CPF(J)=CINP(21)
      CPVAPA(J)=CINP(22)
      CPVAPB(J)=CINP(23)
      CPVAPC(J)=CINP(24)
      CPVAPD(J)=CINP(25)
      DM(J)=CINP(26)
      END IF
 202  CONTINUE
 201  CONTINUE
      RETURN
      END
```

```
C
C     Subroutine to calculate the volumetric flow rate.
C
      SUBROUTINE STRFLOW(TO,FO,VFR)
      DOUBLE PRECISION RHO(50)
      DOUBLE PRECISION TD(50),PP(50),RHOVC(50),FD(20),
     1                 RHOLC(50)
      DIMENSION FM(20),FO(20)
      COMMON/VAR11/NCP
      COMMON/VAR/TIN
      COMMON/FIX1/FIN(20)
      COMMON/UO1/ICC,CSN,PFR,VR,ORT,MD1,PL,RS
      COMMON/EV1/WM(20)
      COMMON/EV2/DS
      COMMON/VAD/PIN,OPR
      COMMON/AL1/IEOS,IPROP
      COMMON/AL3/
      TC(20),PC(20),OMG(20),TB(20),WT(20),ZRA(20)
      COMMON/AL4/CPA(20),CPB(20),CPC(20),CPD(20),CPE(20),
     1           CPF(20)
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
C
C     Transfer the flow rates into FD array
C
      DO 4 I=1,NCP
      IF(ICC.EQ.2.AND.I.EQ.CSN) THEN
      FD(I)=PFR
      GO TO 101
      END IF
      FD(I)=FO(I)
      WRITE(6,*) 'WT(I)=',WT(I)
 101  CONTINUE
 4    CONTINUE
C
C     The pressure and temperature are transferred into
C     the PP, and TD array respectively for input to
C     calculation of density.
C
      PP(1)=OPR/14.504
      TD(1)=TO/1.8
      IF(IPROP.EQ.1.AND.IEOS.EQ.4) THEN
      CALL DENS(FD,NCP,TD,RHO)
      GO TO 20
      END IF
 40   CALL VAPDEN(NCP,TD,PP,FD,RHOVC,RHOLC)
      IF(IPROP.EQ.1) THEN
      DS=RHOLC(1)*62.43
      GO TO 30
      END IF
      DS=RHOVC(1)*62.43
      GO TO 30
 20   DS=RHO(1)*62.43
 30   WRITE(6,*) 'DS=',DS
```

```
      FMW=0.0
      DO 10 I=1,NCP
      FM(I)=FD(I)*WT(I)
      FMW=FM(I)+FMW
 10   CONTINUE
      VFR = FMW/DS
      WRITE(6,*) 'VFR=',VFR
      RETURN
      END
C
C     Subroutine to calculate the rate constants of the
C     reactions.
C
      SUBROUTINE RATEC(TO,RK)
      DIMENSION RK(15)
      COMMON/VAR18/NRX
      COMMON/VAR19/KRX(15)
      COMMON/VAR22/AO(15),AE(15)
      GC=1.986
      DO 10 I=1,NRX
      IF(KRX(I).EQ.2)GO TO 20
      RK(I)=AO(I)*EXP(-AE(I)/(GC*TO))
      WRITE(*,*) 'RK(I)=',RK(I)
 20   CONTINUE
 10   CONTINUE
      RETURN
      END
C
C     Subroutine to develop a rate equation for each
C     reaction.
C
      SUBROUTINE RATERN(TO,VFR,RK,F,RATE)
      DIMENSION RC(15),RK(15),F(20),RATE(15)
      COMMON/VAR31/OCP(20,15)
      COMMON/VAR11/NCP
      COMMON/VAR18/NRX
      COMMON/UO1/ICC,CSN,PFR,VR,ORT,MD1,PL,RS
      COMMON/VAR19/KRX(15)
      DO 20 J=1,NRX
      IF(KRX(J).EQ.2)GO TO 10
      SUM=0.0
      DO 30 I=1,NCP
      SUM=SUM+ABS(OCP(I,J))
 30   CONTINUE
      RC(J)=RK(J)
C
C     Calculate rate of reaction for irreversible reaction.
C
      DO 40 I=1,NCP
      IF(F(I).LE.0.0.OR.OCP(I,J).EQ.0.0)GO TO 40
      IF(ICC.EQ.2.AND.I.EQ.CSN) THEN
      RC(J)=RC(J)*(PFR**(OCP(I,J)))
      GO TO 40
```

```
      END IF
      RC(J)=RC(J)*(F(I)**(OCP(I,J)))
 40   CONTINUE
      RATE(J)=RC(J)/VFR**SUM
      WRITE(*,*) 'RATE(J)=',RATE(J)
 10   CONTINUE
 20   CONTINUE
C
C     Call EQURN to calculate the rate of the reversible
C     reaction.
C
      DO 50 J=1,NRX
      IF(KRX(J).EQ.1)GO TO 60
      CALL EQURN(J,TO,RATE)
      WRITE(*,*) 'RATE(J)=',RATE(J)
 60   CONTINUE
 50   CONTINUE
      RETURN
      END
C
C     Subroutine to set up the total rate expression
C     for each component.
C
      SUBROUTINE RATECOMP(RATE,RCOMP)
      DIMENSION RCOMP(20),RATE(15)
      COMMON/VAR11/NCP
      COMMON/VAR18/NRX
      COMMON/VAR51/STOC(20,15)
      DO 10 I=1,NCP
      RCOMP(I)=0.0
C
C     Rates of the components are calculated from the rates
C     of reactions and the stoichiometric coefficients.
C
      DO 20 J=1,NRX
      RCOMP(I)=RCOMP(I)+STOC(I,J)*RATE(J)
 20   CONTINUE
      WRITE(*,*) 'RCOMP(I)=',RCOMP(I)
 10   CONTINUE
      RETURN
      END
C
C     Subroutine to calculate the difference in temperature
C     between inlet and outlet.
C
      SUBROUTINE TEMPDIF(N,RATE,DT)
      COMMON/VAR11/NCP
      COMMON/FIX1/FO(20)
      COMMON/RT1/HR(15)
      COMMON/VAR18/NRX
      COMMON/VAR/TIN
      COMMON/AL2/IFD(20)
      COMMON/AL3/TC(20),PC(20),OMG(20),TB(20),WT(20),
```

```
     1          ZRA(20)
      COMMON/AL4/CPA(20),CPB(20),CPC(20),CPD(20),CPE(20),
     1          CPF(20)
      COMMON/EN/CPVAPA(20),CPVAPB(20),CPVAPC(20),CPVAPD(20)
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
      COMMON/OL1/DH,FCP
      DIMENSION CP(20),RATE(15)
      TS=TIN+459.67
      DH=0.0
      DO 10 J=1,NRX
      DH=DH+HR(J)*RATE(J)
 10   CONTINUE
      CALL SPHEAT(NCP,TS,CP)
      FCP=0.0
      DO 20 I=1,NCP
      FCP=FCP+CP(I)*FO(I)
 20   CONTINUE
      DT=-(DH/FCP)
      RETURN
      END
C
C
C     Subroutine to set up the non-linear equations.
C
      SUBROUTINE EQUATN(RV,N,X,FX)
      DIMENSION FX(20),X(20),RCOMP(20),RK(15),RATE(15)
      COMMON/FIX1/FO(20)
      COMMON/VAR/TIN
      COMMON/RT2/TOP
      COMMON/VAR11/NCP
      COMMON/RT1/HR(15)
      COMMON/OL1/DH,FCP
      COMMON/UO1/ICC,CSN,PFR,VR,ORT,MD1,PL,RS
      COMMON/AL2/IFD(20)
      COMMON/AL3/TC(20),PC(20),OMG(20),TB(20),WT(20),
     1          ZRA(20)
      COMMON/AL4/CPA(20),CPB(20),CPC(20),CPD(20),CPE(20),
     1          CPF(20)
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
      COMMON/EN/CPVAPA(20),CPVAPB(20),CPVAPC(20),CPVAPD(20)
      COMMON/AL1/IEOS,IPROP
      COMMON/OL2/QGE,QRE
      COMMON/OT1/IST
      IF(TOP.EQ.0) GO TO 40
      IF(ICC.EQ.1) THEN
      TO=ORT+459.67
      GO TO 60
      END IF
      IF(ICC.EQ.0.AND.IST.EQ.0) THEN
      TO=ORT+459.67
      GO TO 60
      END IF
      TO=X(N)+459.67
```

```
      GO TO 60
 40   TO=TIN+459.67

C
C    Calls are given to the various subroutines from this
C    subroutine.
C
60    CALL STRFLOW(TO,X,VFR)
      CALL RATEC(TO,RK)
      CALL RATERN(TO,VFR,RK,X,RATE)
      WRITE(12,61) TO,RATE
 61   FORMAT('AT TEMP=',F8.2,2X,'RATE=',F10.5)
      CALL RATECOMP(RATE,RCOMP)
      IF(ICC.EQ.0.AND.IST.EQ.0) GO TO 11
      IF(ICC.EQ.0) GO TO 11
      IF(ICC.EQ.2) GO TO 12
      DO 160 I=1,NCP
      FX(I)=FO(I)-X(I)+(RCOMP(I)*X(N))
 160  CONTINUE
      GO TO 161
 11   DO 10 I=1,NCP
      FX(I)=FO(I)-X(I)+(RCOMP(I)*RV)
 10   CONTINUE
      GO TO 161
 12   DO 13 I=1,NCP
      IF(ICC.EQ.2.AND.I.EQ.CSN) THEN
      FX(I)=FO(I)-PFR+(RCOMP(I)*X(CSN))
      GO TO 13
      END IF
      FX(I)=FO(I)-X(I)+(RCOMP(I)*X(CSN))
 13   CONTINUE
C
C     Call the subroutine TEMPDIF for adiabatic operation
C     in the reactor.
C
 161  IF(TOP.EQ.0) GO TO 30
      CALL TEMPDIF(N,RATE,DT)
C
C     Calculate the QG and QR values.
C
      IF(ICC.EQ.0.AND.IST.EQ.0) THEN
      QGE=(-DH)*RV
      QRE=(FCP)*(ORT-TIN)
      GO TO 30
      END IF
      QGE=0.0
      QRE=0.0
      WRITE(6,*) 'TIN=',TIN,'X(N)=',X(N)
      WRITE(6,*) 'DT=',DT
      IF(ICC.EQ.1) THEN
      QGE=(-DH)*X(N)
      QRE=(-FCP)*(TIN-ORT)
       FX(N)=TIN-ORT+(DT*X(N))
```

```
      WRITE(3,*) 'ORT=',ORT,'QGE=',QGE,'QRE=',QRE
      GO TO 30
      END IF
      IF(ICC.EQ.2) THEN
      QGE=(-DH)*X(CSN)
      QRE=(-FCP)*(TIN-X(N))
      FX(N)=TIN-X(N)+(DT*X(CSN))
      WRITE(3,*) 'TEMP=',X(N),'QGE=',QGE,'QRE=',QRE
      GO TO 30
      END IF
      QGE=(-DH)*RV
      QRE=(-FCP)*(TIN-X(N))
      FX(N)=TIN-X(N)+(DT*RV)
      WRITE(3,*) 'TEMP=',X(N),'QGE=',QGE,'QRE=',QRE
 30   CONTINUE
      RETURN
      END
C
C
C     Subroutine for checking equilibrium conditions.
C
      SUBROUTINE EQURATE(J,TO,RA,FRA)
      DIMENSION REFK(15),EQU(15),EQF(15)
      COMMON/EMP1/GFE(15)
      COMMON/RT1/HR(15)
      COMMON/VAR11/NCP
      COMMON/VAR51/STOC(20,15)
      COMMON/VAR12/F(20)
      COMMON/VAD/PO,OPR
      R=1.987
C
C     Calculate the equilibrium constant
C
      REFK(J)=EXP(-(GFE(J)/(R*536.4)))
      EQU(J)=REFK(J)*EXP(-(HR(J)/R)*(1./TO-1./536.4))
      SS=0.0
      DO 10 I=1,NCP
      SS=SS+STOC(I,J)
 10   CONTINUE
C
C     Set up the equilibrium criterion.
C
      Y=0.0
      DO 20 I=1,NCP
      EQF(I)=F(I)+STOC(I,J)*RA
      Y=Y+EQF(I)
 20   CONTINUE
      IF(SS.EQ.0)GO TO 30
      EQM=EQU(J)*(Y**SS)*(PO**(-SS))
      GO TO 40
 30   EQM=EQU(J)
 40   EQR=1.0
      DO 50 I=1,NCP
```

```
      IF(STOC(I,J).EQ.0)GO TO 60
      IF(EQF(I).EQ.0)GO TO 60
      EQR=EQR*(ABS(EQF(I))**STOC(I,J))
 60   CONTINUE
 50   CONTINUE
      FRA=EQM-EQR
      RETURN
      END

C
C     Subroutine to set up the equilibrium limitations
C     of the reactions in equilibrium.
C
      SUBROUTINE EQURN(J,TO,RATE)
      DIMENSION RATE(15)
      TOL=0.0001
      ALPHA=0.0
      BETA=1.0
      ICOUNT=1
 10   CONTINUE
C
C     Use of the bisection method for calculation of the
C     rate of the reversible reaction.
C
      CALL EQURATE(J,TO,ALPHA,RALPHA)
      IF(ABS(RALPHA).LE.TOL)GO TO 40
      CALL EQURATE(J,TO,BETA,RBETA)
      RW=(ALPHA+BETA)/2.0
      CALL EQURATE(J,TO,RW,RRW)
      PROD1=RALPHA*RRW
      PROD2=RBETA*RRW
      IF(PROD1.LT.0)GO TO 20
      IF(PROD2.LT.0)GO TO 30
      GO TO 50
 20   BETA=RW
      ICOUNT=ICOUNT+1
      IF(ICOUNT.GE.100)GO TO 50
      GO TO 10
 30   ALPHA=RW
      ICOUNT=ICOUNT+1
      IF(ICOUNT.GE.100)GO TO 50
      GO TO 10
 40   RATE(J)=ALPHA
      GO TO 60
 50   CONTINUE
 60   CONTINUE
      RETURN
      END
C
C
C    Output Subroutine
C
      SUBROUTINE OUTPUT(X)
```

```
      CHARACTER*4
      LCOM(20,15),LCOM1(20,15),CNAME1(20),CNAME2(20)
      CHARACTER*4 RCOM(20,15),RCOM1(20,15)
      DOUBLE PRECISION RHO(50)
      DOUBLE PRECISION
      FR(20),TIC(50),PIC(50),RHOVC(50),RHOLC(50) DIMENSION
      X(20),LEFT(15),NRIGHT(15),NNCP(20)
      COMMON/RT2/TOP
      COMMON/UO1/ICC,CSN,PFR,VR,ORT,MD1,PL,RS
      COMMON/VAR11/NCP
      COMMON/VAR18/NRX
      COMMON/VAR19/KRX(15)
      COMMON/VAR31/OCP(20,15)
      COMMON/VAR51/STOC(20,15)
      COMMON/FIX1/FO(20)
      COMMON/VAR/TIN
      COMMON/VAD/PIN,OPR
      COMMON/EV1/WM(20)
      COMMON/EV2/DS
      COMMON/AL1/IEOS,IPROP
      COMMON/AL2/IFD(20)
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
      COMMON/AL3/TC(20),PC(20),OMG(20),TB(20),WT(20),
     1           ZRA(20)
      COMMON/HI/EQNO(20),A(20),B(20),C(20),D(20)
      COMMON/AL5/CNAME1,CNAME2
      COMMON/AL4/CPA(20),CPB(20),CPC(20),CPD(20),CPE(20),
     1           CPF(20)
      COMMON/OT1/IST
      COMMON/OV/DM(20)
      COMMON/ST1/RPM
      IF(TOP.EQ.1) GO TO 25
      WRITE(14,1)
1     FORMAT(' THE OPERATION IN THE REACTOR IS
     1         ISOTHERMAL',/)
      GO TO 26
25    WRITE(14,2)
2     FORMAT(' THE OPERATION IN THE REACTOR IS
     1         ADIABATIC',/)
26    IF(ICC.EQ.0.AND.IST.EQ.0) GO TO 511
      IF(ICC.EQ.0) GO TO 27
      IF(ICC.EQ.1) GO TO 28
      WRITE(14,3) CSN,PFR
3     FORMAT('THE PROD. RATE OF COMP.#',I3,2X,'IS',
     1        F8.2,2X,'LBMOLES/HR')
      GO TO 29
511   WRITE(14,512) VR
512   FORMAT(' THE SPECIFIED REACTOR VOLUME = ',2X,F8.2)
      WRITE(14,513) ORT
513   FORMAT(' THE SPECIFIED OUTLET TEMPERATURE =
     1          ',2X,F9.2)
      GO TO 29
27    WRITE(14,4) VR
```

```
 4     FORMAT(' THE SPECIFIED REACTOR VOLUME = ',2X,F8.2)
       GO TO 29
 28    WRITE(14,5) ORT
 5     FORMAT(' THE SPECIFIED OUTLET TEMPERATURE =
      1          ',2X,F9.2)
C
C     Set up the reactions for output file.
C
29    DO 114 J=1,NRX
       LEFT(J)=0
       NRIGHT(J)=0
       LNO=1
       RNO=1
       DO 115 I=1,NCP
       IF(STOC(I,J).EQ.0) GO TO 116
       IF(STOC(I,J).LT.0) THEN
       LEFT(J)=LEFT(J)+1
       LCOM(LNO,J)=CNAME1(I)
       LCOM1(LNO,J)=CNAME2(I)
       LNO=LNO+1
       END IF
       IF(STOC(I,J).GT.0) THEN
       NRIGHT(J)=NRIGHT(J)+1
       RCOM(RNO,J)=CNAME1(I)
       RCOM1(RNO,J)=CNAME2(I)
       RNO=RNO+1
       END IF
 116   CONTINUE
 115   CONTINUE
       NNCP(J)=LEFT(J)+NRIGHT(J)
       IF(NNCP(J).EQ.2) GO TO 117
       IF(NNCP(J).EQ.3) GO TO 118
       IF(KRX(J).EQ.1) GO TO 119
       WRITE(14,6) LCOM(1,J),LCOM1(1,J),LCOM(2,J),
      1LCOM1(2,J), RCOM(1,J),RCOM1(1,J),RCOM(2,J),RCOM1(2,J)
       GO TO 160
 119   WRITE(14,7) LCOM(1,J),LCOM1(1,J),LCOM(2,J),
      1LCOM1(2,J), RCOM(1,J),RCOM1(1,J),RCOM(2,J),RCOM1(2,J)
       GO TO 160
 117   IF(KRX(J).EQ.1) GO TO 120
       WRITE(14,8) LCOM(1,J),LCOM1(1,J),RCOM(1,J),RCOM1(1,J)
       GO TO 160
 120   WRITE(14,121) LCOM(1,J),LCOM1(1,J),RCOM(1,J),
      1  RCOM1(1,J)
       GO TO 160
 118   IF(LEFT(J).EQ.2) GO TO 122
       IF(KRX(J).EQ.1) GO TO 123
       WRITE(14,124) LCOM(1,J),LCOM1(1,J),RCOM(1,J),
      1RCOM1(1,J), RCOM(2,J),RCOM1(2,J)
       GO TO 160
 123   WRITE(14,125) LCOM(1,J),LCOM1(1,J),RCOM(1,J),
      1RCOM1(1,J), RCOM(2,J),RCOM1(2,J)
       GO TO 160
```

```
122  IF(KRX(J).EQ.1) GO TO 127
     WRITE(14,126) LCOM(1,J),LCOM1(1,J),LCOM(2,J),
    1LCOM1(2,J), RCOM(1,J),RCOM1(1,J)
     GO TO 160
127  WRITE(14,128) LCOM(1,J),LCOM1(1,J),LCOM(2,J),
    1LCOM1(2,J), RCOM(1,J),RCOM1(1,J)
160  CONTINUE
114  CONTINUE
6    FORMAT(//,1X,2A4,2X,'+',2X,2A4,3X,'=',3X,2A4,
    1        2X,'+',2X,2A4 )
7    FORMAT(//,1X,2A4,2X,'+',2X,2A4,3X,'-
    1         >',3X,2A4,2X,'+',2X,2A4)
8    FORMAT(//,5X,2A4,3X,'=',3X,2A4)
121  FORMAT(//,5X,2A4,3X,'->',3X,2A4)
124  FORMAT(//,3X,2A4,3X,'=',3X,2A4,2X,'+',2X,2A4)
125  FORMAT(//,3X,2A4,3X,'->',3X,2A4,2X,'+',2X,2A4)
126  FORMAT(//,3X,2A4,2X,'+',2X,2A4,3X,'=',3X,2A4)
128  FORMAT(//,3X,2A4,2X,'+',2X,2A4,3X,'->',3X,2A4)
     WRITE(14,80)
80   FORMAT(//,2X,'RXN.',3X,'SEQ.#',3X,'ORDER',
    1          3X,'STOICH.',/)
     DO 31 J=1,NRX
     DO 32 I=1,NCP
     WRITE(14,9) J,I,OCP(I,J),STOC(I,J)
9    FORMAT(2X,I3,4X,I3,5X,F5.2,3X,F6.2)
32   CONTINUE
31   CONTINUE
     IF(NRX.EQ.1) GO TO 70
     WRITE(14,90)
90   FORMAT(//////////////////////////)
70   WRITE(14,10) MD1
10   FORMAT(///,' UNIT OPERATION NO.',I3,2X,'IS A REAC
    1        UNIT',/)
     WRITE(14,11)
11   FORMAT('         FEEDS>>>>>>>>PRODUCTS>>>>')
     WRITE(14,12)
12   FORMAT(' STREAM FLOW RATES ARE LB-MOLES/HR')
     WRITE(14,13) MD1,MD1+2
13   FORMAT(2X,'STREAM NO.',6X,I3,9X,I3)
     WRITE(14,15) MD1,MD1
15   FORMAT(4X,'NAME',11X,'FEED',I2,5X,'PROD.',I2)
34   WRITE(14,16)
16   FORMAT(2X,'COMPONENT')
     DO 18 I=1,NCP
     IF(ICC.EQ.2.AND.I.EQ.CSN) THEN
     WRITE(14,17) CNAME1(I),CNAME2(I),FO(I),PFR
     GO TO 18
     END IF
     WRITE(14,17) CNAME1(I),CNAME2(I),FO(I),X(I)
17   FORMAT(2X,2A4,8X,F7.3,5X,F7.3)
18   CONTINUE
     TOTIN=0.0
     TOTOUT=0.0
```

```
      DO 37 I=1,NCP
      TOTIN=TOTIN+FO(I)
      IF(ICC.EQ.2.AND.I.EQ.CSN) THEN
      TOTOUT=TOTOUT+PFR
      GO TO 37
      END IF
      TOTOUT=TOTOUT+X(I)
37    CONTINUE
      WRITE(14,23) TOTIN,TOTOUT
23    FORMAT(/,4X,'TOTAL',9X,F7.3,5X,F7.3,/)
      IF(TOP.EQ.1) GO TO 39
      WRITE(14,24) TIN,TIN
24    FORMAT(2X,'T,DEG F',9X,F7.2,5X,F7.2)
      GO TO 40
39    N=NCP+1
      IF(ICC.EQ.0.AND.IST.EQ.0) THEN
      N=NCP
      WRITE(14,43) TIN,ORT
      GO TO 40
      END IF
      IF(ICC.EQ.1) THEN
      WRITE(14,43) TIN,ORT
      GO TO 40
      END IF
      WRITE(14,43) TIN,X(N)
43    FORMAT(2X,'T,DEG F',9X,F7.2,5X,F7.2)
40    WRITE(14,44) PIN,OPR
44    FORMAT(2X,'P,PSIA',10X,F7.2,5X,F7.2)
      WMIN=0.0
      WMOUT=0.0
      DO 42 I=1,NCP
      WMIN=WMIN+(FO(I)/TOTIN)*WT(I)
      IF(ICC.EQ.2.AND.I.EQ.CSN) THEN
      WMOUT=WMOUT+(PFR/TOTOUT)*WT(I)
      GO TO 42
      END IF
      WMOUT=WMOUT+(X(I)/TOTOUT)*WT(I)
42    CONTINUE
      WRITE(14,45) WMIN,WMOUT
45    FORMAT(2X,'MOL WEIGHT',6X,F7.4,5X,F7.4)
      PIC(1)=PIN/14.504
      TIC(1)=(TIN+459.67)/1.8
      DO 60 I=1,NCP
      FR(I)=FO(I)
60    CONTINUE
      N=NCP
      IF(IEOS.EQ.4) THEN
      CALL DENS(FR,NCP,TIC,RHO)
      DIN=RHO(1)*62.43
      GO TO 102
      END IF
      CALL VAPDEN(N,TIC,PIC,FR,RHOVC,RHOLC)
      IF(IPROP.EQ.1)GO TO 101
```

```
      DIN=RHOVC(1)*62.43
      GO TO 102
 101  DIN=RHOLC(1)*62.43
 102  WRITE(14,46) DIN,DS
 46   FORMAT(2X,'D,LB/FT3',8X,F7.4,5X,F7.4)
      IF(IPROP.EQ.1) GO TO 19
      WRITE(14,47)
 47   FORMAT(2X,'L/F(MOLAR)',7X,'0.0000',6X,'0.0000')
      GO TO 161
 19   WRITE(14,20)
 20   FORMAT(2X,'L/F(MOLAR)',7X,'1.0000',6X,'1.0000')
 161  CALL POWER(X,POW)
      WRITE(14,201) POW
 201  FORMAT(///,2X,'POWER REQUIRED FOR
      MIXING=',F6.2,2X,'HP') WRITE(14,48) RS
 48   FORMAT(//,2X,'THE REACTOR VOLUME = ',F7.2,2X,'FT3')
      RETURN
      END
C
C
C      Subroutine to calculate the gas viscosity
C
      SUBROUTINE VISCO(F,VISCG)
      REAL F(20),YI(20),TR(20),VISC(20)
      COMMON/VAR11/NCP
      COMMON/RT2/TOP
      COMMON/UO1/ICC,CSN,PFR,VR,ORT,MD1,PL,RS
      COMMON/VAR/TIN
      COMMON/HI/EQNO(20),A(20),B(20),C(20),D(20)
      COMMON/OT1/IST
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
      COMMON/AL3/TC(20),PC(20),OMG(20),TB(20),WT(20),
     1            ZRA(20)
      COMMON/OV/DM(20)
      IF(TOP.EQ.0) THEN
      T=(TIN+459.67)/1.8
      GO TO 40
      END IF
      IF(ICC.EQ.0.AND.IST.EQ.0) THEN
      T=(ORT+459.67)/1.8
      GO TO 40
      END IF
      IF(ICC.EQ.1) THEN
      T=(ORT+459.67)/1.8
      ELSE
      N=NCP+1
      T=(F(N)+459.67)/1.8
      END IF
 40   YSUM=0.0
      DO 60 I=1,NCP
      YSUM=YSUM+F(I)
 60   CONTINUE
      DO 50 I=1,NCP
```

```
      YI(I)=F(I)/YSUM
 50   CONTINUE
      WRITE(*,*) 'YSUM=',YSUM,'T=',T
C
C     Calculate the viscosity of the individual components.
C
      DO 10 I=1,NCP
      TR(I)=T/TC(I)
      DMR=(131.3*DM(I))/((VC(I)*TC(I))**(0.5))
      FC=1-0.2756*OMG(I)+0.05903*(DMR**4)
      TSTAR=1.2593*TR(I)
      SIGV=1.16145*(TSTAR**(-0.14874))+0.52487*(EXP
     1 (-(0.77320*TSTAR)))+2.16178*(EXP(-(2.43787*TSTAR)))
      VISC(I)=(40.785*FC*((WT(I)*T)**0.5))/((VC(I))**(2.0/
     1 3.0)*SIGV)
      WRITE(6,*) 'VISC(I)=',VISC(I)
 10   CONTINUE
C
C     Use of the Herning and Zipperer approximation for
C     calculation of phi required for mixture viscosity.
C
      SUM2=0.0
      DO 20 I=1,NCP
      SUM=0.0
      DO 30 J=1,NCP
      PH=(WT(J)/WT(I))**0.5
      SUM=SUM+YI(J)*PH
 30   CONTINUE
      SUM2=SUM2+(YI(I)*VISC(I))/SUM
 20   CONTINUE
      VISCG=SUM2*1.0E-04
      WRITE(*,*) 'SUM2=',SUM2,'VISCG=',VISCG
      RETURN
      END
C
C     Subroutine to calculate the power required for
C     mixing.
C
      SUBROUTINE POWER(X,POW)
      DIMENSION X(20)
      COMMON/RT2/TOP
      COMMON/EV2/DS
      COMMON/UO1/ICC,CSN,PFR,VR,ORT,MD1,PL,RS
      COMMON/VAR/TIN
      COMMON/HI/EQNO(20),A(20),B(20),C(20),D(20)
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
      COMMON/AL3/TC(20),PC(20),OMG(20),TB(20),WT(20),
     1            ZRA(20)
      COMMON/OV/DM(20)
      COMMON/AL1/IEOS,IPROP
      COMMON/ST1/RPM
      IF(IPROP.EQ.1) THEN
      CALL VISCL(X,VIL)
```

```
      GO TO 20
      END IF
      CALL VISCO(X,VISCG)
      VIL=VISCG
 20   VOL=RS*7.481
C
C     Find the diameter of CSTR based on the volume of
C     the reactor.
C
      IF(VOL.LT.300.0) THEN
      DIA=48.0
      GO TO 10
      END IF
      IF(VOL.LT.500.0) THEN
      DIA=54.0
      GO TO 10
      END IF
      IF(VOL.LT.1000.0) THEN
      DIA=60.0
      GO TO 10
      END IF
      IF(VOL.LT.1200.0) THEN
      DIA=66.0
      GO TO 10
      END IF
      IF(VOL.LT.1250.0) THEN
      DIA=72.0
      GO TO 10
      END IF
      IF(VOL.LT.2200.0) THEN
      DIA=78.0
      GO TO 10
      END IF
      IF(VOL.LT.2500.0) THEN
      DIA=84.0
      GO TO 10
      END IF
      IF(VOL.LT.4000.0) THEN
      DIA=96.0
      GO TO 10
      END IF
      IF(VOL.LT.6000.0) THEN
      DIA=108.0
      GO TO 10
      END IF
      IF(VOL.LT.8000.0) THEN
      DIA=120.0
      GO TO 10
      END IF
      IF(VOL.LT.20000.0) THEN
      DIA=144.0
      GO TO 10
      END IF
```

```
      IF(VOL.LT.30000.0) THEN
      DIA=184.0
      GO TO 10
      END IF
 10   CONTINUE
      WRITE(*,*) 'DIA=',DIA
      IF(VOL.LT.200.0) THEN
      DI=0.5*DIA
      ELSE
      DI=0.33*DIA
      END IF
C
C     Calculate Reynold's number.
C
      WRITE(*,*) 'DI=',DI
      DIS=DI/12.0
      VISC=0.0403*VIL
      REYNO=(DS*RPM*(DIS**2))/VISC
      WRITE(*,*) REYNO
C
C     Calculate the power number from Reynold's number.
C
      IF(REYNO.GE.150.0) THEN
      PON=5.5
      ELSE
      WRITE(6,*) 'REYNO. IS LESS THAN 150.0. ENTER POWER
     1 NO.'
      READ(5,*) PON
      END IF
      WRITE(*,*) PON
C
C     Use of the relation to calculate power required.
C
      POW=1.1*3.52E-03*PON*(DS/62.4)*
     1      ((RPM/60)**3)*((DI/12)**5)+1.0
      WRITE(*,*) POW
      RETURN
      END
C
C
C     Subroutine to calculate the liquid viscosity.
C
      SUBROUTINE VISCL(F,VIL)
      REAL XX(20),F(20)
      COMMON/VAR11/NCP
      COMMON/RT2/TOP
      COMMON/UO1/ICC,CSN,PFR,VR,ORT,MD1,PL,RS
      COMMON/VAR/TIN
      COMMON/HI/EQNO(20),A(20),B(20),C(20),D(20)
      COMMON/OT1/IST
      IF(TOP.EQ.0) THEN
      T=(TIN+459.67)/1.8
      GO TO 40
```

```
      END IF
      IF(ICC.EQ.0.AND.IST.EQ.0) THEN
      T=(ORT+459.67)/1.8
      GO TO 40
      END IF
      IF(ICC.EQ.1) THEN
      T=(ORT+459.67)/1.8
      ELSE
      N=NCP+1
      T=(F(N)+459.67)/1.8
      END IF
 40   SF=0.0
      DO 20 I=1,NCP
      SF=SF+F(I)
 20   CONTINUE
      DO 30 I=1,NCP
      XX(I)=F(I)/SF
 30   CONTINUE
      SUM=0.0
C
C     Calculation of pure component viscosities.
C
      DO 10 I=1,NCP
      IF(EQNO(I).EQ.1.0) THEN
      VIS=A(I)+(B(I)/T)
      GO TO 50
      END IF
      IF(EQNO(I).EQ.2.0) THEN
      VIS=EXP(A(I)+(B(I)/T))
      GO TO 50
      END IF
      VIS=A(I)+(B(I)/T)+C(I)*T+(D(I)/(T*T))
C
C    Calculate the mixture viscosity.
C
 50   SUM=SUM+XX(I)*LOG(VIS)
      WRITE(*,*) VIS
 10   CONTINUE
      VIL=EXP(SUM)
      WRITE(*,*) VIL
      RETURN
      END
C
C     Subroutine to calculate the specific heat of the
C     components.
C
      SUBROUTINE SPHEAT(N,T,CP)
      REAL CP(20),CC(20)
      COMMON/AL2/IFD(20)
      COMMON/AL3/TC(20),PC(20),OMG(20),TB(20),WT(20),
     1           ZRA(20)
      COMMON/AL4/CPA(20),CPB(20),CPC(20),CPD(20),CPE(20),
     1           CPF(20)
```

```
      COMMON/EN/CPVAPA(20),CPVAPB(20),CPVAPC(20),CPVAPD(20)
      COMMON/GH/VC(20),CPLA(20),CPLB(20),CPLC(20)
      COMMON/AL1/IEOS,IPROP
C
C     Use Miller's relation for calculation of liquid
C     specific heat for water and alcohols.
C
      DO 10 I=1,N
      IF(IPROP.EQ.1.AND.IFD(I).GE.61) THEN
      S=T/1.8
      CP(I)=1.986*(CPLA(I)+S*(CPLB(I)*1.0E-03+
     1       S*(CPLC(I)*1.0E-06)))
      GO TO 30
      END IF
      IF(CPA(I).EQ.0.0) THEN
      TM=T/1.8
      CC(I)=CPVAPA(I)+TM*(CPVAPB(I)+TM*(CPVAPC(I)
     2+TM*(CPVAPD(I))))
      MET=0
      GO TO 20
      END IF
      CC(I)=CPB(I)+T*(2.0*CPC(I)*1.0E-04+
     1  T*(3.0*CPD(I)*1.0E-07+T*(4.0*CPE(I)*1.0E-11+
     2  T*(5.0*CPF(I)*1.0E-15))))
      MET=1
C
C     Calculation of liquid heat capacity from ideal gas
C     heat capacity.
C
 20   IF(IPROP.EQ.1) THEN
      TV=T/1.8
      TR=TV/TC(I)
      TRM=1.0-TR
      CP1=1.45+(0.45/TRM)+0.25*OMG(I)*(17.11+
     1      25.2*(TRM**( 1.0/3.0))/TRM+1.742/TRM)
      CP2=EXP(20.1*TR-17.9)
      IF(MET.EQ.1) THEN
      CP(I)=8.314*(CP1-CP2)*0.2389+CC(I)*WT(I)
      GO TO 30
      END IF
      ACCP=8.314*(CP1-CP2)+CC(I)
      CP(I)=ACCP*0.2389
      END IF
      IF(IPROP.EQ.2) THEN
      CP(I)=CC(I)*0.2389
      IF(MET.EQ.1) CP(I)=CC(I)*WT(I)
      END IF
  30  CONTINUE
      WRITE(6,*) 'CP(I)=',CP(I)
  10  CONTINUE
      RETURN
      END
```

VITA

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