INTERACTIVE MODEL OF A HOMOGENEOUS GASEOUS PLUG FLOW REACTOR

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Bachelor of Science

in Chemical Engineering

Oklahoma State University

Stillwater, Oklahoma

1986

Submitted to the Faculty of the Graduate College
of the Oklahoma State University
in partial fulfillment of the requirements
for the Degree of
MASTER OF SCIENCE
December, 1987

INTERACTIVE MODEL OF A HOMOGENEOUS GASEOUS

PLUG FLOW REACTOR

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PREFACE

The purpose of this study was to develop a chemical reactor model. A homogeneous plug flow reactor was introduced into MAXISIM, a process simulator developed and used at Oklahoma State University.

I wish to express my sincere gratitude and appreciation to my major advisor, Dr. Ruth C. Erbar, for her continuous support and assistance throughout all my undergraduate and graduate studies. I am also grateful to my committee members, Dr. Mayis Seapan and Dr. A. H. Johannes for their technical assistance during this work. I thank Mrs. Pamela Hartman for her professional work in typing this thesis.

My deepest appreciation is extended to the Tunisian government and the Scientific Mission of Tunisia for their support all throughout my undergraduate career. And many thanks to Dr. B. L. Crynes and the School of Chemical Engineering for their continuous support and for the excellent education offered.

I wish to express my warm and sincere thanks and appreciation to my dearest family: my loving mother, Hamdouna, my caring sister, Jamila, and her family, and my dear brothers, Wahab and Hamadi, and their families. I would like to express my deepest love and thanks to my memorable father, Hedi, God bless his soul, to whom I dedicate this work.

There are people in my life to whom I owe all the joy and happiness I have had throughout all these years. I would like to express my

gratitude and appreciation to my relatives and all my dear friends, here in the USA and in Tunisia, for their moral support and continued caring.

CHAPTER I

INTRODUCTION

Looking back to the old days when surviving was the only goal mankind searched to achieve, nature seemed to fulfill all our needs. However, as life has evolved, productivity has become a necessity for living. Ever since, man has strived to invent tools and machines for better results and higher achievement. Certainly computers constitute one of the most important and useful tools man has invented to increase not only the productivity of material goods, but also of the mind (1).

In the sixties, computer use was introduced into the domain of education and rapidly started to expand due to the availability of large scale and multiuser digital computers. The traditional teaching method of using chalkboard, projectors, tape recorders, and small teaching devices was criticized to be ineffective and to involve only few students. Whereas the use of educational computer programs allows each and every student to interact with the computer, to follow instructions, and to solve problems (1). This way the student, not only is fully involved in the learning process, but can also feel comfortable if he/she is embarrassed to show his/her "weaknesses" to a teacher or classmates (2). The Computer Assisted Instruction system (CAI), which is the use of the computer for scientific calculations, was first used in many primary or secondary schools and in colleges in the United States of America then reached Europe and Japan (1). Programming Logic for Automated Teaching Operation (PLATO), developed at the University of

Illinois, was the first computer-based educational system to help teach computer topics as well as math and language skills.

The users of these programs usually are not familiar with the software itself which is nothing but a set of mathematical and logical relationships describing a system of interest. These relationships, or equations, based on certain assumptions, constitute a model which is used to gain some understanding of how the corresponding system behaves. In general, models or simulation programs are a two step process. The first step is to convert reality to a model. The simulation is valid if the model adequately represents the real system. The second step is to formulate the model in a code which must do what the model requires for the simulation to be verified. As expected, some real systems are very complex. Depending on the assumptions made, the corresponding models could involve tedious and/or complicated calculations. Fortunately, the presence of desktop computers and modern software allows users with modest mathematical, statistical, and programming backgrounds to represent, explain, predict, and estimate real world phenomena.

Basically, any simulation program presents four main tasks. Firstly, the input data is required from the user in an interactive mode. The input data is usually checked for validity against the program constraints. Secondly, the data is transferred and stored for later use in the program. Thirdly, the program is executed and errors will be detected if present. And finally, the output is made available to the user under request. Despite the development of the computer technology and the advanced software, good models are not readily available, therefore simulation programs should always be used

carefully. And of course, the more technical skills the users have, the better results they obtain.

Chemical engineering simulation systems are interactive computer programs that allow an operator or an engineer to model or to simulate a series of interconnected unit operations in a plant or a single process unit such as a distillation column, a heat exchanger, or a mixed flow reactor. Bonner and Moore, in 1960, published the first chemical simulation system (3). PACER, GEMCS, MAXISIM, SIMSCI, ASPEN, and SIPRO-DTC are other examples of process design simulators. By using such programs, the user is able to set the operating parameters for the unit operations, run the program, review the results, change a few inputs, and run again until an optimum set of results is obtained.

Due to the importance of reactors in the chemical industry, the simulation of chemical reactors had gained considerable attention. Mainly, a reactor model is a set of mathematical relations describing the local production or consumption, the physical properties of the chemicals, the thermodynamics of the system, and the conservation laws (4). 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.

MAXISIM is a complete process design simulator program and is currently used by the students in the School of Chemical Engineering at Oklahoma State University. The focus of this study is to model an ideal gaseous plug flow reactor and include it as a reactor core in MAXISIM. The reactor is designed to handle any type of ten chemical reactions

(elementary and/or nonelementary) and operates isothermally or adiabatically depending on the user's option. The module can be used by students to analyze the performance of the reactor under specified operating conditions. It also allows the users to learn and verify some fundamentals in chemical reactor design.

CHAPTER II

OBJECTIVES

The purpose of this work is to implement a reactor core into MAXISIM, a process design simulation system. The reactor model to be added is a homogeneous gaseous ideal plug flow reactor. It is an interactive program designed for a maximum of ten reactions and fifteen reacting or product components. The chemical reactions can either be elementary or nonelementary, and the reactor can operate both isothermally and adiabatically. Modules from MAXISIM such as "Adder", "Divider", "Compressor", and "Flash" can be used along with the reactor to model a reactor system with recycle.

Once this module is installed in MAXISIM, several tasks can be performed to verify or test some fundamentals in kinetics, reactor and process design. A user would be capable of the following:

1. Determining the required reactor size for a given process and comparing it to known sizes of batch and/or mixed flow reactors.

2. Determining the outlet composition and temperature of a product stream from an operating reactor and comparing it with plant data.

3. Determining the effect of the operation mode (isothermal or adiabatic) on the reactor size or the outlet composition.

4. Determining the effect of recycle on the reactor volume, the outlet composition, the minimum feed required to meet the production specifications.

5. Testing the limitations of a plug flow reactor with recycle.

6. Testing the effect of inerts in the feed.

7. Determining the effect of the feed composition on the product quality.

8. Verifying the kinetics of a process if experimental data is available.

9. Testing the effect of inlet temperature and pressure on reactor performance.

10. Fully describing the process shown in Figure 1 which consists of an adder, a reactor, a high pressure flash, a compressor, and a divider. All the modules except for the reactor are already installed in MAXISIM.

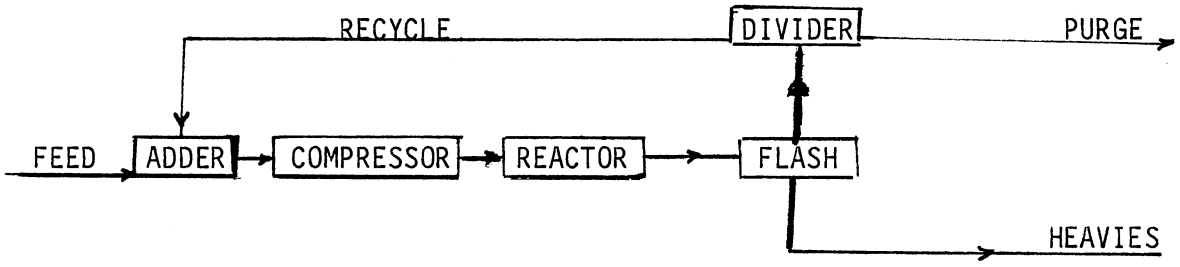


Figure 1. Reactor Loop.

CHAPTER III

LITERATURE REVIEW

Types of Computer Programs

As computer use emerged in education, three main software programs were important: computer-aided instruction, simulators, and small utility packages.

Because of the continuous increase of chemical engineering enrollments in the early eighties, there was a need for computer-based educational instruction techniques. The programs are used to make up for the inability of teachers to give the same level of individualized instruction to the students as they did in former years. These techniques also allow the student to be fully involved and responsible for a complete understanding of the subject and the problem-solving step. PLATO is considered the largest computer-aided instruction program. It has been tested and proven efficient for three chemical engineering courses: stoichiometry, thermodynamics, and unit operations (5). The PLATO system has a unique sophisticated software package which allows the programming of complex highly interactive problems utilizing graphs, diagrams, animations, and even projected slides, in addition to all the usual computational abilities of a large computer. This system is found to be an excellent tool for self-paced instruction of a large number of students who do not need to have any programming background.

On the other hand, process simulators are used in parallel with lectures to verify, test, or criticize some scientific fundamentals and deductions. These programs are also used in industry as an aid for modeling new designs or for improving operating plants. The students or the engineers using these process simulators, usually have a process flow diagram (i.e., flowsheet) to implement. They make use of the interactive mode in these programs to enter the different unit operations and their process data along with feeds specifications and the calculation options. Examples of currently used process simulators are PACER, developed in 1968 (6), CHESS, also developed in 1968 (7), PAS, developed at Oklahoma State University in 1968 (8), and MAXISIM, also developed at Oklahoma State University in 1980 (9). FLOWTRAN, developed at the Monsanto Company, and used in seventy companies and several universities, was introduced in 1973. Quadratic Approximation Programming (QAT), a method based on successive quadratic approximation to the plant objective and constraint function, was used to optimize the FLOWTRAN models (4).

The small utility packages, which form the third type of computer programs used in education and industry, have a rather restricted usage. They cover specified areas in simulations, statistical predictions, and economic analysis. These programs usually do not require any input from the user during the simulation run.

Reactor Simulators

Much of today's industrial technology in petroleum refining, petrochemical processing, and coal conversion center around the use of chemical reactors. Usually, a reactor model is built in several

steps. The first step is to develop a reaction scheme which should be the simplest one that accounts for the observed stoichiometry. The next step is to develop a kinetic model which consists of equations obtained from material and energy balances, activation energies, reaction constants, and physical and thermodynamic properties. The last step is to fit the model to the data by adjusting the parameters. This final step usually involves a number of iterations which are preferably done using a computer.

Mainly such factors as the shape, the numbers of phases, and the flow patterns in the reactor have a great effect on the performance, the design, and the complexity of the calculations. In industry we encounter several types of reactors, such as mixed flow reactors (STR), batch reactors, plug flow reactors (PFR), and others. A detailed description of each is included in Chapter IV. "A Novel Gas-Liquid Stirred Tank Reactor" is an example of an STR model developed by Union Carbide Corporation in 1985 (10). The in-situ coal gasifiers represent a departure from conventional chemical reactors in that their boundaries are not fixed. Such an "unusual" reactor model is being used in several countries including the United States and the Societ Union to recover coal reserves below strip mining depth. Gas or liquid reactors, fixed bed, moving-bed, fluidized-bed, and entrained flow reactors are also frequently used in industry (11).

CHAPTER IV

TYPES OF REACTORS

In order to achieve a good understanding of the kinetics taking place in real reactors, three main ideal reactors are considered: the batch reactor, the Plug Flow Reactor (PFR), and the mixed flow reactor or Stirred Tank Reactor (STR) as shown in Figure 2. A good design shows similar behavior for the real and the ideal reactors.

Batch Reactor

Characteristics

The batch reactor is the simplest of the three and needs the least supporting equipment. It is occasionally used for small-scale experimental studies on reaction kinetics and requires high labor and handling cost. Since there are not any inlet or outlet streams to or from the reactor, and the chemicals are well mixed inside, the composition in the reactor is assumed constant over the reactor at any given instant but varies with time until chemical equilibrium is approached.

Design Equation

From a material balance for any component i, the design equation for a batch reactor can be easily derived and used to solve graphically,

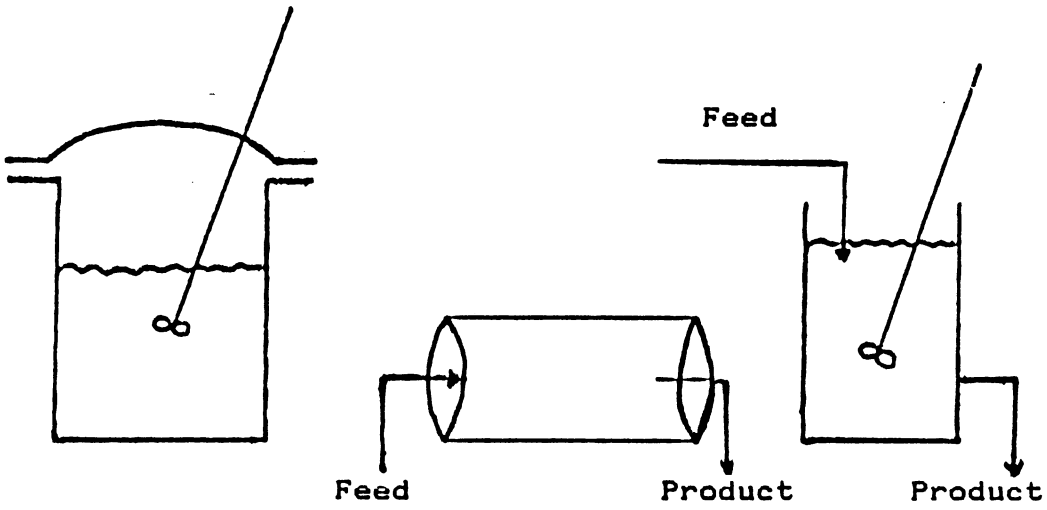


Figure 2. The Three Types of Reactors

analytically, or numerically for the time required to achieve a specified conversion as Equation 1 shows:

$$t = N_{io} \int_{x_{io}}^{x_i} \frac{dX_i}{V(-r_i)} \tag{1}$$

where

X_i = conversion of component i (a reactant) at time t

t = time required to achieve X_i, hr

V = reactor volume, ft^3

$-r_i$ = reaction rate, lbmoles/ft^3 hr

N_{io} = initial number of moles of i, lbmoles

x_{io} = conversion of component i at initial time t_o

Continuous Stirred Tank Reactors (CSTR)

Characteristics

The continuous stirred tank reactor is also called the backmix reactor, or the ideal stirred tank reactor indicating that the contents are well mixed and the composition is uniform. As a result, the composition of the exiting stream is assumed to be the same as the fluid inside the reactor. This type of reactor presents a good control of the reaction speed since the rate of reactions is constant as the reactants are introduced.

Design Equations

Again, from material balance, the design equation can be obtained and used easily to solve for the volume required at steady state

conditions to achieve a desired conversion of some reactant A. A form of this equation is shown below:

$$V = \frac{F_{AO}\,(X_A - X_{AO})}{-r_A} \tag{2}$$

where

X_{AO} = inlet conversion of component A (as reactant)

F_{AO} = inlet molar flow rate of component A, lbmoles/hr.

The space time is an important design criteria and is defined as the time required to process one reactor volume of feed measured at specified conditions as presented in Equation 3:

$$\tau = \frac{V}{v_o} = \frac{C_{AO}\,X_A}{-r_A} \tag{3}$$

where

v_o = inlet volumetric flow rate, ft^3/hr

C_{AO} = inlet concentration of A, $lbmoles/ft^3$.

Plug Flow Reactor (PFR)

Characteristics

In different sources the plug flow reactor is also called a slug flow, a piston flow, an ideal tubular, or an unmixed flow reactor. 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. This type of reactor yields a high quality product and is

capable of processing large quantities of material. For that purpose it is widely used in industry, in particular, within the oil business such as in reforming processes.

Design Equations

By performing a differential component material balance along the reactor on component A, a few key design equations can be derived and used to model such reactors. The following equations express the interrelation between the design parameters and the system kinetics.

$$\frac{V}{F_{AO}} = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A} \tag{4}$$

where

X_{Ai}, X_{af} = inlet and outlet conversions of A

$$\tau = C_{AO} \int_{C_{Ai}}^{C_{Af}} \frac{dC_A}{-r_A} \tag{5}$$

where

C_{Ai}, C_{Af} = inlet and outlet concentrations of A, lbmoles/ft^3.

In this model, all the calculations are based on molar flow rates rather than concentrations or conversions.

CHAPTER V

DESIGN OF PLUG FLOW REACTORS

Material and Energy Balances

Since the emphasis in this work is on tubular reactors, a detailed analysis of the design parameters and equations of such reactors is necessary. The integral design equation, listed as Equation 4 in the previous chapter, allows the determination of the volume of the reactor required to achieve a specified conversion if the rate of reaction can be integrated numerically or analytically within the conversion range. Such task might become very difficult or impossible for certain numbers of chemical reactions occurring simultaneously or presenting complex kinetics. A better method should be used in order to solve for the concentration gradient in the reactor. This method (12) is based on equations derived from differential material and energy balances. By performing a component i material balance around a differential section of the reactor, the following equations can be derived:

$$\text{in} - \text{out} \pm \text{generation} = \text{accumulation} \tag{6a}$$

at steady state, the accumulation term vanishes yielding

$$F_i - F_{i+1} + r_i \, dV = 0 \tag{6b}$$

$$-dF_i = -r_i \, dV \tag{6c}$$

$$\frac{dF_i}{dV} = r_i \tag{6d}$$

where

F_i = molar flow rate of component i, lbmoles/hr at reactor conditions

$$C_i = F_i/v \tag{7}$$

where

v = total volumetric flow rate, ft^3/hr

From kinetics or experimental data, using stoichiometry, and from Equation 7 above, the rates of reactions can be written as a function of temperature and component concentration. If the above equation is written for n components, n ordinary differential equations are obtained. The molar flow rates represent the dependent variables, whereas the reactor volume is the independent variable.

Considering the energy carried in and out by the chemicals, the heat of reactions, and the energy transfer from or to the surroundings, an energy balance equation can be derived. For an adiabatic operation the reactor volume dependence on the temperature in the reactor is given from the following equations:

in - out ± generation = accumulation

at steady state the accumulation term vanishes yielding

$$- \sum_j \Delta H_j \, \varepsilon_j + \sum_i (C_{p_i} \, F_i) dT = 0 \qquad (8a)$$

where

i = component i; i=1, ..., n

j = reaction j; j = 1, ..., m

ΔH_J = heat of reaction j; BTU/lbmoles

ε_j = molar extent of reaction j; lbmoles/hr

C_{p_i} = specific heat of component i; BTU/lbmoles °R

F_i = component i flow rate; lbmoles/hr

dT = differential temperature change in the reactor; °R

The extent of the reaction can be expressed as function of the reaction rate and the differential volume increment as follows:

$$\varepsilon_j = r_j \, dV \qquad (8b)$$

substituting ε_j by its value in Equation 8a gives

$$(- \sum_j \Delta H_j \, r_j) dV + (\sum_i C_{p_i} \, F_i) dT = 0 \qquad (8c)$$

when rearranged

$$\frac{dT}{dV} = \frac{\sum_j \Delta H_j \, r_j}{\sum_i C_{p_i} \, F_i} \qquad (8d)$$

This (n+1)-th ordinary differential equation can be solved simultaneously with the other n equations for the component molar flow rates, the reactor volume, and the temperature profile using an adequate numerical method.

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 or the recycle R is defined as follows:

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

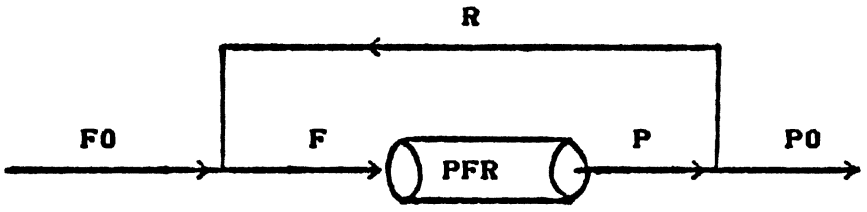
Figure 3 shows a typical recycle reactor scheme. To solve for the recycle effect on the reactor performance, the recycle ratio is first initiated as zero for the first pass through, then set to a desired value, and the calculations are repeated until a constant composition profile is obtained for two executive passes allowing for a desired tolerance. The integral design equation for a plug flow reactor with a recycle stream assuming there are no products in the feed becomes

$$\frac{V}{F_{AO}} = (R+1) \int_{X_{AR}}^{X_{Af}} \frac{dX_A}{-r_A} \tag{9a}$$

where

$$X_{AR} = \frac{R}{R+1} X_{Af} \tag{9b}$$

The above equation can be solved numerically or analytically for simple models. If no recycle is permitted (R=0), the above equation becomes identical to Equation 4, the integral design equation for a simple ideal plug flow reactor. It is important to notice that for infinite recycle, the plug flow reactor performance approaches that of a mixed flow



FO- The feed to the system
F- The feed to the reactor
P- The product from the reactor
PO- The product from the system
R- The recycle stream
PFR- Plug flow reactor

Figure 3. Schematic Representation of a Plug Flow Reactor with Recycle

reactor. Figure 4 shows the limits of a recycle reactor as the recycle ratio varies from zero to infinity (13).

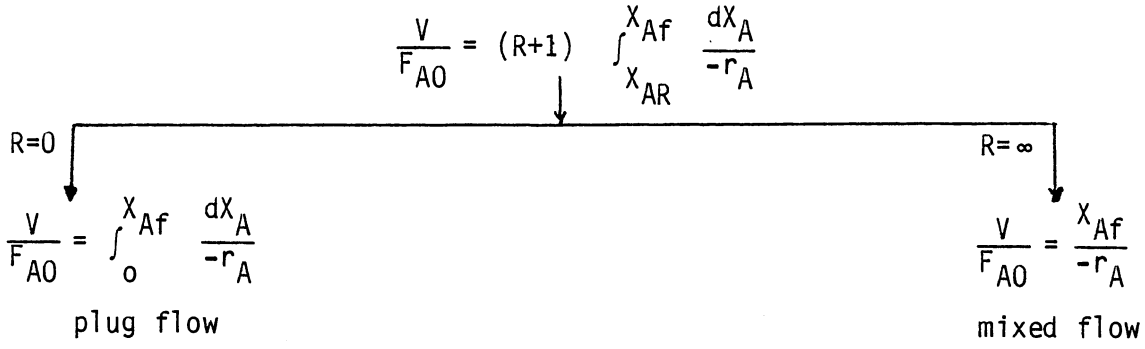


Figure 4. Limitations of a Recycle Reactor

CHAPTER VI

BRIEF DESCRIPTION OF MAXISIM

MAXISIM is an interactive simulation program used for simple thermodynamic equilibrium calculations and/or a complete process design of a system. It was written by Dr. John H. Erbar and revised by Dr. Ruth C. Erbar. Its first version was released in 1983, and its latest revision in 1987.

Like any other process simulator, MAXISIM allows the user to perform calculations and to test the results for simple to complex design models. The interactive nature of the simulator gives the user complete control of the program. He or she can create a model, set units, specify parameters, run the program, review the results, change a few things, and go again.

MAXISIM presents two operating modes -- the "immediate" mode and the "simulation" mode. In the former, quick calculations can be performed such as:

* three-phase bubble point, dew point, and flash equilibrium calculations
* stream manipulation
* gas heating value determination
* hydrate formation prediction
* process unit definition, unit operation deletion, addition and revision

Whereas the simulation mode allows the execution of a specified process model using the following current unit operations available:

* stream adder, divider, and splitter
* isothermal, constant enthalpy, fixed L/F, or three-phase isothermal flash
* expander
* compressor
* pump
* heater
* cooler
* heat exchanger
* short cut, and tray by tray distillation column
* short cut absorber, and tray by tray absorber/stripper
* short cut stabilizer
* plug flow reactor

The inputs to MAXISIM, in an interactive mode, consist of a set of completely specified feed streams (component flow rates, temperature and pressure, etc.), unit operations with their process data, C_{6+} fraction data if present, and unit control information. Checks for validity of the input data are performed. The academic version of MAXISIM can accept a maximum of fifty unit operations and twenty-five components. The outputs from the simulator contain mainly complete results from the immediate mode calculations, detailed description of the unit operations (feeds, products, and process data), and molar balance sheets. Depending on the users option and the set of output control parameters chosen, several other useful outputs are made available.

It is important to mention that MAXISIM leaves no choice to the user but to be well prepared and well organized before simulating any process unit model. A good understanding of the design and a reasonable technical grasp are necessary and vital to avoid bad results, slow convergence, a lot of frustration, and even impossible answers. For those reasons and others, MAXISIM is one of the good simulators for educational purposes.

CHAPTER VII

THE MODEL DESCRIPTION

Introduction

This model simulates an ideal homogeneous gaseous plug flow reactor. The program is coded in such a way that it is easy to include models of other types of reactors such as batch, stirred tank, or a catalytic reactor. A maximum of ten reactions and fifteen reacting or product components are allowed. The introduction of more reactions and more components is just a matter of changing the size of few arrays. As with some other simulators, this program is highly interactive. An effort was made to minimize and simplify the work of the user, but good organization and preparation are highly recommended. The general structure of this model consists of an input file, a calculation routine, and an output file. All these files are introduced into MAXISIM and interact with existing routines and a data base which covers a wide range of industrial chemicals. Appendices A and B include the logic structures for the input file and the calculation subroutines, respectively.

Input Description

First the inlet and outlet stream numbers are specified, and the inlet stream properties are obtained by flashing the stream using MAXISIM at the inlet reactor conditions. If more than one inlet or

outlet stream is defined an error message will be prompted. The number of reactions is entered next. The user is then asked by just looking at the rate equations, to enter the rate constants, the stoichiometric coefficients, and the components powers in the reaction rate expressions. The average heats of reactions are requested in the case of adiabatic operation in the reactor. Once all the information about the kinetics are fully specified, the user is given several options concerning the operation mode, the pressure drop specifications, and the convergence criteria. Both isothermal and adiabatic operations are available to control the variation of temperature along the reactor. The pressure difference between inlet and outlet is determined either by specifying a pressure drop across the reactor, or by setting the pressure of the outlet stream. Three possible convergence criteria are available to the user. The reactor volume can be fixed if the performance of an installed reactor is to be tested. But usually, the user is interested in or asked to determine a reactor size in order to produce a desired yield of a substance of interest. In this case, the outlet flow rate of that substance can be specified to set the convergence criteria. In a few cases, especially for exothermic reactions, the temperature change in the reactor is very large, consequently, to avoid overheating or freezing, the user might want to set an upper or lower limit on the exit temperature as a convergence criteria. An update menu is available in case the user decides to try different values of the reactor volume, the exit temperature, the outlet flow rate of a specified component, the operation mode, or the inlet temperature to the reactor.

Output Description

By the virtue of using MAXISIM, several output features are already available. A topology of the process can be viewed to check the stream numbers and their destinations. An echo of the input process data is also available to check for possible typing errors when entering the inputs. Also, a complete description of the inlet and output streams, including components flow rates, temperature, pressure, and a few other extensive and intensive properties, is given. Finally, the required reactor volume for the process and the heat load on the reactor are listed.

Subroutines Description

Input Subroutine: REAC(II)

This subroutine constitutes the major interactive part of the model. All the inputs, mentioned earlier, are read in and stored in a permanent array. The frequency factors, the activation energies, the Gibb's free energies, and the heats of reactions are stored in single dimensional arrays. Whereas the stoichiometric coefficients and the orders of each reaction with respect to the components are stored in two dimensional working arrays. All the other variables are stored as constants. Every input is transferred into the process data, PD, array which is permanent in MAXISIM and can be viewed before executing the simulation. All inputs are checked against appropriate limitations. Appendix A, as mentioned before, lists a logic structure for this routine.

Flow Subroutine: VFLOW

This subroutine simply picks up the molar flow rates from the stream, the components' molecular weights from the data base, and the stream density to determine the total volumetric flow rate of the stream for later use.

$$v = \frac{\sum_i F_i (MW)_i}{\rho_s} \tag{10}$$

where

$(MW)_i$ = the molecular weight of component i, lbm/lbmole

ρ_s = density of the stream, lbm/ft^3

A flow chart describing the logic structure of this subroutine is included in Appendix B.

Rate Constant Subroutine: RCONST

This routine sets up the rate constants as functions of temperature, T, using the inputs of the activation energies E_A's, and the frequency factors, k_o's, sometimes referred to as pre-exponential terms in the rate constant expressions. If the rate constant is evaluated at an average fixed temperature, then the activation energy input is entered as a dummy variable equal to zero.

$$k = k_o \exp(-E_A/RT) \tag{11}$$

The Extent of Reaction Subroutine: RRXN

Picking up the stoichiometric coefficients and the order of each reaction with respect to each component from the PD array, and using the

calculated value of the rate constant from RCONST, this routine sets up a unit rate change for each reaction, this is called the reaction coordinate or the extent of the reaction.

This concept is very important and useful in solving for the effect of several gaseous chemical reactions occurring simultaneously. Once the extents of all the reactions are determined, the outlet composition is easily computed by considering for each component, the changes due to respective reactions. Also if the extent of reaction method is used, the expansion effect from temperature changes is counted for inherently.

The Component Rate of Change
Subroutine: RRCOMP

This routine sums up the rates of change for each component in all the reactions. This is simply done by multiplying the unit rates of change for the reactions by the respective stoichiometric coefficient of the component, then summing the calculated changes for each component separately.

The Temperature Subroutine: RTEMP

Depending on the nature of the reaction and the operation mode, the temperature may rise or drop along the length of the reactor. This change is a function of the rate of change for the reactions from RRXN, the component flow rates, the heat capacities calculated using MAXISIM data base, and the heats of reactions from the PD array. The component heat capacities are derived using the SRK equation of state, as shown in Appendix C (14).

Differential Equation Solver: RUNGE

This constitutes the core of the reactor calculation file. Basically, all the mentioned subroutines, play the role of setting up a differential equation describing the change of each component flow rate along the reactor. These differential equations for all the components, plus the one describing the temperature change, are solved using the routine RUNGE. This routine uses Runge-Kutta fourth-order algorithm. Updates values of the component flow rates and the temperature are returned to the main program at each increment along the reactor.

A numerical routine is needed to solve the differential equations generated. There are basically three types of such numerical methods. The first class includes simple methods that are very easy to use and to understand. However, these routines are not highly recommended for general purpose usage. Such a class includes Euler's method. The second class consists of improved and elaborate first class methods. These methods are used to solve most differential equations encountered, but still are unable to adequately describe a few complicated equations. The modified Newton's method or Heun formula, the three-term Taylor series method, the Runge-Kutta first-, second-, third-, and fourth-order methods are some examples of the second class methods. It is important to notice that all the methods above compute the updated value of the function knowing only the previous value of the function. Such methods are called single-step methods. However, the third class routines are called the multistep methods because several previous points are used to determine the updated value of the function (15). Adam-Moulton's method and Gears method are example of those routines.

Choosing among the methods is not usually a clear-cut decision. Basically there are three decision factors that should be considered:

i) the complication of the differential equations at hand,

ii) the amount of computation involved, and

iii) the accuracy limitations.

In this work, the Runge-Kutta fourth-order method was chosen to solve for the component flow rates along the length of the reactor. This method was chosen over Euler's basically because the latter might fail to solve the differential equations generated if the stoichiometric coefficients and the orders of the components in the reactions are not integers. Also Runge-Kutta gives better accuracy for the same volume increment. Halving the differential increment reduces the local error by a factor of 1/32, as compared to 1/2 using Euler's method. The trade-off of using Runge-Kutta over Euler's method consists of evaluating the function four times in one increment, as opposed to once, but this is not very crucial with the presence and the availability of high-speed computers which are able to perform such calculations in a few seconds for any except extremely complicated and lengthy functions. A natural question to ask is why not use a multistep method such as Adam's and Moulton's over Runge-Kutta since, not only the orders of accuracy are the same, but also the former method evaluates the function only twice in each increment and is capable of solving very stiff differential equations (16). The answer is that there exists a drawback in using Adam's method, which consists of the inconvenience of changing the step size as the calculation proceeds. This change of the step size necessitates the calculation of new points consistent with the new step size. For this reason, and the fact that Runge-Kutta is much

easier to code than is Adam's and Moulton's method, the former method is used in this work.

Equilibrium Criteria Subroutine: RTRY

This subroutine simply sets up the equilibrium criteria for the reactions in equilibrium. In the general case, the chemical equilibrium is expressed in function of the fugacity coefficients of the components in the gas mixture, their mole fractions and the system pressure, as given by Equation 12:

$$KP^{-\nu} = \prod_{i=1}^{n} (y_i \hat{\phi}_i)^{\nu_i} \tag{12}$$

where

K = chemical equilibrium constant

P = system pressure

y_i = mole fraction of component i

ν_i = stoichiometric coefficient of component i

ν = sum of the stoichiometric coefficients in the reaction

n = number of the components in the mixture

$\hat{\phi}_i$ = the fugacity coefficient of component i in the gas mixture

If the gases are assumed to be ideal, the fugacity coefficients are set to one, and if the mole fractions are expressed in terms of the flow rates, Equation 12 becomes

$$KP^{-\nu} \left(\sum_{i=1}^{n} F_i \right)^{\nu} - \prod_{i=1}^{n} F_i^{\nu_i} = 0 \tag{13}$$

Finally, the chemical equilibrium constant can be expressed as a function of Gibb's free energy, ΔG° as follows:

$$\ln K_o = - \frac{\Delta G^0}{RT_o} \tag{14}$$

where R is the ideal gas constant; 1.987 BTU/lbmoles °R.

The equilibrium constant calculated above is at a reference temperature, T_o, corresponding to the Gibb's free energy (13). Then, Van Hoff's law is used to determine the equilibrium constant at any specified temperature T from Equation 13. And

$$\ln \frac{K}{K_o} = - \frac{\Delta H_{rxn}}{R} \left(\frac{1}{T} - \frac{1}{T_o}\right) \tag{15}$$

where

ΔH_{rxn} = constant heat of reaction in the temperature interval.

Once the thermodynamic equilibrium constant is evaluated from Gibb's free energy and the temperature, the left-hand side of Equation 13 can be evaluated from each given set of the component flow rates. However, the reactions in equilibrium are very fast compared to the rest of the reactions in the process. If the reactor volume increment is small, then, at the entrance to each increment in the reactor, the contribution of the reactions in equilibrium can be determined before the consideration of the rest of the reactions.

Therefore, the component flow rates in Equation 13 can be written as follows:

$$F_i = (F_i)_o + \nu_{ij} r_j \tag{16}$$

where

F_i = updated component flow rate

$(F_i)_o$ = previous component flow rate

ν_{ij} = stoichiometric coefficient of component i in reaction j

r_j = molar extent of the equilibrium reaction j

If the F_i's are substituted in Equation 13, the equilibrium criterion equation can be formulated

$$K P^{-\nu} \left(\sum_i [(F_i)_o + \nu_{ij}\, r_j]^{\nu} \right) - \prod_i [(F_i)_o + \nu_{ij}\, r_j]^{\nu_i} = 0 \qquad (17)$$

The only unknown in Equation 17 is the extent of the equilibrium reaction. It is obvious that there is not an analytical solution, therefore a numerical method for solving an algebraic equation is needed.

Equation 17 can be very complicated to solve if the stoichiometric coefficients are not integers and if the reaction in equilibrium occurs among several components. However, in most cases four types of reactions in equilibrium are encountered:

$$A = B \qquad (18a)$$

$$A = B + C \qquad (18b)$$

$$A + B = C \qquad (18c)$$

$$A + B = C + D \qquad (18d)$$

All these reactions yield to a thermodynamic equilibrium criterion which is reasonably easy to solve.

Extent of Equilibrium Reaction

Calculation Subroutine: RXEQU(J)

This routine uses a numerical method to solve for the extent of reaction in equilibrium. Basically, this constitutes a guessing process. Each time a value of the extent of reaction is picked, the subroutine RTRY is called to check if the left-hand side of Equation 17 is close enough to zero. In essence, solving the thermodynamic equilibrium criteria is finding a numerical method to solve for the roots of the function $f(x) = 0$. The obvious method is the so-called "marching routine". It consists of picking an initial guess and increasing it by a small increment, while checking the value of the function each time, until a root is found. This routine has the advantage of hitting every root of the function. However, in some cases this method could be very slow, especially if the increment chosen is very small. Another method, called bisection, 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 certain cases if the lower and/or the upper limit is not carefully chosen. The existence of multiple roots reveals the problem of choosing the right or the appropriate root. In general the choice between such methods depends strongly on the problem at hand.

For this task, solving for the appropriate extent of reaction in equilibrium, a few observations can be made in order to facilitate the choice. First the equilibrium reactions which are usually encountered are of the forms shown in Equation 18a through 18d. The thermodynamic

equilibrium criteria, in those cases, are polynomial functions with highest degree of two. The bisection method is used to solve for the correct root fairly quickly and accurately. The component flow rates determine the lower and the upper limits of the extents of reactions, i.e., of the roots of the function.

The Main Calculation Subroutine: REACR

This subroutine uses all the subprograms mentioned earlier. The calls to the different subroutines are first put in the appropriate order. The product stream from the i-th volume increment or differential is flashed at the updated temperature and outlet pressure to pick up a new stream density, then the heat capacities for the components are updated as they are functions of temperature. Respectively, the subroutines VFLOW, RCONST, RRXN, RRCOMP, RTEMP, and RUNGE are then called to update the flow rates, and the temperature before entering the (i+1)-th volume increment. The testing for the convergence criteria, the operation mode, and the pressure specifications are dealt with within this subroutine.

The Output Subroutine: REACO

This subroutine accomplishes two major printing objectives. First, it echos all the inputs to the reactor unit. This process design (PD) description allows the user to cross-check the numbers he/she has entered. First the operation mode, the volume increment, the inlet pressure to the reactor, the outlet pressure, and the conversion criteria are listed. Then the chemical reactions are displayed with the component names shown as reactants and/or products, e.g., $C + O_2 \rightarrow$

CO_2. Finally, an input table for the process is presented in order to compare it to the one the user has used to enter the stoichiometric coefficients and the orders of the components in each reaction. At this point, the user can detect input errors in the kinetics. Once the program is executed and the feed and the product streams are fully described, the output routine prints out these streams, the reactor volume, and the heat load on the reactor.

CHAPTER VIII

THE USER MANUAL

How to Create a File

The procedure to simulate a process containing a single reactor or any number of reactors is the same as the one described in MAXISIM manual. Basically, the feed is initiated and flashed at some specified inlet conditions. It is then saved or stored in a numbered stream. At this stage, a choice of the unit operations from MAXISIM menu is made.

The Input Process

The Reactor Process Inputs

If the user has chosen to define a plug flow reactor as one of his/her unit operations, the following pieces of information have to be known in advance:

* Reactor inlet and outlet stream numbers
* The number of reactions
* The volume increment
* The frequency factor of each nonequilibrium reaction
* The activation energy of each nonequilibrium reaction
* The heat of each reaction
* The Gibb's free energy for each equilibrium reaction
* The option of operating isothermally or adiabatically

* The option of specifying the outlet pressure from reactor, or the pressure drop across the reactor
* The option of specifying the reactor volume, the exit temperature, or the outlet flow rate of a specified component
* The order of reaction with respect to each component
* The stoichiometric coefficient of each component in each reaction

Organization

It is important to have the input data for the reactor well organized. First of all, it is highly recommended to have the inputs prepared in the order shown in the previous section. Once the components are chosen from the MAXISIM data base, the order in which they follow is fixed, therefore it is helpful to make a list of the components with their corresponding sequence numbers. Once this is done, the chemical reactions should be written in a form where the component names are replaced by their sequence numbers. This helps read off the stoichiometric coefficients. In the same manner, the rate expression for each reaction, which must be a power law type, should be rewritten and the component names again represented in those expressions by their sequence numbers. This, again, facilitates the picking up of the order of the components in each reaction. At this stage, it is highly recommended to set up an input table as shown in Table I. The input mode is set up so that the numbers are entered starting from the upper left corner across the rows down the columns.

TABLE I

THE INPUT TABLE

Reaction Number	Component Sequence Number	The Power of the Component Concentration in the Rate Expression	Stoichiometric Coefficient of the Component
I	1	#	##
	2	#	##
	.	.	.
	.	.	.
	.	.	.
	N	#	##
II	1	#	##
	2	#	##
	.	.	.
	.	.	.
	.	.	.
	N	#	##
M	1	#	##
	2	#	##
	.	.	.
	.	.	.
	.	.	.
	N	#	##

#, ## - the inputs to the model
- can be a positive real number or a zero for inerts
- is a positive integer for a product
- is a negative integer for a reactant
- is zero if the component is not involved in the reaction

Information Storage

Once the inputs to the reactor and the other unit operations are entered, the user is ready to set up a data file by simply entering "FL" and giving a file name after the request. By doing so, the user will have avoided the tedious work of reentering the input data to the process every time he/she needs to run the simulation. Detailed options, included in MAXISIM manual, can allow the user to alter the input data to the unit operations.

The Update Mode

There are five inputs to the reactor that can be updated. Following the menu, the operation mode in the reactor, (adiabatic or isothermal), the reactor volume, the exit temperature, the volume increment, and the outlet flow rate of a specified component can be altered if needed.

Useful Remarks

It is important to make sure that the feed to the reactor is a gas. Once the choice of units is made, it is crucial to enter the inputs such as the frequency factors, the activation energies, and the heats of reactions in the chosen units, as requested in the input instructions.

An Input Example

The hydrodealkylation of toluene is a common way to make benzene. Usually more than one reaction occurs simultaneously, but for the sake of this example, only the main reaction

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$$

is assumed to take place. To model a reactor to handle this process, first a feed is specified, flashed at the inlet conditions of the reactor, then stored in a feed stream. Usually, in MAXISIM, the user will choose components from most to least volatile. Following this rule, the components in this reaction are numbered as follows

H_2 - Component #1

CH_4 - Component #2

C_6H_6 - Component #3

C_7H_8 - Component #4

N_2 - Component #5

The nitrogen is thrown in the reaction as an inert. The following reaction rate expression is given (17):

$$\text{rate} = 1.82\text{x}10^{15}\ C_{H_2}^{1/2}\ C_{tol.}\ \exp(-96{,}560/RT)\ \frac{\text{lbmoles}}{\text{ft}^3\ \text{hr}}$$

From the rate expression, the frequency factor is equal to $1.82\text{x}10^{15}$ lbmoles/ft^3 hr, the activation energy value is 96,560 BTU/lbmole. The input data for the kinetics of this reaction is shown in Table II.

TABLE II

INPUT TABLE FOR THE EXAMPLE PROBLEM

Reaction Number	Component Sequence Number	The Power of the Component Concentration in the Rate Expression	Stoichiometric Coefficient of the Component
I	1	0.5	-1
	2	0	1
	3	0	1
	4	1	-1
	5	0	0

CHAPTER IX

THE MODEL PERFORMANCE AND TESTING

Introduction

Since this model is primarily going to be used for educational purposes, the "friendliness" of the interactive mode, the verification of reactor design fundamentals, the flexibility of the program, and the accuracy of the results have been tested. The hydrodealkylation of toluene to produce benzene is the main test case treated in this chapter. It constitutes a good example to work with because, not only does it present three chemical reactions, but also it can be tested to verify several reactor design principles and process design techniques.

Input Units

By the virtue of using MAXISIM, four sets of units are available to the user. Once he/she chooses a set of units the input instructions follow consistently the user's choice of units. Since the units of the frequency factor, or the so-called pre-exponential term in the rate expression, depend on the kinetics, two options of units are offered to the user. Usually the rate of reaction is given in gmole/l sec, and occasionally the units are lbmoles/ft^3 hr. Appendix D shows the conversion from one set of units for the rate constant to the other for any given kinetics.

Input Display

As described in Chapter VII, the output subroutine displays the inputs for error detection. A sample of a process diagram for the hydrodealkylation of toluene is given in Appendix E.

Update Menu

An update menu is available to the user. Several options are given, and the user can test the performance of the model by changing the outlet reactor temperature, the reactor volume, the operating mode, the volume increment, or the production rate of a specified component. Appendix F contains outputs for several runs performed with the three reactions occurring in the hydrodealkylation of toluene. The computer outputs correspond to the following operating conditions.

i) the reactor volume is set to 500 ft^3, and the operation is adiabatic,

ii) the production rate of benzene is set to 200 lbmoles/hr,

iii) the operation mode is switched to isothermal keeping the same conversion factor, and

iv) the operation is switched back to adiabatic, and the outlet temperature is set to 1400°F.

Verification of Some Reactor
Design Principles

Referring to the outputs for the runs described above:

* When the production rate of benzene is specified to be equal to 200 lbmoles/hr, a smaller reactor is needed than when the

volume was set at 500 ft^3 (or the feed may be decreased by the user iteratively to optimize the feed rate).

* Since the overall process is exothermic, when the operation in the reactor is switched to isothermal, a much larger reactor is needed to meet the same benzene production rate of 200 lbmoles/hr for the same inlet temperature.
* From i), under adiabatic operation and with a volume equal to 500 ft^3, the reactor exit temperature is about 1413°F. When an upper limit of 1400°F on the reactor outlet temperature is set, less production is obtained since the reactor volume can not reach the full 500 ft^3.

A Plug Flow Reactor with Recycle

Using an adder, a flash unit, a compressor, and a divider from the MAXISIM unit operation menu, a plug flow reactor with recycle, so-called "Reactor Loop" as shown in Figure 1, is simulated. Appendix G contains the output for such a process. A process topology, a process design for each unit operation, a full description of the feed and product streams in the process, and the unit operations' characteristics or sizes are included in the printout.

Accuracy of the Model

In this model, as mentioned previously, the SRK equation of state is used to determine the properties of the streams and the compnoents; also the differential equations describing the changes along the reactor are solved using a fourth-order Runge-Kutta method. Due to those two

reasonably powerful methods, the results from the model are found to be accurate.

Appendix H shows two identical runs except the volume increment for the second run has been cut to one-fourth that of the original run. In the first simulation, with the volume increment equal to 1 ft^3, the production rate of benzene and the outlet temperature from the reactor are equal to 215.97 lbmoles/hr and 1413.23°F, respectively; whereas, in the second run (dv = 0.25 ft^3), they are equal to 215.98 lbmoles/hr and 1415.5°F, respectively, showing very small variation due to increment size because of the accuracy of the fourth-order Runge-Kutta.

Two identical plug flow reactors are simulated in series, and their performance is tested against a single reactor twice as large as shown in Figure 5. The topology of the system, the process data, and the outputs are shown in Appendix I. Using an inlet temperature and pressure equal to 1200°F and 495 psia, respectively, identical yields of benzene are obtained using the two reactors in series and the single reactor alone.

Two identical plug flow reactors are simulated in parallel using a divider and an adder from MAXISIM. The divider splits the feed in half between the reactors, and the products of the reactors are combined using the adder to yield the overall process product as shown in Figure 6. For given feeds and inlet conditions, the benzene production from a single reactor with a volume equal to 500 ft^3 was 232.94 lbmoles/hr. For the same feed and inlet conditions, and using two reactors in parallel with a volume equal to 250 ft^3 each, the benzene production was 232.91 lbmoles/hr, showing about 0.02% difference. The

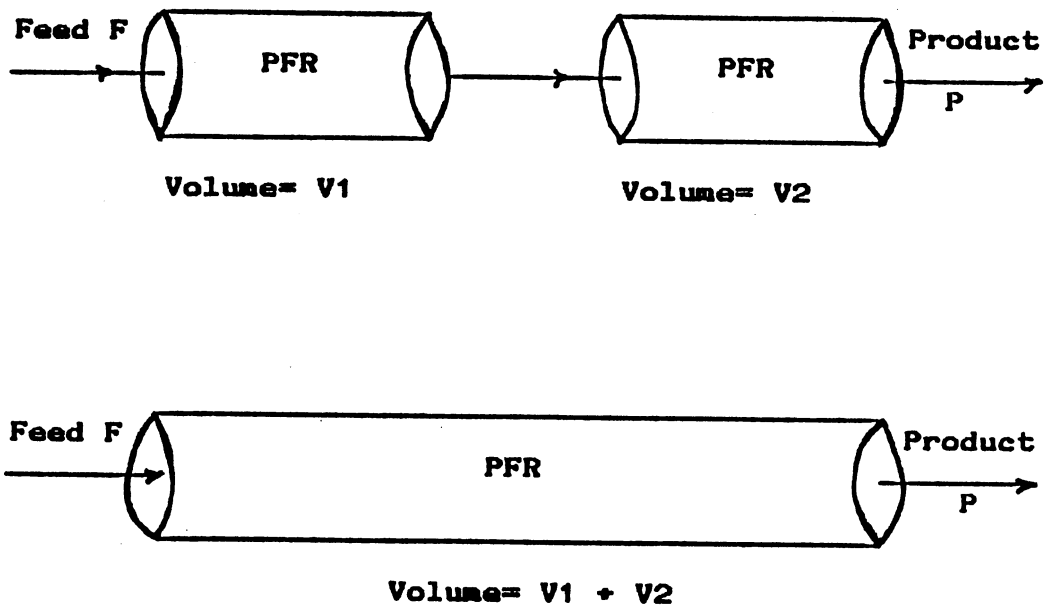


Figure 5. Equivalence of Plug Flow Reactors in Series

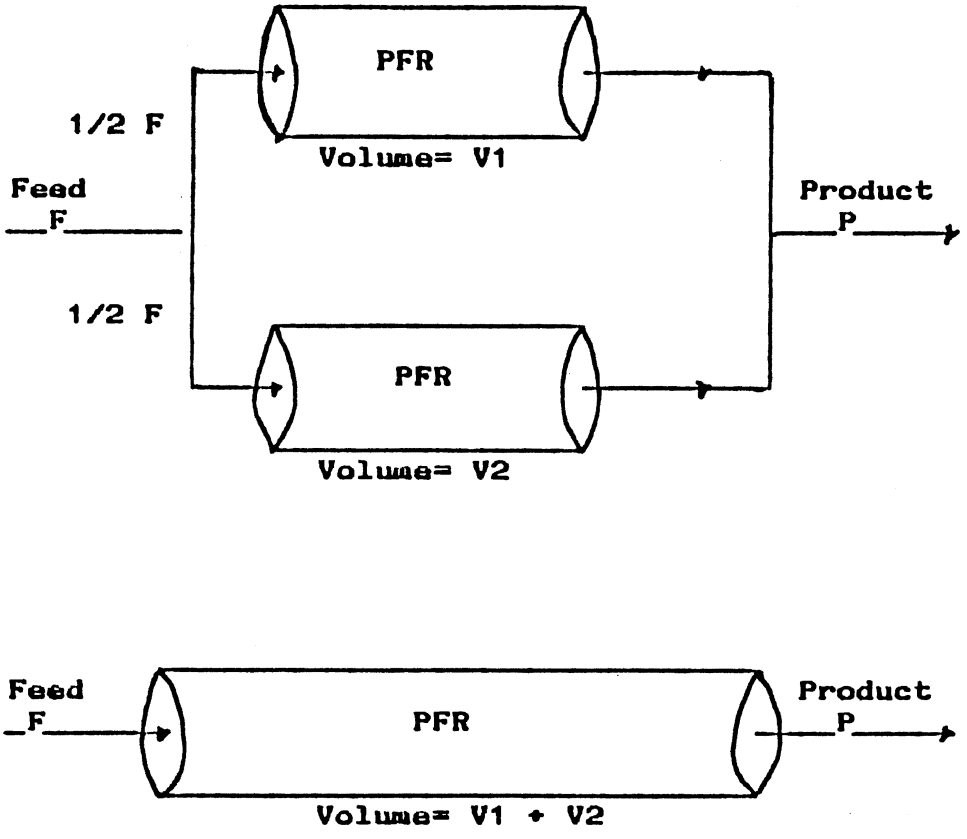


Figure 6. Equivalence of Plug Flow Reactors in Parallel

topology of the system, the process data, and the outputs from MAXISIM are shown in Appendix J.

To avoid coking in the reactor (17), the ratio of hydrogen to aromatics should be at least three to one (usually it is five to one). If a single pass through the reactor is chosen, at least 650 lbmoles/hr of hydrogen are required to produce 203 lbmoles/hr of benzene. To avoid the large amount of hydrogen in the feed, i.e., the operating cost, a portion of the reactor product is recycled. The drawback of the recycle is the increase of the reactor volume, but this is not crucial because this cost is included in the capital cost which is paid only once in a lifetime. Appendix K shows two simulations producing 203 lbmoles/hr of benzene from the reactor. The first run represents a single pass through the reactor, and the second set of results are obtained using a 79% recycle stream. The purge and the recycle percentages can be optimized by performing different runs. The user should change one of the two percentages each time and check the reactor volume and the feed rate.

CHAPTER X

CONCLUSIONS AND RECOMMENDATIONS

The purpose behind this work is to develop a plug flow reactor model and include it as a reactor core into MAXISIM. The computer code of the model is included in Appendix L. Based on the structure and the performance of this model, several conclusions are drawn.

1. Despite the enormous number of calculations involved, a simulation of a plug flow reactor with several equilibrium and/or nonequilibrium reactions can be performed with little I/O time, i.e., it takes about five seconds if the reactor volume is equal to 500 ft^3 in the hydrodealkylation of toluene case.

2. Some reactor design principles and process design techniques can be illustrated using the reactor model with MAXISIM for the example given.

   a. Increasing the inlet temperature to the reactor, if exothermic reactions are present, will increase the yield or the conversion for irreversible reactions.

   b. Changing the operating pressure in the reactor will change the output.

   c. Recycling a percentage of the product stream will alter the feed to the system required to meet the purity specifications.

3. A complete chemical process containing plug flow reactors within its unit operations can be simulated on MAXISIM, and the optimum operating variables of the modules can be investigated.

Since several assumptions are made within this plug flow reactor model calculation, few recommendations will serve to improve parts of this work.

1. The maximum number of reactions and components allowed can be increased by simply changing the size of the PD array and making the necessary changes in the working arrays in the calculation routine of the reactor.

2. The modeling of a fixed-bed catalytic reactor or a fluidized bed can be simply introduced by creating calculation subroutine for such reactors, and calling them from the main calculation routine. Obviously, a few other inputs will be requested from the user and stored in the PD array. The numerical methods (Runge-Kutta fourth-order and the bisection method) can both be used to solve the differential equations generated to describe the changes along the reactor.

3. The ideal gas assumption is made only when the extent of the reaction in equilibrium is calculated. This assumption can be avoided if both the forward and the reverse rate constants in the reversible reaction are known. In that case, such a reaction should be modeled as two irreversible reactions to avoid the ideal gas assumption and the bisection numerical method calculations.

4. Since SRK equation of state is available in MAXISIM, the fugacity coefficients of the components in the mixture can be picked up and used in the thermodynamic equilibrium criteria. Such an improvement should be checked for necessity since in most cases the phase of

interest is well in the gaseous phase far from the envelope; in which case the ideal gas assumption is probably safe.

5. Again, using the SRK equation of state for the gas and liquid phases, or the split approach if activity correlations are available, a heterogeneous reactor model can be introduced.

6. Using the SRK equation of state or an activity coefficient correlation for a liquid phase, a plug flow reactor that handles chemical reactions occurring in the liquid phase can be simulated.

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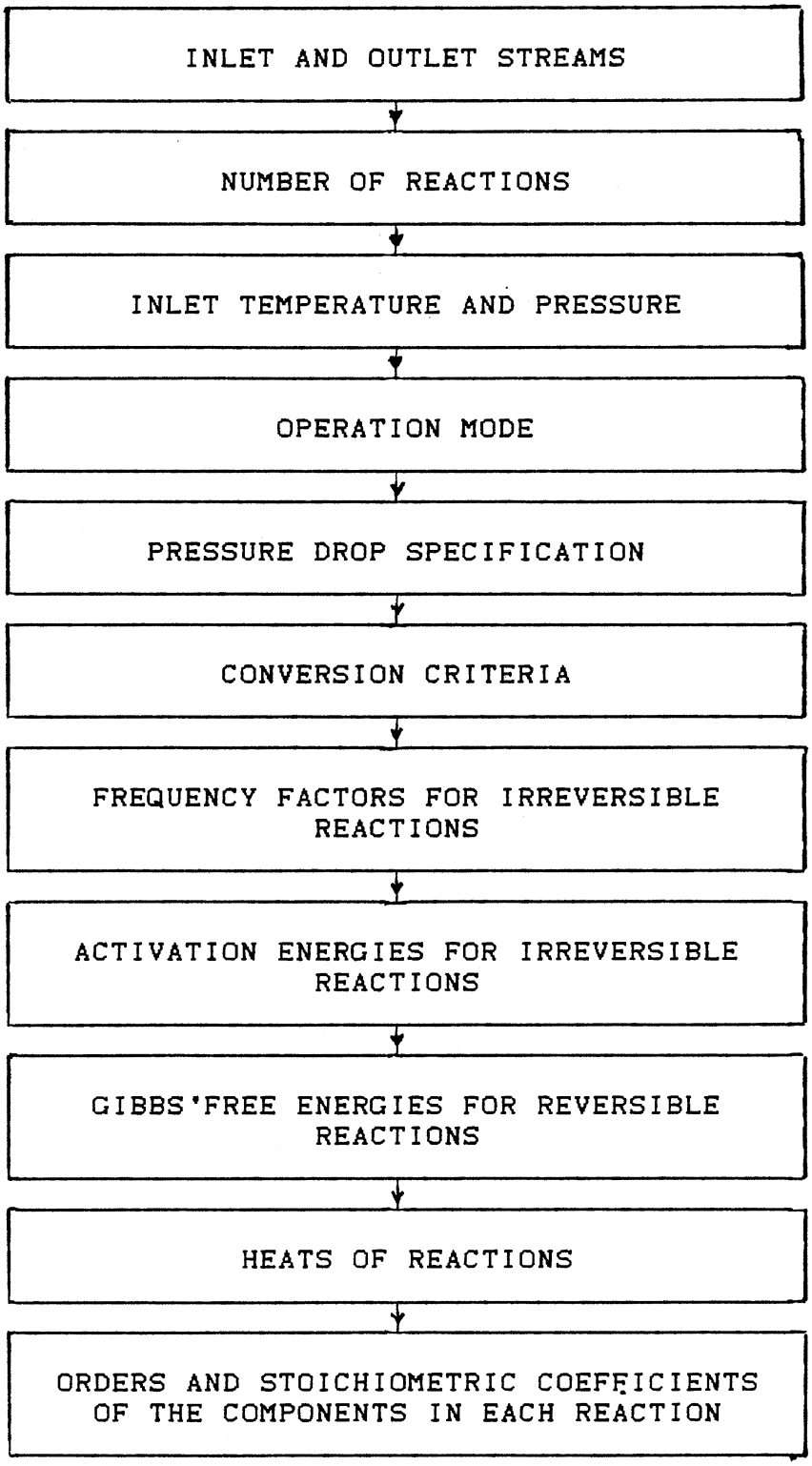
APPENDIX A

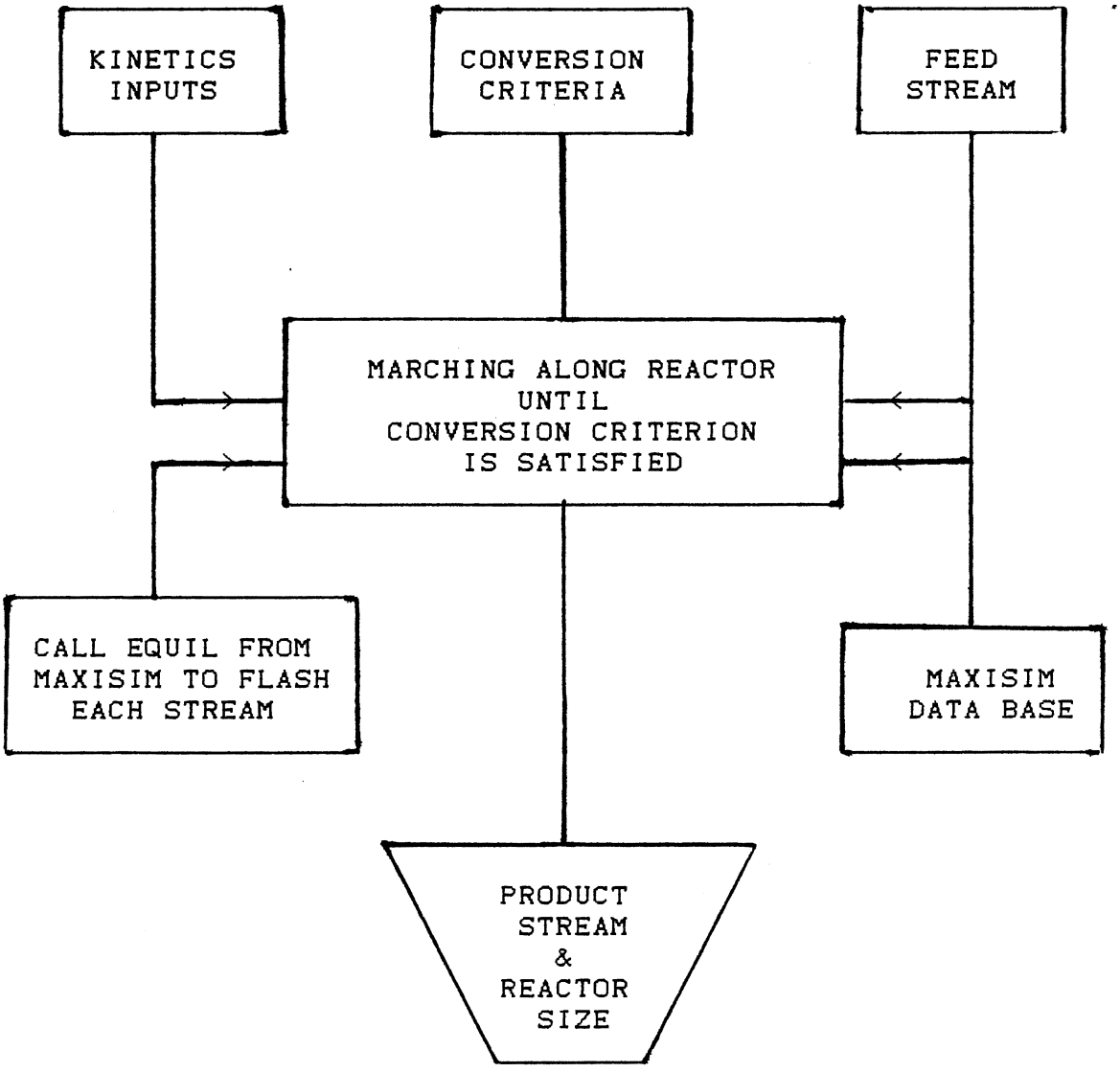
LOGIC STRUCTURE FOR THE INPUT SUBROUTINE REAC(II)



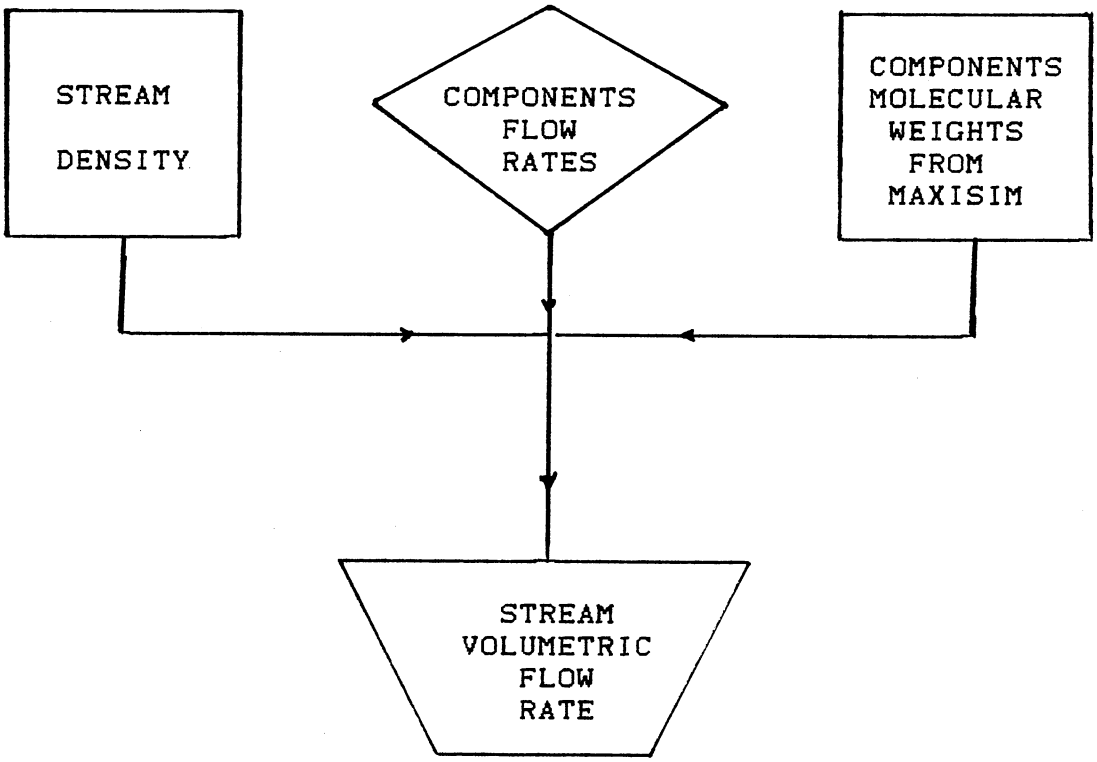
LOGIC STRUCTURE FOR REAC(II)

APPENDIX B

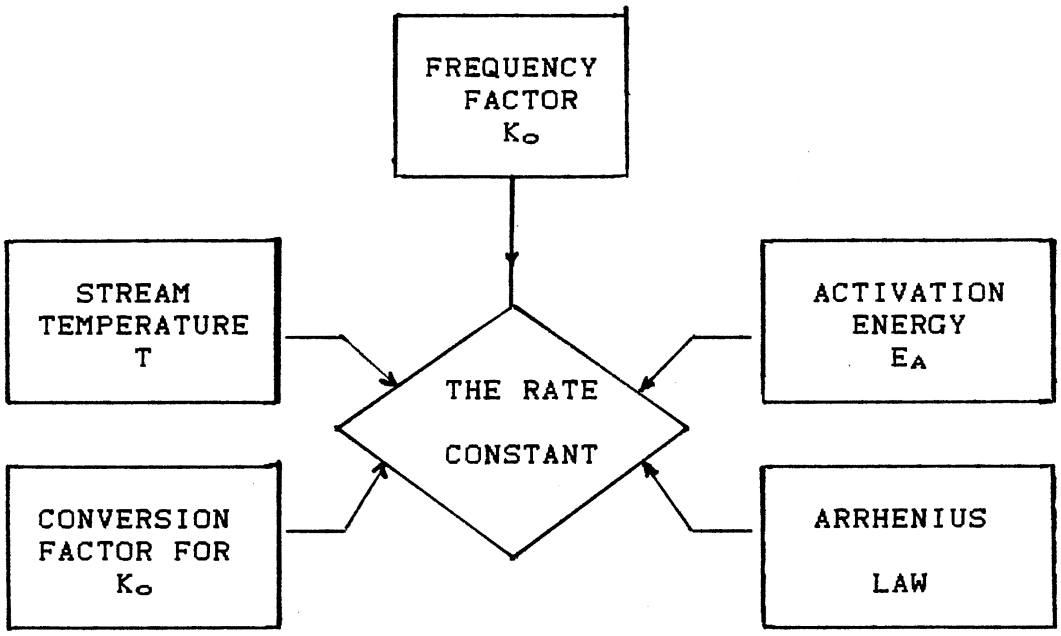
LOGIC STRUCTURE FOR THE CALCULATION SUBROUTINES IN REACR



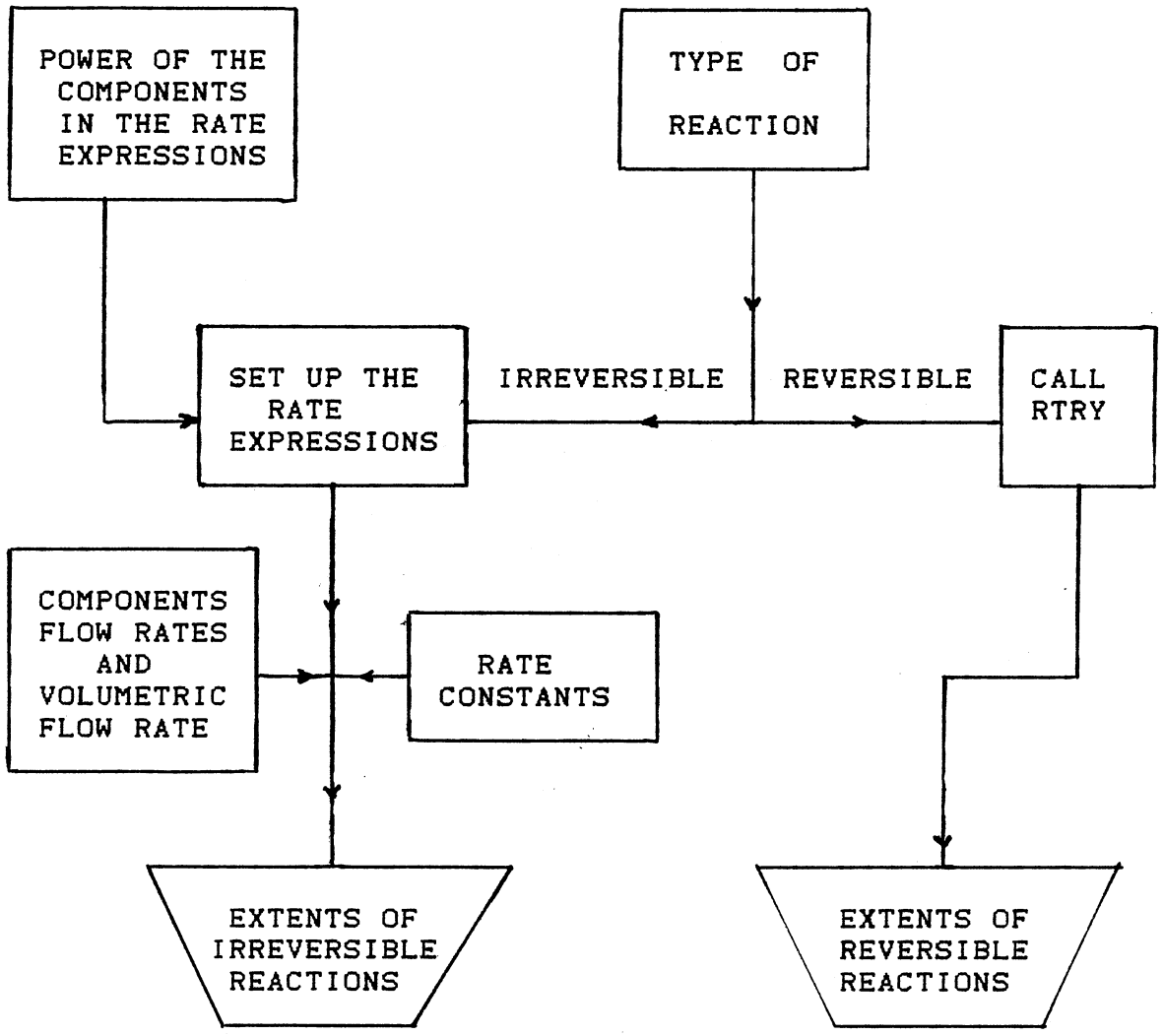
LOGIC STRUCTURE FOR SUBROUTINE REACR



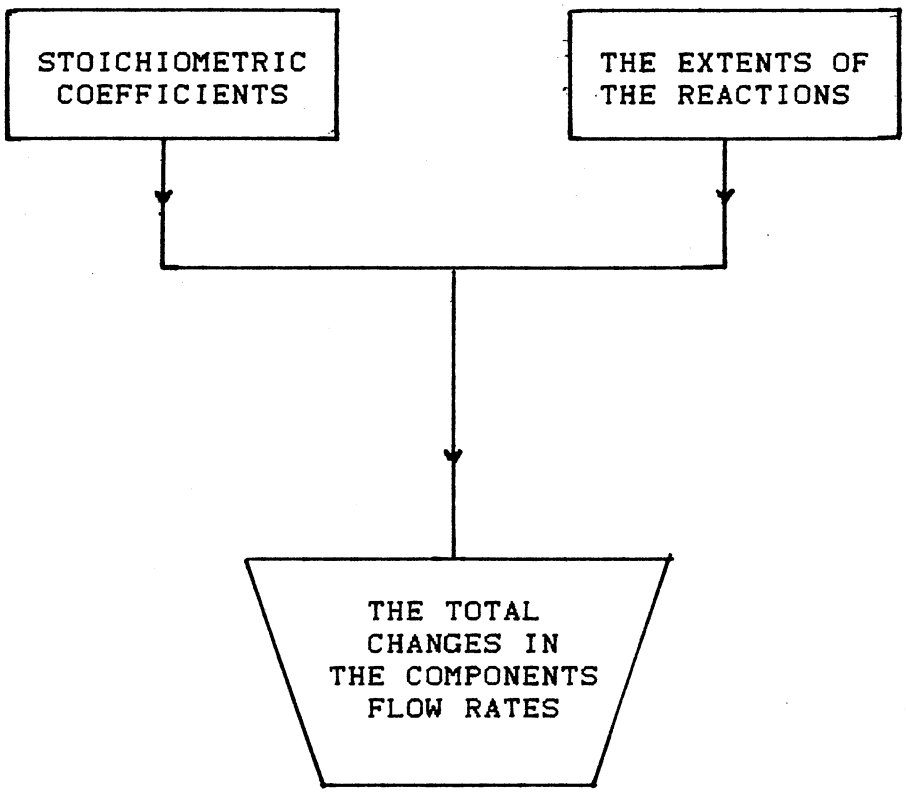
LOGIC STRUCTURE FOR VFLOW



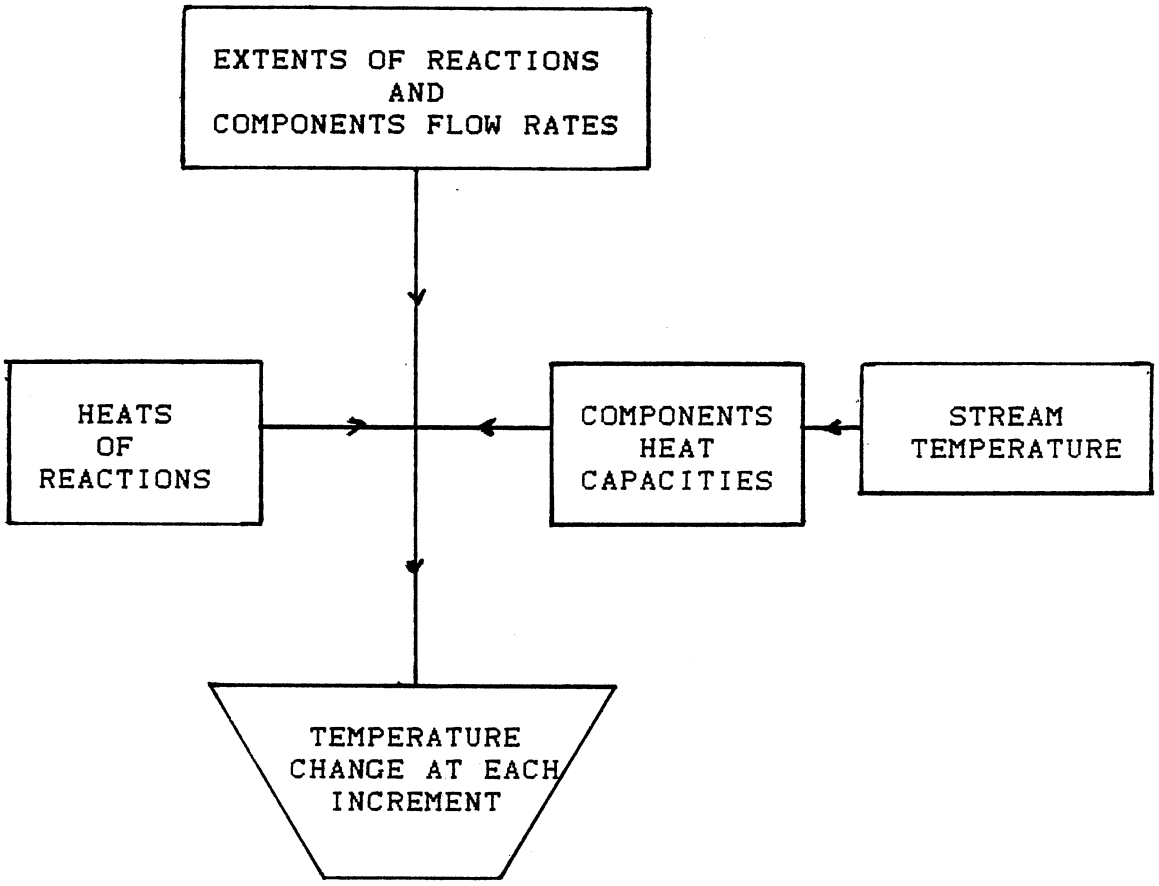
LOGIC STRUCTURE FOR RCONST



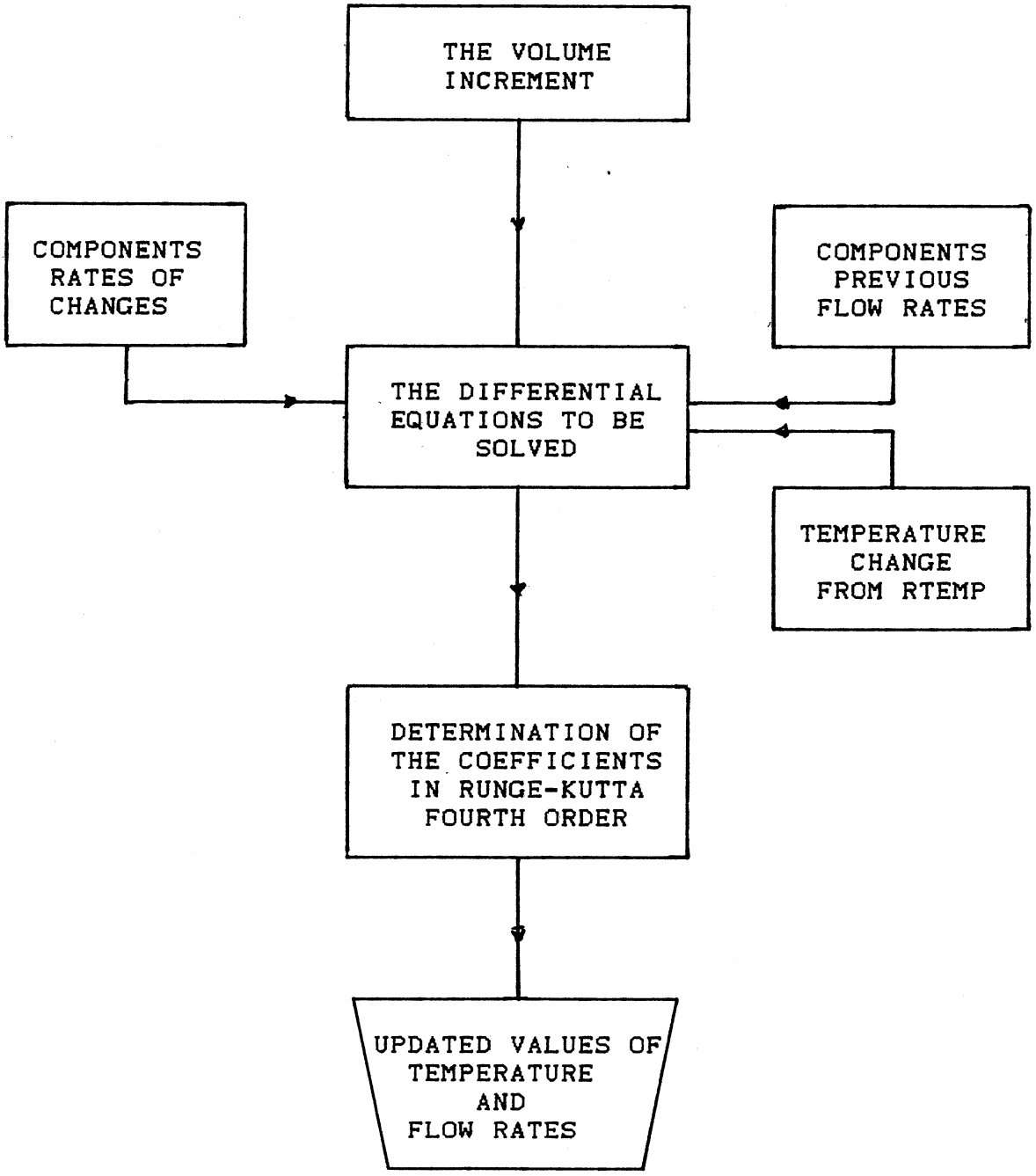
LOGIC STRUCTURE FOR RRXN



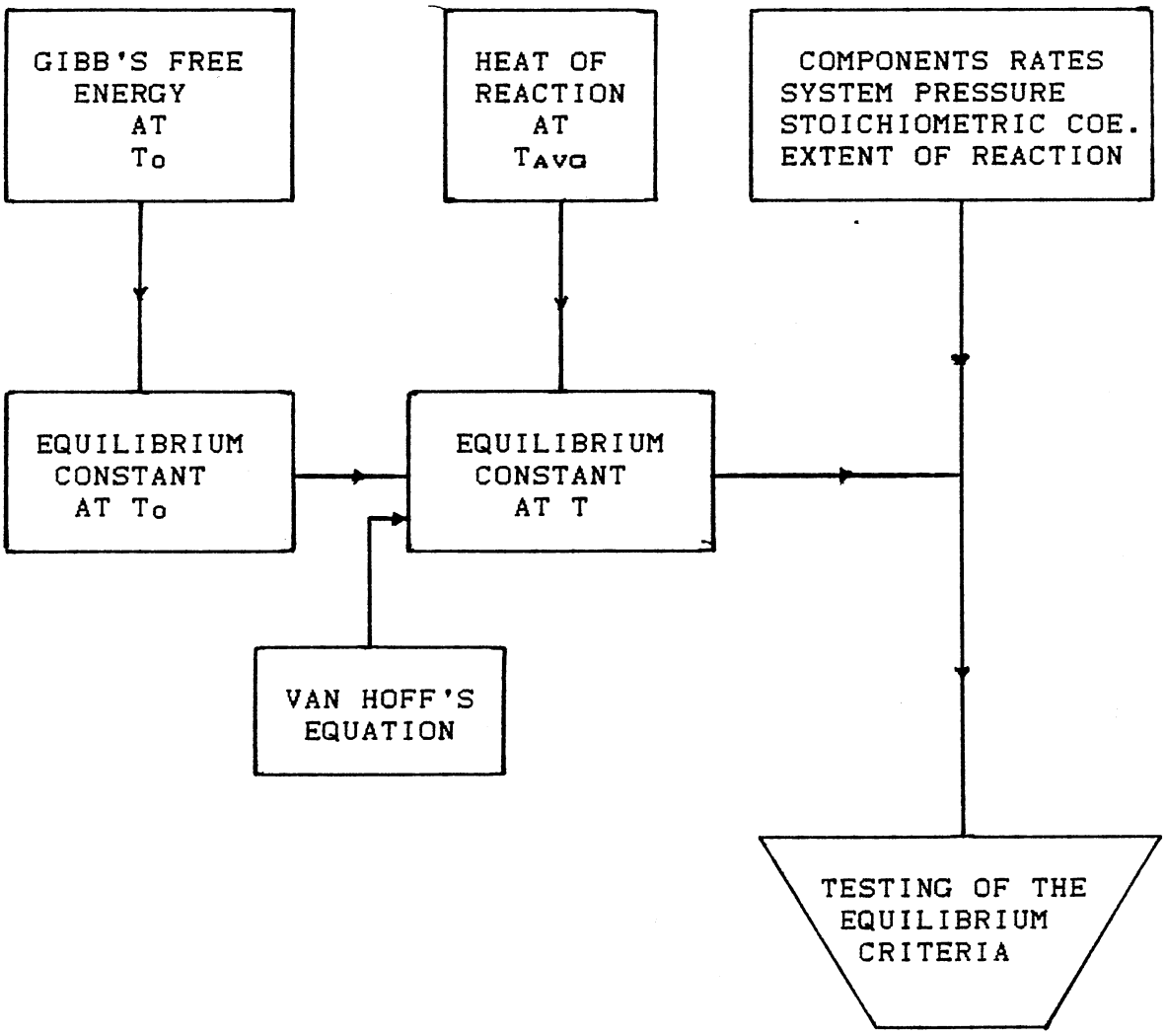
LOGIC STRUCTURE FOR RCOMP



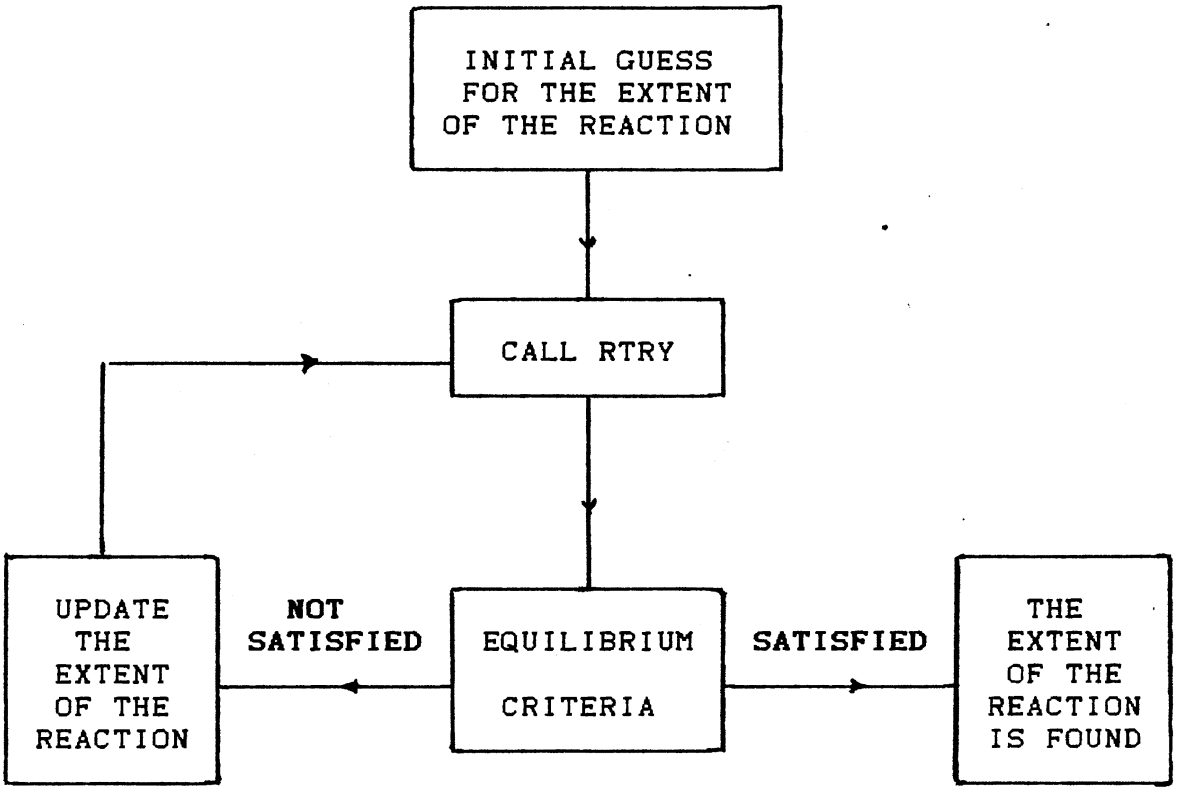
LOGIC STRUCTURE FOR RTEMP



LOGIC STRUCTURE FOR RUNGE



LOGIC STRUCTURE FOR RTRY



LOGIC STRUCTURE FOR RXEQU

APPENDIX C

DERIVATION OF HEAT CAPACITY FROM SRK EQUATION OF STATE

Constant Pressure Heat Capacity, C_p

$$C_p = C_p^0 - C_p'$$

where

C_p^0 = the ideal gas state heat capacity.

The departure function C_p' can be calculated if C_v' (the constant volume heat capacity heat departure function) is known from

$$C_p' - C_v' = \frac{T\,[(\partial P/\partial T)_v]^2}{(\partial P/\partial v)_T}$$

C_p^0 is available from the temperature derivative of the ideal gas state enthalpy equation

$$H^0 = a_1 T + a_2 T^2 + a_3 T^3 + \ldots$$

$$C_p^0 = a_1 + 2a_2 T + 3a_3 T^2 + \ldots$$

For a mixture

$$(C_p^0)_{mix} = \sum_i C_{p_i}^o X_i$$

where X_i is the mole fraction of each species in the mixture.

The SRK equation of state is used to evaluate the partial derivative of pressure with respect to temperature and pressure. Figure 7 shows the expression of the SRK equation of state.

$$\ln \phi_i = \frac{b_i}{b} (Z - 1) - \ln (Z - B) - \frac{A}{B} \left[\frac{2(ac\alpha)_i}{(ac\alpha)} - \frac{b_i}{b}\right] \ln \left(1 + \frac{B}{Z}\right)$$

$$- \frac{\Delta H}{RT} = \left[\frac{A}{B} - \frac{\beta}{Rb}\right] \ln \left(1 + \frac{B}{Z}\right) + 1 - Z$$

$$\frac{\Delta S}{R} = \sum x_i \ln \phi_i - \frac{\Delta H}{RT} + \sum x_i \ln x_i + \ln P/P_o$$

$$Z^3 - Z^2 + (A - B - B^2)Z - AB = 0.0$$

$$A = \frac{(ac\alpha)P}{R^2 T^2} \; ; \; B = b \frac{P}{T}; \; b = \sum x_i b_i$$

$$b_i = 0.08667 \frac{RT_{ci}}{P_{c_i}} \; ; \; a_{c_i} = 0.42747 \frac{R^2 T_{c_i}^2}{P_{c_i}} \; ; \; \alpha_i^{0.5} = 1 + m_i (1 - T_{r_i}^{0.5})$$

$$m_i = 0.480 + 1.574 w_i - 0.176 w_i^2$$

$$(ac\alpha) = \sum_i \sum_j x_i x_j a_{c_i}^{0.5} a_{c_j}^{0.5} \alpha_i^{0.5} \alpha_j^{0.5} (1 - k_{ij})$$

$$(\alpha c \alpha)_i = \sum_{j=1}^{n} x_j a_{c_i}^{0.5} a_{c_j}^{0.5} \alpha_i^{0.5} \alpha_j^{0.5} (1 - k_{ij})$$

$$\beta = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j \left[\frac{a_{c_i}^{0.5} a_{c_j}^{0.5} \alpha_j^{0.5} m_i}{2 T_{c_j} T_{r_i}} + \frac{a_{c_i}^{0.5} a_{c_i}^{0.5} \alpha_i^{0.5} m_j}{2 T_{c_i} T_{r_j}}\right] (1 - k_{ij})$$

$$k_i = \phi_i^L / \phi_i^V$$

Figure 7. SRK Equation of State

APPENDIX D

GENERAL KINETICS CONVERSION FACTORS

The rate expression is usually given in mole/lit sec. For general kinetics, the rate expression is as follows:

$$\text{rate} = k_o \exp(-A/RT)\ C_A^{\nu_A}\ C_B^{\nu_B}\ C_C^{\nu_C} \ \ldots \text{ moles/lit sec}$$

where ν_A, ν_B, ν_C = the stoichiometric coefficients of components A, B, and C, respectively, if the concentration is written as a function of the flow rate.

$$\text{rate} = k_o \exp(-A/RT)\ \left\{\frac{F_A^{\nu_A}\ F_B^{\nu}\ \ldots}{v^{\nu_A + \nu_B \ldots}}\right\} \text{ moles/lit sec}$$

where v = total volumetric flow rate.

The units of the rate constant can be determined as follows:

$$[k_o] = \left(\frac{\text{mole}}{\text{lit sec}}\right)\ \left\{\frac{V^{\nu_A + \nu_B + \ldots}}{F_A^{\nu_A}\ F_B^{\nu_B}\ \ldots}\right\}$$

if the units of the volumetric flow rate and the molar flow rates are substituted in

$$[k_o] = \left(\frac{\text{mole}}{\text{lit sec}}\right)\ \left\{\frac{(\text{lit/sec})^{\nu_A + \nu_B + \ldots}}{\left(\frac{\text{mole}}{\text{sec}}\right)^{\nu_A + \nu_B + \ldots}}\right\}$$

$$= \left(\frac{\text{mole}}{\text{lit sec}}\right)\ \left\{\frac{\text{lit}}{\text{mole}}\right\}^{\nu_A + \nu_B + \ldots}$$

$$[k_o] = \left(\frac{\text{lit}}{\text{mole}}\right)^{\nu_A + \nu_B + \cdots - 1} \left(\frac{1}{\text{sec}}\right)$$

If the rate expression is given in lbmole/ft^{3}hr, then the rate constant units are

$$[k_o]' = \left(\frac{\text{ft}^3}{\text{lbmole}}\right)^{\nu_A + \nu_B + \cdots - 1} \left(\frac{1}{\text{hr}}\right)$$

From the two previous equations

$$[k_o]' = [k_o] \left\{\left(\frac{454 \text{ mole}}{\text{lbmole}}\right)\left(\frac{0.03532 \text{ ft}^3}{\text{lit}}\right)\right\}^{\nu_A + \nu_B + \cdots - 1} \left(\frac{3600 \text{ sec}}{\text{hr}}\right)$$

$$[k_o]' = [k_o] \, (16.04)^{\nu_A + \nu_B + \cdots - 1} \, (3600)$$

APPENDIX E

PROCESS DIAGRAM DISPLAY AND UPDATE MENU

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 6-AUG-1987
PAGE 5 USER:

REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 500.000 CUFT

H2 + C7H8 -> CH4 + C6H6

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00

```
ENTER NEXT COMMAND?

ENTER NEXT COMMAND?
UP1
** ERROR ** SELECTION UP NOT FOUND

 ENTER NEXT UPDATE COMMAND ?

         1

                ** UPDATE MENU**

 ENTER    CC   TO CHANGE THE CONVERSION CRITERIA
 ENTER    OP   TO CHANGE OPERATION MODE
 ENTER    VI   TO CHANGE VOLUME INCREMENT
 ENTER    MN   TO DISPLAY MENU
 ENTER    QT   TO STOP UPDATE  ?

 ENTER NEXT UPDATE COMMAND ?
```

APPENDIX F

THE OVERALL PROCESS OF HYDRODEALKYLATION OF TOLUENE

In the hydrodealkylation process, the following three chemical reactions occur:

$$H_2 + C_7H_8 \rightarrow CH_4 + C_6H_6$$

$$H_2 + \text{o-xylene} \rightarrow CH_4 + C_7H_8$$

$$2C_6H_6 \rightleftarrows H_2 + \text{diphenyl}$$

The main reaction is the hydrogenation of toluene, whereas the other two form the side reactions in the system. The feed to the reactor consists of mainly hydrogen and toluene with a trace of ortho-xylene.

Four outputs are included testing the three conversion criteria (reactor volume, outlet temperature, and the benzene production rate) and the two operation modes (adiabatic and isothermal).

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REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 500.000 CUFT

H2 + C7H8 -> CH4 + C6H6

H2 + O-X -> CH4 + C7H8

C6H6 = H2 + DIPHENYL

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00
1	5	0.00	0.00
1	6	0.00	0.00
2	1	0.50	-1.00
2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00
2	5	1.00	-1.00

2	6	0.00	0.00
3	1	0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

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UNIT OPERATION NO 1 IS A REAC UNIT**

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	450.0000	221.3273
CH4	18.7000	247.3728
C6H6	0.0000	215.9727
C7H8	203.3000	0.0272
O-X	12.7000	0.0000
DIPHENYL	0.0000	0.0000
TOTAL	684.7000	684.7000
T,DEG F	1200.00	1413.23
P,PSIA	495.00	490.00
H,KBTU	18378.55	20866.16
S,KBTU/R	41.9603	43.8732
MOL WEIGHT	31.0685	31.0837
D,LB/FT3	0.8533	0.7495
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 500.00 CUFT

```
DO YOU WANT TO PRINT MOL BALANCE SHEETS;YES OR NO?

         1

                ** UPDATE MENU**

 ENTER    CC   TO CHANGE THE CONVERSION CRITERIA
 ENTER    OP   TO CHANGE OPERATION MODE
 ENTER    VI   TO CHANGE VOLUME INCREMENT
 ENTER    MN   TO DISPLAY MENU
 ENTER    QT   TO STOP UPDATE  ?

 ENTER NEXT UPDATE COMMAND ?
CC
 ENTER THE CONVERSION CRITERIA
          0   FOR REACTOR VOLUME
          1   FOR OUTLET TEMPERATURE
          2   FOR PRODUCTION RATE (P/F)

2
ENTER THE DISIRED PRODUCTION RATE IN  LB  MOLES/HR

200
SPECIFY THE COMPONENT SEQUENCE NUMBER

3
 ENTER NEXT UPDATE COMMAND ?
QT
ENTER NEXT COMMAND?
```

SCI MAXI*SIM JOB ID:
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REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA

THE PRODUCTION RATE OF COMP.# 3 IS 200.00 LB MOLES/HR

H2 + C7H8 -> CH4 + C6H6

H2 + O-X -> CH4 + C7H8

C6H6 = H2 + DIPHENYL

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00
1	5	0.00	0.00
1	6	0.00	0.00
2	1	0.50	-1.00
2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00

2	5	1.00	-1.00
2	6	0.00	0.00
3	1	0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

SCI MAXI*SIM JOB ID:
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UNIT OPERATION NO 1 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	450.0000	237.3010
CH4	18.7000	231.3991
C6H6	0.0000	200.0647
C7H8	203.3000	15.8696
O-X	12.7000	0.0657
DIPHENYL	0.0000	0.0000
TOTAL	684.7000	684.7001
T,DEG F	1200.00	1398.89
P,PSIA	495.00	490.00
H,KBTU	18378.55	20701.59
S,KBTU/R	41.9603	43.8980
MOL WEIGHT	31.0685	31.0820
D,LB/FT3	0.8533	0.7552
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 284.00 CUFT

```
DO YOU WANT TO PRINT MOL BALANCE SHEETS;YES OR NO?

         1

               ** UPDATE MENU**

 ENTER    CC   TO CHANGE THE CONVERSION CRITERIA
 ENTER    OP   TO CHANGE OPERATION MODE
 ENTER    VI   TO CHANGE VOLUME INCREMENT
 ENTER    MN   TO DISPLAY MENU
 ENTER    QT   TO STOP UPDATE  ?

 ENTER NEXT UPDATE COMMAND ?
OP

    ENTER    0     FOR ISOTHERMAL OPERATION
    ENTER    1     FOR ADIABATIC  OPERATION

0
 ENTER NEXT UPDATE COMMAND ?
QT
ENTER NEXT COMMAND?
```

SCI MAXI*SIM JOB ID:
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REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ISOTHERMAL
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA

THE PRODUCTION RATE OF COMP.# 3 IS 200.00 LB MOLES/HR

H2 + C7H8 -> CH4 + C6H6

H2 + O-X -> CH4 + C7H8

C6H6 = H2 + DIPHENYL

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00
1	5	0.00	0.00
1	6	0.00	0.00
2	1	0.50	-1.00
2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00

2	5	1.00	-1.00
2	6	0.00	0.00
3	1	0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

SCI MAXI*SIM JOB ID:
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UNIT OPERATION NO 1 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	450.0000	237.3507
CH4	18.7000	231.3492
C6H6	0.0000	200.0135
C7H8	203.3000	15.9221
O-X	12.7000	0.0645
DIPHENYL	0.0000	0.0000
TOTAL	684.7000	684.7000
T,DEG F	1200.00	1200.00
P,PSIA	495.00	490.00
H,KBTU	18378.55	17384.24
S,KBTU/R	41.9603	42.0098
MOL WEIGHT	31.0685	31.0780
D,LB/FT3	0.8533	0.8465
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS -11124.56 KBTU per HR
THE REACTOR VOLUME= 1764.00 CUFT

SCI MAXI*SIM JOB ID:
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REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR OUTLET TEMPERATURE= 1400.000 DEG F

H2 + C7H8 -> CH4 + C6H6

H2 + O-X -> CH4 + C7H8

C6H6 = H2 + DIPHENYL

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00
1	5	0.00	0.00
1	6	0.00	0.00
2	1	0.50	-1.00
2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00
2	5	1.00	-1.00

2	6	0.00	0.00
3	1	0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

SCI MAXI*SIM JOB ID:
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UNIT OPERATION NO 1 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	450.0000	236.4900
CH4	18.7000	232.2101
C6H6	0.0000	200.8693
C7H8	203.3000	15.0714
O-X	12.7000	0.0593
DIPHENYL	0.0000	0.0000
TOTAL	684.7000	684.7002
T,DEG F	1200.00	1399.62
P,PSIA	495.00	490.00
H,KBTU	18378.55	20709.98
S,KBTU/R	41.9603	43.8985
MOL WEIGHT	31.0685	31.0821
D,LB/FT3	0.8533	0.7549
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 286.00 CUFT

APPENDIX G

SIMULATION OF A PLUG FLOW REACTOR WITH RECYCLE

```
SCI MAXI*SIM    JOB ID:
VERSION #2.2    DATE:   7-AUG-1987
PAGE       15  USER:




UNIT OPERATION   1 IS A ADDR UNIT
  2 FEED(S) TO UNIT OPERATION   1 HAVE BEEN DEFINED:
              1,   8,
  1 PRODUCT(S) FROM UNIT OPERATION   1 HAVE BEEN DEFINED:
              2,

UNIT OPERATION   2 IS A COMP UNIT
  1 FEED(S) TO UNIT OPERATION   2 HAVE BEEN DEFINED:
              2,
  1 PRODUCT(S) FROM UNIT OPERATION   2 HAVE BEEN DEFINED:
              3,

UNIT OPERATION   3 IS A REAC UNIT
  1 FEED(S) TO UNIT OPERATION   3 HAVE BEEN DEFINED:
              3,
  1 PRODUCT(S) FROM UNIT OPERATION   3 HAVE BEEN DEFINED:
              4,

UNIT OPERATION   4 IS A FLSH UNIT
  1 FEED(S) TO UNIT OPERATION   4 HAVE BEEN DEFINED:
              4,
  2 PRODUCT(S) FROM UNIT OPERATION   4 HAVE BEEN DEFINED:
              5,   6,

UNIT OPERATION   5 IS A DVDR UNIT
  1 FEED(S) TO UNIT OPERATION   5 HAVE BEEN DEFINED:
              5,
  2 PRODUCT(S) FROM UNIT OPERATION   5 HAVE BEEN DEFINED:
              7,   8,

THE FOLLOWING STREAM(S) ARE EXTERNAL FEEDS TO THE SIMULATION:
              1,
THE FOLLOWING STREAM(S) ARE PRODUCTS FROM THE SIMULATION:
              6,   7,



STREAM NO   8 IS A RECYCLE STREAM
LOOP   1 ENDS WITH UNIT OPERATION NO   5
```

```
SCI MAXI*SIM    JOB ID:
VERSION #2.2    DATE:   6-AUG-1987
PAGE        6   USER:




ADDR #  1
  ADDR UNIT OPERATION REQUIRES NO PROCESS DATA

COMP #  2
  DISCHARGE PRES     =  495.00 PSIA
  DISCHARGE TEMP     = 1200.00 DEG F
  1=REV ADB;2=POLYTR =    1.00

 REAC #   3


*** THIS IS THE PD FOR THE REACTOR UNIT ****


THE OPERATION IN THE REACTOR IS ADIABATIC
 THE VOLUME INCREMENT=     1.00   CUFT
  THE  INLET PRESSURE TO REACTOR=      495.0000    PSIA
  THE OUTLET PRESSURE FROM REACTOR=      490.0000     PSIA
 THE SPECIFIED REACTOR VOLUME=       500.000  CUFT


H2        +  C7H8       ->   CH4       +  C6H6


H2        +  O-X        ->   CH4       +  C7H8


  C6H6       =   H2         +  DIPHENYL


RXN.   SEQ.#   ORDER   STOCHIO>

  1       1     0.50     -1.00

  1       2     0.00      1.00

  1       3     0.00      1.00

  1       4     1.00     -1.00

  1       5     0.00      0.00

  1       6     0.00      0.00

  2       1     0.50     -1.00
```

2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00
2	5	1.00	-1.00
2	6	0.00	0.00
3	1	.0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

FLSH # 4
CALCULATION TYPE = 1.0
SPEC OR ESTM T = 100.00 DEG F
SPEC PRESSURE = 485.00 PSIA
SPEC OR ESTM L/F = 0.20000

DVDR # 5

PERCENT OF TOTAL FEED TO PRODUCT	PRODUCT NUMBER
20.400	1
79.600	2

SCI MAXI*SIM JOB ID:
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UNIT OPERATION NO 1 IS A ADDR UNIT***

FEEDS>>>>>>>>>>>>>>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	8	2
NAME	FEED	RECYCLE	CMINLET
COMPONENT			
H2	450.0000	1416.6345	1854.1699
CH4	18.7000	340.5688	359.5650
C6H6	0.0000	4.4993	4.5012
C7H8	203.3000	3.2738	206.5448
O-X	12.7000	0.0361	12.7356
DIPHENYL	0.0000	0.0000	0.0000
TOTAL	684.7000	1765.0125	2437.5164
T,DEG F	1200.00	100.00	681.47
P,PSIA	495.00	485.00	485.00
H,KBTU	18385.02	6990.10	25328.35
S,KBTU/R	41.9722	50.0933	96.4254
MOL WEIGHT	31.0866	5.0857	12.4059
D,LB/FT3	0.8538	0.4041	0.4851
L/F(MOLAR)	0.00000	0.00000	0.00000

SCI MAXI*SIM JOB ID:
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UNIT OPERATION NO 2 IS A COMP UNIT***

FEEDS>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	2	3
NAME	CMINLET	TOLUENE
COMPONENT		
H2	1854.1699	1854.1699
CH4	359.5650	359.5650
C6H6	4.5012	4.5012
C7H8	206.5448	206.5448
O-X	12.7356	12.7356
DIPHENYL	0.0000	0.0000
TOTAL	2437.5164	2437.5164
T,DEG F	681.47	1200.00
P,PSIA	485.00	495.00
H,KBTU	25328.35	41359.41
S,KBTU/R	96.4254	107.8463
MOL WEIGHT	12.4059	12.3983
D,LB/FT3	0.4851	0.3407
L/F(MOLAR)	0.00000	0.00000

VALUES AT DELTA S = 0.0
TEMP = 685.45 DEG F
L/F(MOLAR) = 0.00000

WORK = -6300.44 HP AT 0.71 % EFFICIENCY

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
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UNIT OPERATION NO 3 IS A REAC UNIT*** 0

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	3	4
NAME	TOLUENE	BENZENE
COMPONENT		
H2	1854.1699	1781.7428
CH4	359.5650	431.9936
C6H6	4.5012	70.2432
C7H8	206.5448	147.4893
O-X	12.7356	6.0491
DIPHENYL	0.0000	0.0000
TOTAL	2437.5164	2437.5178
T,DEG F	1200.00	1235.29
P,PSIA	495.00	490.00
H,KBTU	41359.41	42177.20
S,KBTU/R	107.8463	108.8405
MOL WEIGHT	12.3983	12.3997
D,LB/FT3	0.3407	0.3304
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 500.00 CUFT

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 20 USER:

UNIT OPERATION NO 4 IS A FLSH UNIT***

FEEDS>>>>>>>PRODUCTS>>>>>>>>>>>>>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	4	5	6
NAME	BENZENE	VAPOR	HEAVY
COMPONENT			
H2	1781.7428	1779.6915	2.0512
CH4	431.9936	427.8503	4.1433
C6H6	70.2432	5.6524	64.5908
C7H8	147.4893	4.1129	143.3765
O-X	6.0491	0.0453	6.0038
DIPHENYL	0.0000	0.0000	0.0000
TOTAL	2437.5178	2217.3523	220.1655
T,DEG F	1235.29	100.00	100.00
P,PSIA	490.00	485.00	485.00
H,KBTU	42177.20	8781.53	-1594.29
S,KBTU/R	108.8405	62.9313	11.3657
MOL WEIGHT	12.3997	5.0857	86.1323
D,LB/FT3	0.3304	0.4041	52.7411
L/F(MOLAR)	0.00000	0.00000	1.00000

HEAT TRANSFERRED -34989.96 KBTU

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 21 USER:

UNIT OPERATION NO 5 IS A DVDR UNIT***

FEEDS>>>>>>>PRODUCTS>>>>>>>>>>>>>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	5	7	8
NAME	VAPOR	PURGE	RECYCLE
COMPONENT			
H2	1779.6915	363.0571	1416.6345
CH4	427.8503	87.2814	340.5688
C6H6	5.6524	1.1531	4.4993
C7H8	4.1129	0.8390	3.2738
O-X	0.0453	0.0092	0.0361
DIPHENYL	0.0000	0.0000	0.0000
TOTAL	2217.3523	452.3399	1765.0125
T,DEG F	100.00	100.00	100.00
P,PSIA	485.00	485.00	485.00
H,KBTU	8781.53	1791.43	6990.10
S,KBTU/R	62.9313	12.8380	50.0933
MOL WEIGHT	5.0857	5.0857	5.0857
D,LB/FT3	0.4041	0.4041	0.4041
L/F(MOLAR)	0.00000	0.00000	0.00000

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
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OVERALL PROCESS MATERIAL BALANCE

COMPONENT NAME	TOTAL FEEDS	TOTAL PRODUCTS	RATIO (PD/FD)
H2	450.0000	365.1083	0.81135
CH4	18.7000	91.4247	4.88902
C6H6	0.0000	65.7439	0.00000
C7H8	203.3000	144.2155	0.70937
O-X	12.7000	6.0130	0.47346
DIPHENYL	0.0000	0.0000	0.00000
TOTAL	684.7000	672.5054	0.98219

APPENDIX H

THE EFFECT OF THE VOLUME INCREMENT ON THE RESULTS

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 9-AUG-1987
PAGE 10 USER:

REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 500.000 CUFT

H2 + C7H8 -> CH4 + C6H6

H2 + O-X -> CH4 + C7H8

C6H6 = H2 + DIPHENYL

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00
1	5	0.00	0.00
1	6	0.00	0.00
2	1	0.50	-1.00
2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00
2	5	1.00	-1.00

2	6	0.00	0.00
3	1	0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 9-AUG-1987
PAGE 6 USER:

UNIT OPERATION NO 1 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	450.0000	221.3273
CH4	18.7000	247.3728
C6H6	0.0000	215.9727
C7H8	203.3000	0.0272
O-X	12.7000	0.0000
DIPHENYL	0.0000	0.0000
TOTAL	684.7000	684.7000
T,DEG F	1200.00	1413.23
P,PSIA	495.00	490.00
H,KBTU	18378.55	20866.16
S,KBTU/R	41.9603	43.8732
MOL WEIGHT	31.0685	31.0837
D,LB/FT3	0.8533	0.7495
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 500.00 CUFT

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 9-AUG-1987
PAGE 12 USER:

REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 0.25 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 500.000 CUFT

H2 + C7H8 -> CH4 + C6H6

H2 + O-X -> CH4 + C7H8

C6H6 = H2 + DIPHENYL

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00
1	5	0.00	0.00
1	6	0.00	0.00
2	1	0.50	-1.00
2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00
2	5	1.00	-1.00

2	6	0.00	0.00
3	1	0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 9-AUG-1987
PAGE 8 USER:

UNIT OPERATION NO 1 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	450.0000	221.3194
CH4	18.7000	247.3812
C6H6	0.0000	215.9811
C7H8	203.3000	0.0187
O-X	12.7000	0.0000
DIPHENYL	0.0000	0.0000
TOTAL	684.7000	684.7004
T,DEG F	1200.00	1415.50
P,PSIA	495.00	490.00
H,KBTU	18378.55	20905.06
S,KBTU/R	41.9603	43.8938
MOL WEIGHT	31.0685	31.0837
D,LB/FT3	0.8533	0.7486
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 500.00 CUFT

APPENDIX I

SIMULATION OF TWO PLUG FLOW REACTORS IN SERIES

The first run shows the results from the simulation of one single reactor with a volume equal to 500 ft^3. The second run shows the results from the simulation of two reactors in series. For comparison, look at stream number 2 in the first run, and stream number 3 in the second run.

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 4 USER:

REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 500.000 CUFT

H2 + C7H8 -> CH4 + C6H6

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 6 USER:

UNIT OPERATION NO 1 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	450.0000	217.0577
CH4	0.0000	232.9424
C6H6	0.0000	232.9424
C7H8	233.0000	0.0576
TOTAL	683.0000	683.0001
T,DEG F	1200.00	1408.17
P,PSIA	495.00	490.00
H,KBTU	18865.59	21383.47
S,KBTU/R	42.5316	44.6471
MOL WEIGHT	32.7408	32.7541
D,LB/FT3	0.8995	0.7920
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 500.00 CUFT

```
UNIT OPERATION   1 IS A REAC UNIT
  1 FEED(S) TO UNIT OPERATION   1 HAVE BEEN DEFINED:
              1,
  1 PRODUCT(S) FROM UNIT OPERATION   1 HAVE BEEN DEFINED:
              2,

UNIT OPERATION   2 IS A REAC UNIT
  1 FEED(S) TO UNIT OPERATION   2 HAVE BEEN DEFINED:
              2,
  1 PRODUCT(S) FROM UNIT OPERATION   2 HAVE BEEN DEFINED:
              3,

THE FOLLOWING STREAM(S) ARE EXTERNAL FEEDS TO THE SIMULATION:
              1,
THE FOLLOWING STREAM(S) ARE PRODUCTS FROM THE SIMULATION:
              3,
```

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 7 USER:

REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 492.5000 PSIA
THE SPECIFIED REACTOR VOLUME= 250.000 CUFT

H2 + C7H8 -> CH4 + C6H6

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00

REAC # 2

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 492.5000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 250.000 CUFT

H2 + C7H8 -> CH4 + C6H6

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00

1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 8 USER:

UNIT OPERATION NO 1 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	FEED1	PROD.1
COMPONENT		
H2	450.0000	258.0125
CH4	0.0000	191.9874
C6H6	0.0000	191.9874
C7H8	233.0000	41.0126
TOTAL	683.0000	682.9999
T,DEG F	1200.00	1372.39
P,PSIA	495.00	492.50
H,KBTU	18865.59	20957.63
S,KBTU/R	42.5316	44.6117
MOL WEIGHT	32.7408	32.7523
D,LB/FT3	0.8995	0.8114
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 250.00 CUFT

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 9 USER:

UNIT OPERATION NO 2 IS A REAC UNIT*** v1.3

FEEDS>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	2	3
NAME	PROD.1	PROD.2
COMPONENT		
H2	258.0125	217.0548
CH4	191.9874	232.9451
C6H6	191.9874	232.9451
C7H8	41.0126	0.0548
TOTAL	682.9999	682.9998
T,DEG F	1372.39	1408.16
P,PSIA	492.50	490.00
H,KBTU	20957.63	21383.25
S,KBTU/R	44.6117	44.6469
MOL WEIGHT	32.7523	32.7541
D,LB/FT3	0.8114	0.7920
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 250.00 CUFT

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 10 USER:

OVERALL PROCESS MATERIAL BALANCE

COMPONENT NAME	TOTAL FEEDS	TOTAL PRODUCTS	RATIO (PD/FD)
H2	450.0000	217.0548	0.48234
CH4	0.0000	232.9451	0.00000
C6H6	0.0000	232.9451	0.00000
C7H8	233.0000	0.0548	0.00024
TOTAL	683.0000	682.9998	1.00000

APPENDIX J

SIMULATION OF TWO PLUG FLOW REACTORS IN PARALLEL

The first run shows the results from the simulation of one single reactor with a volume equal to 500 ft^3. The second run shows the results from the simulation of two reactors in parallel. For comparison, look at stream number 2 in the first run, and stream number 6 in the second run.

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 4 USER:

REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 500.000 CUFT

H2 + C7H8 -> CH4 + C6H6

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 5 USER:

UNIT OPERATION NO 1 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	450.0000	217.0577
CH4	0.0000	232.9424
C6H6	0.0000	232.9424
C7H8	233.0000	0.0576
TOTAL	683.0000	683.0001
T,DEG F	1200.00	1408.17
P,PSIA	495.00	490.00
H,KBTU	18865.59	21383.47
S,KBTU/R	42.5316	44.6471
MOL WEIGHT	32.7408	32.7541
D,LB/FT3	0.8995	0.7920
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 500.00 CUFT

```
SCI MAXI*SIM    JOB ID:
VERSION #2.2    DATE:   7-AUG-1987
PAGE        2  USER:



UNIT OPERATION   1 IS A DVDR UNIT
  1 FEED(S) TO UNIT OPERATION   1 HAVE BEEN DEFINED:
              1,
  2 PRODUCT(S) FROM UNIT OPERATION   1 HAVE BEEN DEFINED:
              2,   3,

UNIT OPERATION   2 IS A REAC UNIT
  1 FEED(S) TO UNIT OPERATION   2 HAVE BEEN DEFINED:
              2,
  1 PRODUCT(S) FROM UNIT OPERATION   2 HAVE BEEN DEFINED:
              4,

UNIT OPERATION   3 IS A REAC UNIT
  1 FEED(S) TO UNIT OPERATION   3 HAVE BEEN DEFINED:
              3,
  1 PRODUCT(S) FROM UNIT OPERATION   3 HAVE BEEN DEFINED:
              5,

UNIT OPERATION   4 IS A ADDR UNIT
  2 FEED(S) TO UNIT OPERATION   4 HAVE BEEN DEFINED:
              4,   5,
  1 PRODUCT(S) FROM UNIT OPERATION   4 HAVE BEEN DEFINED:
              6,

THE FOLLOWING STREAM(S) ARE EXTERNAL FEEDS TO THE SIMULATION:
              1,
THE FOLLOWING STREAM(S) ARE PRODUCTS FROM THE SIMULATION:
              6,
```

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 3 USER:

DVDR # 1

PERCENT OF TOTAL FEED TO PRODUCT	PRODUCT NUMBER
50.000	1
50.000	2

REAC # 2

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 250.000 CUFT

H2 + C7H8 -> CH4 + C6H6

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00

REAC # 3

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA
THE SPECIFIED REACTOR VOLUME= 250.000 CUFT

H2 + C7H8 -> CH4 + C6H6

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00

ADDR # 4
ADDR UNIT OPERATION REQUIRES NO PROCESS DATA

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 4 USER:

UNIT OPERATION NO 1 IS A DVDR UNIT***

FEEDS>>>>>>>PRODUCTS>>>>>>>>>>>>>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2	3
NAME	FEED	1/2FEED	1/2FEED
COMPONENT			
H2	450.0000	225.0000	225.0000
CH4	0.0000	0.0000	0.0000
C6H6	0.0000	0.0000	0.0000
C7H8	233.0000	116.5000	116.5000
TOTAL	683.0000	341.5000	341.5000
T,DEG F	1200.00	1200.00	1200.00
P,PSIA	495.00	495.00	495.00
H,KBTU	18871.37	9432.79	9432.79
S,KBTU/R	42.5422	21.2658	21.2658
MOL WEIGHT	32.7572	32.7408	32.7408
D,LB/FT3	0.9000	0.8995	0.8995
L/F(MOLAR)	0.00000	0.00000	0.00000

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 5 USER:

UNIT OPERATION NO 2 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	2	4
NAME	1/2FEED	PROD.1
COMPONENT		
H2	225.0000	108.5427
CH4	0.0000	116.4572
C6H6	0.0000	116.4572
C7H8	116.5000	0.0427
TOTAL	341.5000	341.4999
T,DEG F	1200.00	1405.46
P,PSIA	495.00	490.00
H,KBTU	9432.79	10667.94
S,KBTU/R	21.2658	22.3110
MOL WEIGHT	32.7408	32.7540
D,LB/FT3	0.8995	0.7932
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 250.00 CUFT

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 6 USER:

UNIT OPERATION NO 3 IS A REAC UNIT***

FEEDS>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	3	5
NAME	1/2FEED	PROD.2
COMPONENT		
H2	225.0000	108.5427
CH4	0.0000	116.4573
C6H6	0.0000	116.4573
C7H8	116.5000	0.0427
TOTAL	341.5000	341.5000
T,DEG F	1200.00	1405.46
P,PSIA	495.00	490.00
H,KBTU	9432.79	10667.92
S,KBTU/R	21.2658	22.3110
MOL WEIGHT	32.7408	32.7541
D,LB/FT3	0.8995	0.7932
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 250.00 CUFT

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 7 USER:

UNIT OPERATION NO 4 IS A ADDR UNIT***

FEEDS>>>>>>>>>>>>>>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	4	5	6
NAME	PROD.1	PROD.2	OVERALL
COMPONENT			
H2	108.5427	108.5427	217.0854
CH4	116.4572	116.4573	232.9145
C6H6	116.4572	116.4573	232.9145
C7H8	0.0427	0.0427	0.0854
TOTAL	341.4999	341.5000	682.9999
T,DEG F	1405.46	1405.46	1405.29
P,PSIA	490.00	490.00	490.00
H,KBTU	10667.94	10667.92	21335.86
S,KBTU/R	22.3110	22.3110	44.6248
MOL WEIGHT	32.7540	32.7541	32.7614
D,LB/FT3	0.7932	0.7932	0.7934
L/F(MOLAR)	0.00000	0.00000	0.00000

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 7-AUG-1987
PAGE 8 USER:

OVERALL PROCESS MATERIAL BALANCE

COMPONENT NAME	TOTAL FEEDS	TOTAL PRODUCTS	RATIO (PD/FD)
H2	450.0000	217.0854	0.48241
CH4	0.0000	232.9145	0.00000
C6H6	0.0000	232.9145	0.00000
C7H8	233.0000	0.0854	0.00037
TOTAL	683.0000	682.9999	1.00000

APPENDIX K

THE NEED OF THE REACTOR WITH RECYCLE

SCI MAXI*SIM JOB ID:
VERSION #2.2 DATE: 9-AUG-1987
PAGE 5 USER:

REAC # 1

*** THIS IS THE PD FOR THE REACTOR UNIT ****

THE OPERATION IN THE REACTOR IS ADIABATIC
THE VOLUME INCREMENT= 1.00 CUFT
THE INLET PRESSURE TO REACTOR= 495.0000 PSIA
THE OUTLET PRESSURE FROM REACTOR= 490.0000 PSIA

THE PRODUCTION RATE OF COMP.# 3 IS 203.00 LB MOLES/HR

H2 + C7H8 -> CH4 + C6H6

H2 + O-X -> CH4 + C7H8

C6H6 = H2 + DIPHENYL

RXN.	SEQ.#	ORDER	STOCHIO>
1	1	0.50	-1.00
1	2	0.00	1.00
1	3	0.00	1.00
1	4	1.00	-1.00
1	5	0.00	0.00
1	6	0.00	0.00
2	1	0.50	-1.00
2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00

2	5	1.00	-1.00
2	6	0.00	0.00
3	1	0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

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UNIT OPERATION NO 1 IS A REAC UNIT*** .

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	2
NAME	TOLUENE	BENZENE
COMPONENT		
H2	629.3000	413.5182
CH4	18.7000	234.4818
C6H6	0.0000	203.1246
C7H8	203.3000	12.8326
O-X	12.7000	0.0428
DIPHENYL	0.0000	0.0000
TOTAL	864.0000	863.9999
T,DEG F	1200.00	1388.11
P,PSIA	495.00	490.00
H,KBTU	20466.50	22832.64
S,KBTU/R	47.8736	50.0149
MOL WEIGHT	25.0379	25.0490
D,LB/FT3	0.6872	0.6120
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 367.00 CUFT

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UNIT OPERATION   1 IS A ADDR UNIT
  2 FEED(S) TO UNIT OPERATION   1 HAVE BEEN DEFINED:
              1,   8,
  1 PRODUCT(S) FROM UNIT OPERATION   1 HAVE BEEN DEFINED:
              2,

UNIT OPERATION   2 IS A COMP UNIT
  1 FEED(S) TO UNIT OPERATION   2 HAVE BEEN DEFINED:
              2,
  1 PRODUCT(S) FROM UNIT OPERATION   2 HAVE BEEN DEFINED:
              3,

UNIT OPERATION   3 IS A REAC UNIT
  1 FEED(S) TO UNIT OPERATION   3 HAVE BEEN DEFINED:
              3,
  1 PRODUCT(S) FROM UNIT OPERATION   3 HAVE BEEN DEFINED:
              4,

UNIT OPERATION   4 IS A FLSH UNIT
  1 FEED(S) TO UNIT OPERATION   4 HAVE BEEN DEFINED:
              4,
  2 PRODUCT(S) FROM UNIT OPERATION   4 HAVE BEEN DEFINED:
              5,   6,

UNIT OPERATION   5 IS A DVDR UNIT
  1 FEED(S) TO UNIT OPERATION   5 HAVE BEEN DEFINED:
              5,
  2 PRODUCT(S) FROM UNIT OPERATION   5 HAVE BEEN DEFINED:
              7,   8,

THE FOLLOWING STREAM(S) ARE EXTERNAL FEEDS TO THE SIMULATION:
              1,
THE FOLLOWING STREAM(S) ARE PRODUCTS FROM THE SIMULATION:
              6,   7,



STREAM NO   8 IS A RECYCLE STREAM
LOOP   1 ENDS WITH UNIT OPERATION NO   5
```

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ADDR #  1
  ADDR UNIT OPERATION REQUIRES NO PROCESS DATA

COMP #  2
  DISCHARGE PRES     =  495.00 PSIA
  DISCHARGE TEMP     = 1200.00 DEG F
  1=REV ADB;2=POLYTR =    1.00

 REAC #   3


*** THIS IS THE PD FOR THE REACTOR UNIT ****


THE OPERATION IN THE REACTOR IS ADIABATIC
 THE VOLUME INCREMENT=     1.00   CUFT
  THE  INLET PRESSURE TO REACTOR=      495.0000    PSIA
  THE OUTLET PRESSURE FROM REACTOR=      490.0000     PSIA

 THE PRODUCTION RATE OF COMP.#    3   IS        203.00       LB  MOLES/HR


H2        +  C7H8       ->   CH4       +  C6H6


H2        +  O-X        ->   CH4       +  C7H8


  C6H6        =   H2         +  DIPHENYL


RXN.   SEQ.#   ORDER   STOCHIO>

  1       1     0.50     -1.00

  1       2     0.00      1.00

  1       3     0.00      1.00

  1       4     1.00     -1.00

  1       5     0.00      0.00

  1       6     0.00      0.00
```

2	1	0.50	-1.00
2	2	0.00	1.00
2	3	0.00	0.00
2	4	0.00	1.00
2	5	1.00	-1.00
2	6	0.00	0.00
3	1	0.00	1.00
3	2	0.00	0.00
3	3	0.00	-2.00
3	4	0.00	0.00
3	5	0.00	0.00
3	6	0.00	1.00

FLSH # 4
CALCULATION TYPE = 1.0
SPEC OR ESTM T = 100.00 DEG F
SPEC PRESSURE = 485.00 PSIA
SPEC OR ESTM L/F = 0.20000

DVDR # 5

PERCENT OF TOTAL FEED TO PRODUCT	PRODUCT NUMBER
20.400	1
79.600	2

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UNIT OPERATION NO 1 IS A ADDR UNIT***

FEEDS>>>>>>>>>>>>>>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	1	8	2
NAME	FEED	RECYCLE	COMPINL
COMPONENT			
H2	450.0000	873.1261	1299.6881
CH4	18.7000	813.0051	829.4761
C6H6	0.0000	14.1494	13.9856
C7H8	203.3000	0.6928	203.9788
O-X	12.7000	0.0013	12.7013
DIPHENYL	0.0000	0.0000	0.0000
TOTAL	684.7000	1700.9749	2359.8301
T,DEG F	1200.00	100.00	654.15
P,PSIA	495.00	485.00	485.00
H,KBTU	18385.02	6995.70	25279.18
S,KBTU/R	41.9722	55.5203	101.9957
MOL WEIGHT	31.0866	9.3897	15.7473
D,LB/FT3	0.8538	0.7574	0.6319
L/F(MOLAR)	0.00000	0.00000	0.00000

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UNIT OPERATION NO 2 IS A COMP UNIT***

FEEDS>>>>>>>PRODUCTS>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	2	3
NAME	COMPINL	TOLUENE
COMPONENT		
H2	1299.6881	1299.6881
CH4	829.4761	829.4761
C6H6	13.9856	13.9856
C7H8	203.9788	203.9788
O-X	12.7013	12.7013
DIPHENYL	0.0000	0.0000
TOTAL	2359.8301	2359.8301
T,DEG F	654.15	1200.00
P,PSIA	485.00	495.00
H,KBTU	25279.18	43888.88
S,KBTU/R	101.9957	115.4028
MOL WEIGHT	15.7473	15.7397
D,LB/FT3	0.6319	0.4323
L/F(MOLAR)	0.00000	0.00000

VALUES AT DELTA S = 0.0
TEMP = 657.69 DEG F
L/F(MOLAR) = 0.00000

WORK = -7313.88 HP AT 0.58 % EFFICIENCY

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UNIT OPERATION NO 3 IS A REAC UNIT*** ,

FEEDS>>>>>>>PRODUCTS>>>>
STREAM FLOW RATES ARE LB-MOLS

STREAM NO	3	4
NAME	TOLUENE	BENZENE
COMPONENT		
H2	1299.6881	1098.1405
CH4	829.4761	1031.0270
C6H6	13.9856	203.0260
C7H8	203.9788	27.4484
O-X	12.7013	0.1915
DIPHENYL	0.0000	0.0000
TOTAL	2359.8301	2359.8335
T,DEG F	1200.00	1286.43
P,PSIA	495.00	490.00
H,KBTU	43888.88	46145.32
S,KBTU/R	115.4028	116.9566
MOL WEIGHT	15.7397	15.7432
D,LB/FT3	0.4323	0.4072
L/F(MOLAR)	0.00000	0.00000

THE HEAT LOAD ON REACTOR IS 0.00 KBTU per HR
THE REACTOR VOLUME= 1914.00 CUFT

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UNIT OPERATION NO 4 IS A FLSH UNIT***

FEEDS>>>>>>>PRODUCTS>>>>>>>>>>>>>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	4	5	6
NAME	BENZENE	VAPOR	HEAVY
COMPONENT			
H2	1098.1405	1096.8921	1.2484
CH4	1031.0270	1021.3632	9.6638
C6H6	203.0260	17.7756	185.2504
C7H8	27.4484	0.8704	26.5780
O-X	0.1915	0.0017	0.1898
DIPHENYL	0.0000	0.0000	0.0000
TOTAL	2359.8335	2136.9031	222.9304
T,DEG F	1286.43	100.00	100.00
P,PSIA	490.00	485.00	485.00
H,KBTU	46145.32	8788.58	-1546.46
S,KBTU/R	116.9566	69.7493	9.9499
MOL WEIGHT	15.7432	9.3897	76.6933
D,LB/FT3	0.4072	0.7574	52.4747
L/F(MOLAR)	0.00000	0.00000	1.00000

HEAT TRANSFERRED -38903.20 KBTU

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UNIT OPERATION NO 5 IS A DVDR UNIT***

FEEDS>>>>>>>PRODUCTS>>>>>>>>>>>>>>>>

STREAM FLOW RATES ARE LB-MOLS

STREAM NO	5	7	8
NAME	VAPOR	PURGE	RECYCLE
COMPONENT			
H2	1096.8921	223.7660	873.1261
CH4	1021.3632	208.3581	813.0051
C6H6	17.7756	3.6262	14.1494
C7H8	0.8704	0.1776	0.6928
O-X	0.0017	0.0003	0.0013
DIPHENYL	0.0000	0.0000	0.0000
TOTAL	2136.9031	435.9282	1700.9749
T,DEG F	100.00	100.00	100.00
P,PSIA	485.00	485.00	485.00
H,KBTU	8788.58	1792.87	6995.70
S,KBTU/R	69.7493	14.2288	55.5203
MOL WEIGHT	9.3897	9.3897	9.3897
D,LB/FT3	0.7574	0.7574	0.7574
L/F(MOLAR)	0.00000	0.00000	0.00000

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OVERALL PROCESS MATERIAL BALANCE

COMPONENT NAME	TOTAL FEEDS	TOTAL PRODUCTS	RATIO (PD/FD)
H2	450.0000	225.0144	0.50003
CH4	18.7000	218.0219	11.65892
C6H6	0.0000	188.8766	0.00000
C7H8	203.3000	26.7556	0.13161
O-X	12.7000	0.1902	0.01497
DIPHENYL	0.0000	0.0000	0.00000
TOTAL	684.7000	658.8586	0.96226

APPENDIX L

THE COMPUTER CODE OF THE MODEL

```
      C
      C
      CCCCCCC
      C       SUBROUTINE INPUT FOR REACTOR
      C
      C123456
            SUBROUTINE REAC(II)
      C
            DIMENSION IFDB(11),IPDB(11),KMD(5)
            COMMON/PRD1/F1(500),IDCS(25),IDPRO(50),IFD(50),
           1 IFDL(200),IPD(50),IPDL(200),IPRC(70),IRC(50),
           2 ISIZ(25),ITCNT(100),JPD(50),MHB(50),NRECL(10),
           3 PD(1250),PROP(3000),RCNT(100),TEMP(410),X(5000)
            COMMON/SIZE2/ISIZ2(100)
            COMMON/UPDATE/IUPDT(50)
            COMMON/COMIO/NI,NO,IYES,INO,PNAM(15),NPAGE
            COMMON/UNITA1/UDA(3),ULA(3),UVA(3),ULB(3),UHT(9),UDF(6),HPU(3
     )
            COMMON/UNITA2/TU(4),PU(6),HU(3),SU(6),RU(6),UM(3),PUX(6)
            COMMON/UNITA3/UARE(3),UVIS(6),UTHC(9),UHPA(3),UVB(3),USG(6)
            COMMON/UNITDM/IU1,IU2,IU3,IU21,IU31
            EQUIVALENCE(ITCNT(18),N2),(ITCNT(21),NCP),(ITCNT(22),NCPU),
           1 (ITCNT(23),NCPT  ),(ITCNT(24),NCPP  ),(ITCNT(25),NCPH  ),
           2 (ITCNT(26),NCPS  ),(ITCNT(27),NCPF  ),(ITCNT(28),NCPD  ),
           3 (ITCNT(29),NCPN  ),(ITCNT(30),NCP5  ),(ITCNT(31),NEL   ),
           4 (ITCNT(32),NARFD ),(ITCNT(33),NARPD ),(ITCNT(34),NARPV ),
           5 (ITCNT(35),NMAX  ),(ITCNT(36),NEOS  ),(ITCNT(37),NHELP ),
           6 (ITCNT(38),NST   ),(ITCNT(39),NND   ),(ITCNT(46),NOPT   )
            EQUIVALENCE(RCNT(1),RTOL),(RCNT(2),RACC),(RCNT(3),QIJC),
           1 (RCNT( 4),RHOV ),(RCNT( 5),YMW  ),(RCNT( 6),XMW),
           2 (RCNT(51),TST  ),(RCNT(52),TEND ),(RCNT(53),PST),
           3 (RCNT(54),PEND ),(RCNT(55),DELT ),(RCNT(56),DELP),
           4 (RCNT(57),TLMU ),(RCNT(58),TLML ),(RCNT(59),PLMU),
           5 (RCNT(60),HSPEC),(RCNT(61),FRAC )
            COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
            COMMON/INPR2/NNCP,M
            COMMON/EQRXN/NRX(10),GRX(10)
            DATA KMD/2HCC,2HOP,2HVI,2HMN,2HQT/
        1   FORMAT(' ENTER FEED STREAM ID NO TO REACTOR UNIT',I3,'?')
        2   FORMAT(11I5)
        3   FORMAT(' ENTER PRODUCT STREAM ID NO FROM REACTOR',I3,'?')
        5   FORMAT(F20.0)
        6   FORMAT(
           1 /'                  ** UPDATE MENU**          ',/
           4 /'  ENTER    CC   TO CHANGE THE CONVERSION CRITERIA ',
           7 /'  ENTER    OP   TO CHANGE OPERATION MODE ',
           2 /'  ENTER    VI   TO CHANGE VOLUME INCREMENT    ',
           5 /'  ENTER    MN   TO DISPLAY MENU ',
           6 /'  ENTER    QT   TO STOP UPDATE  ? '/)
        7   FORMAT(A2)
        8   FORMAT('   ENTER THE VOLUME INCREMENT IN  ',A4/)
        9   FORMAT( '  ENTER THE INLET TEMPERATURE IN  ',A4)
        10  FORMAT( '  ENTER THE INLET PRESSURE IN  ',A4)
        11  FORMAT( '  NO OF FEEDS SHOULD BE ONE '/)
```

```
 2513        12  FORMAT( '  NO OF PRODUCTS SHOULD BE ONE '/)
 2514        14  FORMAT( '  ENTER NEXT UPDATE COMMAND ? ')
 2515        15  FORMAT( '  ONLY ONE FEED ALLOWED TO REACTOR UNIT',I3/)
 2516        17  FORMAT( '  PRODUCT STREAM IS ',I3,/)
 2517        18  FORMAT( '  UNIT',I3,' HAS PRODUCTS AS FEEDS '/)
 2518        20  FORMAT( '  ENTER ORDER OF COMP.#     ',I3,'    IN RXN.   ',I3
,/)
 2519        21  FORMAT( '  ENTER THE NUMBER OF REACTIONS '/)
 2520        23  FORMAT( '  ENTER THE STOICHIOMETRIC COEFFICIENT ',
 2521           1 'OF COMPONENT     ',I3,'    IN REACTION     ',I3,/)
 2522        24  FORMAT( '  THE MAXIMUM NUMBER OF REACTIONS IS TEN'/)
 2523        41  FORMAT( '  ARE THE UNITS OF THE FREQUENCY FACTOR IN TERMS ',
 2524           1 /'  0-gmoles,lit,sec         1-lbmoles,cuft,hr '/)
 2525        26  FORMAT( '  ENTER THE FREQUENCY FACTOR OF REACTION ',I3,/)
 2526        27  FORMAT( '  ENTER THE ACTIVATION ENERGY OF REACTION   ',I3
 2527           1 ,'  IN  ',A4,'/',A4,'MOLES'/)
 2528        28  FORMAT( ' ENTER THE HEAT OF REACTION   ',I3,'  IN  ',
 2529           1 A4,'/',A4,'MOLES'/)
 2530        35  FORMAT( '  ENTER THE OUTLET PRESSURE OPTION',
 2531           1 /'   ENTER  1  IF PRESSURE DROP IS TO BE SPECIFIED',
 2532           2 /'   ENTER  0  IF OUTLET PRESSURE IS TO BE SPECIFIED'/)
 2533        36  FORMAT( '  ENTER PRESSURE DROP ACROSS THE REACTOR IN    ',A4/
)
 2534        37  FORMAT( '  ENTER OUTLET PRESSURE FROM REACTOR IN    ',A4/)
 2535        30  FORMAT(
 2536           1 /'     ENTER    0     FOR ISOTHERMAL OPERATION ',
 2537           2 /'     ENTER    1     FOR ADIABATIC  OPERATION '/)
 2538        31  FORMAT( '  ENTER THE CONVERSION CRITERIA ',
 2539           1 / '            0   FOR REACTOR VOLUME ',
 2540           2 / '            1   FOR OUTLET TEMPERATURE ',
 2541           3 / '            2   FOR PRODUCTION RATE (P/F) '/)
 2542        32  FORMAT( ' SPECIFY THE COMPONENT SEQUENCE NUMBER '/)
 2543        33  FORMAT( ' ENTER THE DESIRED REACTOR VOLUME ',A4/)
 2544        34  FORMAT(' ENTER THE DISIRED PRODUCTION RATE IN  ',A4,'MOLES/HR
'/)
 2545        38  FORMAT( ' ENTER THE OUTLET REACTOR TEMPERATURE  IN DEG    ',A
1/)
 2546        39  FORMAT( ' IS REACTION   ',I3, '    IN EQUILIBRIUM ',
 2547           1 /'     ENTER     1:NO          2:YES  '/)
 2548        40  FORMAT( ' ENTER THE GIBB_S FREE ENERGY FOR RXN.     'I3
 2549           1 ,'  IN',A4,'/',A4,'MOLE'/)
 2550            IF(II.EQ.0) GO TO 70
 2551            IPOS=JPD(NEL)
 2552            WRITE(6,*)IPOS
 2553            IF (II.LT.0)GO TO 91
 2554            GO TO 95
 2555        70  IPOS=NARPV
 2556            WRITE(6,*)IPOS
 2557       212 KFD=0
 2558            DO 245 I=1,11
 2559            IFDB(I)=0
 2560       245 CONTINUE
 2561      9001 WRITE(NO,1) NEL
 2562            READ(NI,2,ERR=9001)(IFDB(I),I=1,1)
 2563            CALL FPSTAK(IFD,IFDB,IFDL,NARFD,NEL,KFD)
```

```
2564            IF(KFD.NE.0) GO TO 210
2565            WRITE(NO,11)
2566            GO TO 212
2567          210 IF(KFD.EQ.1) GO TO 228
2568            WRITE(NO,15)NEL
2569            GO TO 212
2570          228 DO 310 K=1,KFD
2571            IDEST=(IFDB(K)-1)*NCP5 + NCPD
2572            X(IDEST)=NEL
2573          310 CONTINUE
2574          214 KPD=0
2575            DO 9002 I=1,11
2576            IPDB(I)=0
2577         9002 CONTINUE
2578            WRITE(NO,3) NEL
2579            READ(NI,2,ERR=214)(IPDB(I),I=1,1)
2580            CALL FPSTAK(IPD,IPDB,IPDL,NARPD,NEL,KPD)
2581          215 IF(KPD.EQ.1) GO TO 191
2582            WRITE(NO,12)
2583            GO TO 214
2584          191 WRITE(NO,17)(IPDB(1))
2585          216 IDUP=0
2586            CALL FPSCAN(KFD,KPD,IFDB,IPDB,IDUP)
2587            IF(IDUP.EQ.0) GO TO 246
2588            WRITE(NO,18) NEL
2589            GO TO 214
2590          246 NARFD=NARFD + KFD +1
2591            NARPD=NARPD + KPD +1
2592            MHB(NEL)=1
2593           91  CONTINUE
2594         C
2595         C
2596         C***        READ IN THE INPUT DATA AND STORE IN PD ARRAY
2597         C
2598         C
2599                NNCP=NCP
2600          100 WRITE(NO,21)
2601            READ(NI,2,ERR=100)M
2602            IF (M) 100,100,101
2603          101 IF(M.GT.10) GO TO 103
2604            PD(IPOS)=M
2605            IF(II.GT.0)GO TO 3000
2606            GO TO 110
2607          103 WRITE(NO,24)
2608            GO TO 100
2609          110 WRITE(NO,9)TU(IU1)
2610            READ(NI,5,ERR=110)TTRINT
2611            PD(IPOS+4)=TTRINT
2612          119 WRITE(NO,10)PU(IU2)
2613            READ(NI,5,ERR=119)PTRINT
2614            PD(IPOS+364)=PTRINT
2615          120 WRITE(NO,30)
2616            READ(NI,2,ERR=120)NOP
2617            IF(NOP)120,122,122
2618          122 IF(NOP.GT.1)GO TO 120
```

```
2619            PD(IPOS+3)=NOP
2620            IF(II.GT.0) GO TO 3000
2621          130 WRITE(NO,35)
2622            READ(NI,2,ERR=130)NPS
2623            PD(IPOS+40)=NPS
2624            IF(NPS)130,131,132
2625          131 WRITE(NO,37)PU(IU2)
2626            READ(NI,5,ERR=131)ORP
2627            IF(ORP)131,131,133
2628          133 PD(IPOS+5)=ORP
2629            IF(II.GT.0)GO TO 3000
2630            GO TO 140
2631          132 IF(NPS.GT.1)GO TO 130
2632          134 WRITE(NO,36)PU(IU2)
2633             READ(NI,5,ERR=134) PRDROP
2634            IF (PRDROP)134,135,135
2635          135 PD(IPOS+7)=PRDROP
2636            IF (II.GT.0) GO TO 3000
2637          140 WRITE(NO,31)
2638            READ(NI,2,ERR=140) NCC
2639            PD(IPOS+41)=NCC
2640            IF(NCC)140,141,142
2641          141 WRITE(NO,33),UVB(IU3)
2642            READ(NI,5,ERR=141) RV
2643            IF(RV)141,141,143
2644          143 PD(IPOS+2)=CONVRT(12,IU3,1,RV)
2645            IF(II.GT.0)GO TO 3000
2646          915 WRITE(NO,8),UVB(IU3)
2647            READ(NI,5,ERR=915)DV
2648            IF(DV)915,915,916
2649          916 PD(IPOS+1)=CONVRT(12,IU3,1,DV)
2650            IF(II.GT.0)GO TO 3000
2651            GO TO 150
2652          142 IF(NCC.GT.2)GO TO 140
2653            IF(NCC.EQ.2) GO TO 147
2654          145 WRITE(NO,38)TU(IU1)
2655            READ(NI,5,ERR=145) ROT
2656            PD(IPOS+6)=CONVRT(1,IU1,2,ROT)
2657            IF(II.GT.0)GO TO 3000
2658          115 WRITE(NO,8),UVB(IU3)
2659            READ(NI,5,ERR=115)DV
2660            IF(DV)115,115,116
2661          116 PD(IPOS+1)=CONVRT(12,IU3,1,DV)
2662            IF(II.GT.0)GO TO 3000
2663            GO TO 150
2664          147 WRITE(NO,34)UM(IU3)
2665            READ(NI,5,ERR=147)FP
2666            IF(FP)147,146,146
2667          146 PD(IPOS+9)=CONVRT(3,IU3,1,FP)
2668          144 WRITE(NO,32)
2669            READ(NI,2,ERR=144)NS
2670            IF(NS)144,144,149
2671          149 PD(IPOS+8)=NS
2672            IF(II.GT.0)GO TO 3000
2673          117 WRITE(NO,8),UVB(IU3)
```

```
2674            READ(NI,5,ERR=117)DV
2675            IF(DV)117,117,118
2676          118 PD(IPOS+1)=CONVRT(12,IU3,1,DV)
2677            IF(II.GT.0)GO TO 3000
2678            GO TO 150
2679          C
2680          C
2681          C**    INPUT OF KINETICS
2682          C
2683          150 DO 4000 I=1,M
2684          165 WRITE(NO,39) I
2685            READ(NI,2,ERR=165)NRX(I)
2686            PD(IPOS+41+I)=NRX(I)
2687            IF(NRX(I))165,165,154
2688          154 IF(NRX(I).EQ.2)GO TO 166
2689          151 WRITE(NO,26) I
2690            READ(NI,5,ERR=151)F(I)
2691            PD(IPOS+9+I)=F(I)
2692            IF(II.GT.0)GO TO 3000
2693          155 WRITE(NO,41)
2694            READ(NI,2,ERR=155)LFUN
2695            PD(IPOS+363)=LFUN
2696            IF(II.GT.0)GO TO 3000
2697          152 WRITE(NO,27)I,HU(IU3),UM(IU3)
2698            READ(NI,5,ERR=152)A(I)
2699            PD(IPOS+19+I)=CONVRT(4,IU3,1,A(I))
2700            IF(II.GT.0)GO TO 3000
2701          153 WRITE(NO,28) I,HU(IU3),UM(IU3)
2702            READ(NI,5,ERR=153)HR(I)
2703            PD(IPOS+29+I)=CONVRT(4,IU3,1,HR(I))
2704            IF (II.GT.0)GO TO 3000
2705            GO TO 4002
2706          166 WRITE(NO,40)I,HU(IU3),UM(IU3)
2707            READ(NI,5,ERR=166)GRX(I)
2708            PD(IPOS+51+I)=CONVRT(4,IU3,1,GRX(I))
2709            IF(II.GT.0)GO TO 3000
2710          167 WRITE(NO,28)I
2711            READ(NI,5,ERR=167)HR(I)
2712            PD(IPOS+29+I)=CONVRT(4,IU3,1,HR(I))
2713            IF(II.GT.0)GO TO 3000
2714         4002 CONTINUE
2715         4000 CONTINUE
2716            DO 5000 J=1,M
2717            DO 6000 I=1,NNCP
2718            IF(NRX(J).EQ.2)GO TO 161
2719          160 WRITE(NO,20) I,J
2720            READ(NI,5,ERR=160)ONEX(I,J)
2721            PD(IPOS+10*J+51+I)=ONEX(I,J)
2722          161 WRITE(NO,23) I, J
2723            READ(NI,5,ERR=161) STO(I,J)
2724            PD(IPOS+10*J+201+I)=STO(I,J)
2725         6000 CONTINUE
2726         5000 CONTINUE
2727          C
2728          C**    NOW ALL INPUT DATA IS IN PD,NEX,STO ARRAYS
```

```
      C
            IF(II.GT.0)GO TO 3000
            IF(II.LT.0)GO TO 90
            JPD(NEL)=NARPV
            NARPV=NARPV+ISIZ(16)
            ISIZ2(NEL)=ISIZ(16)
            GO TO 90
         95 WRITE(NO,6)
       3000 WRITE(NO,14)
            READ(NI,7,ERR=3000) KE
            CALL SCOUT(5,KMD,KE,KAD)
            IF(KAD.EQ.0) GO TO 3000
            GO TO (140,120,117,95,90),KAD
         90 CONTINUE
         99 IRC(NEL)  =1
            IUPDT(NEL)=1
            RETURN
            END
*
```

```
      C
      C123456
            SUBROUTINE REACR
      C
            COMMON/BUG1/ILV,ITYPE,IQ,IHORS,IEXTQ,IPRT
            COMMON/PRD1/F1(500),IDCS(25),IDPRD(50),IFD(50),
           1 IFDL(200),IPD(50),IPDL(200),IPRC(70),IRC(50),
           2 ISIZ(25),ITCNT(100),JPD(50),MHB(50),NRECL(10),
           3 PD(1250),PROP(3000),RCNT(100),TEMP(410),X(5000)
            COMMON/UPDATE/IUPDT(50)
            COMMON/COMIO/NI,NO,IYES,INO,PNAM(15),NPAGE
            COMMON/UNITA2/TU(4),PU(6),HU(3),SU(6),RU(6),UM(3),PUX(6)
            COMMON/UNITA1/UDA(3),ULA(3),UVA(3),ULB(3),UHT(9),UDF(6)
            COMMON/UNITA3/UARE(3),UVIS(6),UTHC(9),UHPA(3),UVB(3),USG(6)
            COMMON/UNITDM/IU1,IU2,IU3,IU21,IU31
            COMMON/CWRK/WK(6600),IWK(100)
            COMMON/DBB/IFDB(11),IPDB(11),KMD(5)
            EQUIVALENCE(ITCNT(18),N2),(ITCNT(21),NCP),(ITCNT(22),NCPU),
           1 (ITCNT(23),NCPT  ),(ITCNT(24),NCPP  ),(ITCNT(25),NCPH  ),
           2 (ITCNT(26),NCPS  ),(ITCNT(27),NCPF  ),(ITCNT(28),NCPD  ),
           3 (ITCNT(29),NCPN  ),(ITCNT(30),NCP5  ),(ITCNT(31),NEL   ),
           4 (ITCNT(32),NARFD ),(ITCNT(33),NARPD ),(ITCNT(34),NARPV ),
           5 (ITCNT(35),NMAX  ),(ITCNT(36),NEQS  ),(ITCNT(37),NHELP ),
           6 (ITCNT(38),NST   ),(ITCNT(39),NND   ),(ITCNT(40),IIQ   ),
           7 (ITCNT(41),JJQ   ),(ITCNT(42),NPDMAX),(ITCNT(43),NFDMAX),
           8 (ITCNT(44),NPVMAX),(ITCNT(45),NPRNT ),(ITCNT(46),NOPT  ),
           9 (ITCNT(47),LIMIT ),(ITCNT(48),IWARN )
            EQUIVALENCE(RCNT(1),RTOL),(RCNT(2),RACC),(RCNT(3),QIJC),
           1 (RCNT( 4),RHOV ),(RCNT( 5),YMW  ),(RCNT( 6),XMW),
           2 (RCNT(51),TST  ),(RCNT(52),TEND ),(RCNT(53),PST),
           3 (RCNT(54),PEND ),(RCNT(55),DELT ),(RCNT(56),DELP ),
           4 (RCNT(57),TLMU ),(RCNT(58),TLML ),(RCNT(59),PLMU ),
           5 (RCNT(60),HSPEC),(RCNT(61),FRAC )
            COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
            COMMON/INPR2/NNCP,M
            COMMON/CALC2/TO,DF,FF(15),DV
            COMMON/TRACK/OLD(15),CHANGE(15)
            COMMON/SELEC/NOP,NCC,NPS
            COMMON/CRIT/FFOUT(15),PROD(15)
            COMMON/ALI/HCAP,CPP(15)
            COMMON/EQRXN/NRX(10),GRX(10)
            COMMON/EQRXN1/PO
            COMMON/OUTP/VO
            COMMON/RPRINT1/SIGMA(10)
            COMMON/RPRINT2/LFUN
            REAL DPROP(10)
      C
      C
         1  FORMAT('  REAC # ',I2)
            WRITE(NO,1)NEL
            IPOS=JPD(NEL)
            NNCP=NCP
            IPRT=1
            FFTOL=.001
```

```
1336            TTOL=.5
1337            VTOL=.01
1338      C
1339      C   TRANSFER OF FLOW RATES FROM X-ARRAY TO FF-ARRAY
1340      C
1341            NL=IFD(NEL)
1342            NSF=IFDL(NL+1)
1343            NTOP=(NSF-1)
1344            NLP=IPD(NEL)
1345            NSP=IPDL(NLP+1)
1346            NTOF=NSP-1
1347            DO 1111 I=1,NCP
1348            FF(I)=X(NTOP*NCP5+I)
1349      C     WRITE(NO,*)FF(I)
1350       1111 CONTINUE
1351            TO=X(NTOP*NCP5+NCP+2)
1352            DF=X(NTOP*NCP5+NCP+7)
1353            PO=X(NTOP*NCP5+NCP+3)
1354      C     WRITE(NO,*)TO,PO
1355      C
1356      C  PD ARRAY TRANSFER
1357      C
1358            NOP=PD(IPOS+3)
1359            NPS=PD(IPOS+40)
1360            NCC=PD(IPOS+41)
1361            ORP=CONVRT(2,IU2,1,PD(IPOS+5))
1362            PRDROP=CONVRT(2,IU2,1,PD(IPOS+7))
1363            LFUN=PD(IPOS+363)
1364            M=PD(IPOS)
1365            DO 70 I=1,M
1366            GRX(I)=1000*PD(IPOS+51+I)
1367            NRX(I)=PD(IPOS+41+I)
1368            DO 101 J=1,NNCP
1369            SIGMA(J)=STO(J,I)
1370         101 CONTINUE
1371            F(I)=PD(IPOS+9+I)
1372            A(I)=1000*PD(IPOS+19+I)
1373            HR(I)=1000*PD(IPOS+29+I)
1374        70  CONTINUE
1375            DO 130 JJ=1,M
1376            DO 140 MPW=1,NNCP
1377            ONEX(MPW,JJ)=PD(IPOS+10*JJ+51+MPW)
1378            STO(MPW,JJ)=PD(IPOS+10*JJ+201+MPW)
1379         140 CONTINUE
1380         130 CONTINUE
1381            IF(NPS.EQ.0)POUT=ORP
1382            IF(NPS.EQ.1)POUT=PO-PRDROP
1383            IF(NCC.EQ.0)RV=PD(IPOS+2)
1384            IF(NCC.EQ.1)TMAX=PD(IPOS+6)
1385            IF(NCC.EQ.2)FP=PD(IPOS+9)
1386            IF(NCC.EQ.2)NS=PD(IPOS+8)
1387            FTOL=5.0
1388            ICOUNT=1
1389            DV=PD(IPOS+1)
1390            VO=DV
```

```
1391            NOPT=5
1392            TST=T0
1393            TEND=0.0
1394            DELT=0.0
1395            PST=P0
1396            PEND=0.0
1397            DELP=0.0
1398            IEXT2=2
1399            NLPH=1
1400            IF(NH2O.NE.0)NLPH=2
1401            CALL XMOVER(NSF,1)
1402            CALL CALC
1403            CALL FMOVER(1,NSF)
1404            IF(NOP.EQ.0)GO TO 200
1405            CALL SRKPD(DPROP)
1406            HCAP=DPROP(1)
1407          200 CONTINUE
1408            DO 30 I=1,3000
1409            DO 40 J=1,NNCP
1410            OLD(J)=FF(J)
1411           40 CONTINUE
1412            CALL RUNGE
1413            DO 150 NN=1,NNCP
1414            X(NTOF*NCP5+NN)=FF(NN)
1415          150 CONTINUE
1416            NOPT=5
1417            TST=T0
1418            TEND=0.0
1419            DELT=0.0
1420            PST=POUT
1421            PEND=0.0
1422            DELP=0.0
1423            IEXT2=2
1424            NLPH=1
1425            IF(NH2O.NE.0)NLPH=2
1426            CALL XMOVER(NSP,1)
1427            CALL CALC
1428            CALL FMOVER(1,NSP)
1429            IF(NOP.EQ.0)GO TO 210
1430            CALL SRKPD(DPROP)
1431            HCAP=DPROP(1)
1432          210 DF=X(NTOF*NCP5+NCP+7)
1433            IF(NCC.EQ.0)GO TO 80
1434            IF(NCC.EQ.1)GO TO 90
1435            IF(NCC.EQ.2)GO TO 100
1436           80  IF((RV-V0).LE.VTOL)GO TO 110
1437            GO TO 33
1438           90  IF((TMAX-T0).LE.TTOL)GO TO 110
1439            GO TO 33
1440          100  IF((FF(NS)-FP).GE.FFTOL)GO TO 110
1441           33  ICOUNT=ICOUNT+1
1442            V0=V0+DV
1443           30  CONTINUE
1444           110 CONTINUE
1445            DO 220 I=1,NNCP
```

```
C     WRITE(NO,*)X(NTOF*NCP5+I)
  220 CONTINUE
      IPRT=0
      RXHT=0.0
      DO 2 JHT=1,M
      DO 3 IHT=1,NNCP
      IF(STO(IHT,JHT).GE.0)GO TO 4
      RXHT=RXHT+HR(JHT)*(X(NTOP*NCP5+IHT)-FF(IHT))
    4 CONTINUE
    3 CONTINUE
    2 CONTINUE
      PD(IPOS+362)=RXHT
      IF(NOP.EQ.1)PD(IPOS+362)=0.0
      RETURN
      END
C
C**   SUBROUTINE TO SUM UP THE VOLUMETRIC FLOW RATES
C
      SUBROUTINE VFLOW
      COMMON/PRD1/F1(500),IDCS(25),IDPRD(50),IFD(50),
     1 IFDL(200),IPD(50),IPDL(200),IPRC(70),IRC(50),
     2 ISIZ(25),ITCNT(100),JPD(50),MHB(50),NRECL(10),
     3 PD(1250),PROP(3000),RCNT(100),TEMP(410),X(5000)
      COMMON/CALC2/TO,DF,FF(15),DV
      COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
      COMMON/INPR2/NNCP,M
      COMMON/CALC4/VF,FFM(15)
      EQUIVALENCE(ITCNT(18),N2),(ITCNT(21),NCP),(ITCNT(22),NCPU),
     1 (ITCNT(23),NCPT),(ITCNT(24),NCPP  ),(ITCNT(25),NCPH  ),
     2 (ITCNT(26),NCPS),(ITCNT(27),NCPF  ),(ITCNT(28),NCPD  ),
     3 (ITCNT(29),NCPN),(ITCNT(30),NCP5  ),
     4 (ITCNT(38),NST ),(ITCNT(39),NND   )
      EQUIVALENCE(IPRC(1),MLCXA),(IPRC(2),MLCY),(IPRC(3),MLCXB),
     1 (IPRC( 4),MLTXA),(IPRC( 5),MLTY),(IPRC( 6),MLTXB),
     2 (IPRC( 7),MLPXA),(IPRC( 8),MLPY ),(IPRC( 9),MLPXB),
     3 (IPRC(10),MLHO),(IPRC(11),MLSO),(IPRC(12),MLCZF),
     4 (IPRC(13),MLKVA),(IPRC(14),MLKVB),(IPRC(15),MPHSP),
     5 (IPRC(16),MPRC1),(IPRC(17),MPRC2),(IPRC(18),MPRC3),
     6 (IPRC(19),MPRC4),(IPRC(20),MPRC5),
     7 (IPRC(26),MPRA1),
     8 (IPRC(36),MM   ),
     1 (IPRC(62),MECU ),(IPRC(63),MECP ),(IPRC(64),LOCKP)
      REAL WE(15)
      VF=0.0
      FMM=0.0
      DO 5 I=NST,NND
      NN=(I-1)*N2+MPHSP
      WE(I)=PROP(NN+8)
    5 CONTINUE
      DO 10 I=1,NNCP
      FFM(I)=FF(I)*WE(I)
   10 CONTINUE
      DO 20 I=1,NNCP
      FM=FFM(I)+FMM
      FMM=FM
```

```
1501          20 CONTINUE
1502             VF=FMM/DF
1503             RETURN
1504             END
1505       C
1506       C**   SUBROUTINE RCONST-TO DEVELOP THE EXPRESSIONS FOR
1507       C     THE RATE CONSTANTS OF THE REACTIONS
1508       C
1509             SUBROUTINE RCONST
1510             COMMON/CALC2/TO,DF,FF(15),DV
1511             COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
1512             COMMON/INPR2/NNCP,M
1513             COMMON/CALC3/RK(10)
1514             COMMON/EQRXN/NRX(10),GRX(10)
1515             COMMON/RPRINT2/LFUN
1516             RC=1.986
1517             CTERM=1.0
1518             DO 10 I=1,M
1519             IF(NRX(I).EQ.2)GO TO 20
1520       C     WRITE(6,*)LFUN
1521             IF(LFUN.EQ.1)GO TO 21
1522             DO 2 J=1,NNCP
1523             PSS=PSS+STO(J,I)
1524           2 CONTINUE
1525             IF(PSS.EQ.1)CTERM=3600
1526             IF(PSS.NE.1)CTERM=3600*(16.04**(PSS-1))
1527          21 RK(I)=CTERM*F(I)*EXP(-A(I)/(RC*TO))
1528          20 CONTINUE
1529          10 CONTINUE
1530             RETURN
1531             END
1532       C
1533       C**   SUBROUTINE RRXN-TO DEVELOP A "UNIT" RATE EQUATION
1534       C     FOR EACH REACTION
1535       C
1536             SUBROUTINE RRXN
1537             COMMON/CALC4/VF,FFM(15)
1538             COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
1539             COMMON/INPR2/NNCP,M
1540             COMMON/CALC3/RK(10)
1541             COMMON/CALC2/TO,DF,FF(15),DV
1542             COMMON/CALC5/R(10)
1543             COMMON/EQRXN/NRX(10),GRX(10)
1544             DIMENSION RR(10)
1545             DO 40 J=1,M
1546             IF(NRX(J).EQ.1)GO TO 41
1547             CALL RXEQU(J)
1548          41 CONTINUE
1549          40 CONTINUE
1550             DO 10 J=1,M
1551             IF(NRX(J).EQ.2)GO TO 15
1552             S=0.0
1553             DO 30 I=1,NNCP
1554             S=S+ABS(ONEX(I,J))
1555          30 CONTINUE
```

```
1556            RR(J)=RK(J)
1557            DO 20 I=1,NNCP
1558            IF(FF(I).LE.0)GO TO 20
1559            IF(ONEX(I,J).EQ.0)GO TO 20
1560            RR(J)=RR(J)*(FF(I)**(ONEX(I,J)))
1561          20 CONTINUE
1562            R(J)=RR(J)/VF**S
1563          15 CONTINUE
1564          10 CONTINUE
1565            RETURN
1566            END
1567      C
1568      C
1569      C**   SUBROUTINE RCOMP-TO SET UP THE TOTAL RATE EXPRESSION
1570      C     FOR EACH COMPONENT
1571      C
1572            SUBROUTINE RRCOMP
1573            COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
1574            COMMON/INPR2/NNCP,M
1575            COMMON/CALC5/R(10)
1576            COMMON/CALC6/RCOMP(15)
1577            DO 10 I=1,NNCP
1578            RCOMP(I)=0.0
1579            DO 20 J=1,M
1580            RCOMP(I)=RCOMP(I)+STO(I,J)*R(J)
1581         20 CONTINUE
1582         10 CONTINUE
1583            RETURN
1584            END
1585      C
1586      C**   SUBROUTINE RTEMP-TO EVALUATEM
1587      C**   SUBROUTINE RTEMP-TO EVALUATE THE TEMPERATURE
1588      C     CHANGE ALONG THE REACTOR
1589      C
1590            SUBROUTINE RTEMP
1591            COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
1592            COMMON/INPR2/NNCP,M
1593            COMMON/CALC2/T0,DF,FF(15),DV
1594            COMMON/CALC5/R(10)
1595            COMMON/CALC7/DT
1596            COMMON/SELEC/NOP,NCC,NPS
1597            COMMON/ALI/HCAP,CPP(15)
1598            REAL XHR(10)
1599            DHR=0.0
1600            DO 10 J=1,M
1601            DHR=DHR + HR(J)*R(J)
1602          10 CONTINUE
1603            FC=0.0
1604            DO 20 I=1,NNCP
1605            FC=FC + FF(I)*CPP(I)
1606          20 CONTINUE
1607      C     WRITE(6,*)R(1),DHR,FC,DT
1608            DT=-(DHR/FC)*DV
1609            RETURN
1610            END
```

```
1611      C
1612      C  SUBROUTINE RUNGE-TO SOLVE DE.'S USING 4-TH ORDER RUNGA-KUTTA
1613      C
1614            SUBROUTINE RUNGE
1615            DIMENSION S1(15),S2(15),S3(15),S4(15)
1616            COMMON/CALC6/RCOMP(15)
1617            COMMON/CALC2/T0,DF,FF(15),DV
1618            COMMON/INPR2/NNCP,M
1619            COMMON/TRACK/OLD(15),CHANGE(15)
1620            COMMON/CALC7/DT
1621            COMMON/SELEC/NOP,NCC,NPS
1622            REAL FFPRE(15)
1623            CALL VFLOW
1624            CALL RCONST
1625            CALL RRXN
1626            CALL RRCOMP
1627            DO 70 I=1,NNCP
1628            FFPRE(I)=FF(I)
1629         70 CONTINUE
1630            DO 10 I=1,NNCP
1631            S1(I)=DV*RCOMP(I)
1632            FF(I)=FF(I)+.5*S1(I)
1633         10 CONTINUE
1634            CALL VFLOW
1635            CALL RCONST
1636            CALL RRXN
1637            CALL RRCOMP
1638            DO 20 I=1,NNCP
1639            S2(I)=DV*RCOMP(I)
1640            FF(I)=FF(I)+.5*S2(I)
1641         20 CONTINUE
1642            CALL VFLOW
1643            CALL RCONST
1644            CALL RRXN
1645            CALL RRCOMP
1646            DO 30 I=1,NNCP
1647            S3(I)=DV*RCOMP(I)
1648            FF(I)=FF(I)+S3(I)
1649         30 CONTINUE
1650            CALL VFLOW
1651            CALL RCONST
1652            CALL RRXN
1653            CALL RRCOMP
1654            DO 60 I=1,NNCP
1655            S4(I)=DV*RCOMP(I)
1656         60 CONTINUE
1657            DO 40 I=1,NNCP
1658            CHANGE(I)=(1/6.0)*(S1(I)+2*S2(I)+2*S3(I)+S4(I))
1659            FF(I)=FFPRE(I)+CHANGE(I)
1660         40 CONTINUE
1661            IF(NOP.EQ.0)GO TO 50
1662            CALL RTEMP
1663            T0=T0+DT
1664      C     WRITE(6,*)DT,T0
1665         50 CONTINUE
```

```
      RETURN
      END
C
C
C    SUBROUTINE TO SET UP THE EQUILIBRIUM LIMITATIONS
C          OF THE REACTIONS IN EQUILIBRIUM
C
      SUBROUTINE RXEQU (J)
      COMMON/CALC5/R(10)
      PTOL=.0001
      ALPHA=0.0
      BETA=100.0
      ICOUNT=1
   10 CONTINUE
C     WRITE(6,*)ALPHA,BETA,RALPHA,RBETA
      CALL RTRY(ALPHA,RALPHA)
      IF(ABS(RALPHA).LE.PTOL)GO TO 41
      CALL RTRY(BETA,RBETA)
      RW=(ALPHA+BETA)/2.0
      CALL RTRY(RW,RRW)
      PROD1=RALPHA*RRW
      PROD2=RBETA*RRW
      IF(PROD1.LT.0) GO TO 20
      IF(PROD2.LT.0) GO TO 30
      GO TO 70
   20 BETA=RW
      ICOUNT=ICOUNT+1
      IF(ICOUNT.GE.100) GO TO 70
      GO TO 10
   30 ALPHA=RW
      ICOUNT=ICOUNT+1
      IF(ICOUNT.GE.100) GO TO 70
      GO TO 10
   41 R(J)=ALPHA
C     WRITE(6,*)R(J)
      GO TO 71
   70 WRITE(6,*)'ROOT IS NOT FOUND'
   71 CONTINUE
      RETURN
      END
C
C
C  SUBROUTINE TO SET UP THE EXTENSION OF REACTIONS IN
C              EQUILIBRIUM
C
      SUBROUTINE XREQU(J)
      COMMON/CALC5/R(10)
      PTOL=.000001
      SIG1=0.0
      IFLAG=1
   30 CALL RTRY(SIG1,RSIG1)
      IF(ABS(RSIG1).LE.PTOL) GO TO 20
      SIG1=SIG1+.01
      IFLAG=IFLAG+1
      IF(IFLAG.GT.100)GO TO 31
```

```
1721            GO TO 30
1722         31 R(J)=0.0
1723            GO TO 21
1724         20 CONTINUE
1725            R(J)=SIG1
1726         21 CONTINUE
1727            RETURN
1728            END
1729      C
1730      C  SUBROUTINE FOR CHECKING EQUILIBRIUM CONDITIONS
1731      C
1732            SUBROUTINE RTRY(RA,FRA)
1733            COMMON/CALC2/TO,DF,FF(15),DV
1734            COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
1735            COMMON/INPR2/NNCP,M
1736            COMMON/CALC5/R(10)
1737            COMMON/EQRXN/NRX(10),GRX(10)
1738            COMMON/EQRXN1/PO
1739            REAL EQUIK(10),EQUIK1(10),EQFF(15),OLDR(10),OLDF(10)
1740            RC=1.987
1741            EQUIK(J)=EXP(-(GRX(J)/(RC*536.4)))
1742            EQUIK1(J)=EQUIK(J)*EXP(-(HR(J)/RC)*(1/TO-1/536.4))
1743            SS=0.0
1744            DO 20 I=1,NNCP
1745            SS=SS+STO(I,J)
1746         20 CONTINUE
1747         22 Y=0.0
1748            DO 30 I=1,NNCP
1749            EQFF(I)=FF(I)+STO(I,J)*RA
1750            Y=Y+EQFF(I)
1751         30 CONTINUE
1752            IF(SS.EQ.0)GO TO 25
1753            EQL=EQUIK1(J)*(PO**(-SS))*(Y**SS)
1754            GO TO 26
1755         25 EQL=EQUIK1(J)
1756         26 EQR=1.0
1757            DO 50 I=1,NNCP
1758            IF(STO(I,J).EQ.0)GO TO 31
1759            IF(EQFF(I).EQ.0)GO TO 31
1760      C     WRITE(6,*)I,EQFF(I),STO(I,J)
1761            EQR=EQR*(EQFF(I)**STO(I,J))
1762         31 CONTINUE
1763         50 CONTINUE
1764            FRA=EQL-EQR
1765            RETURN
1766            END
1767      C
1768      C
1769      C     SUBROUTINE REACO-TO DISPLAY SOME OF THE PD INFORMATION
1770      C                 REATOR VOLUME AND HEAT LOAD
1771      C
1772            SUBROUTINE REACO
1773            COMMON/PRD1/F1(500),IDCS(25),IDPRO(50),IFD(50),
1774           1 IFDL(200),IPD(50),IPDL(200),IPRC(70),IRC(50),
1775           2 ISIZ(25),ITCNT(100),JPD(50),MHB(50),NRECL(10),
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1776            3 PD(1250),PROP(3000),RCNT(100),TEMP(410),X(5000)
1777             COMMON/COMIO/NI,NO,IYES,INO,PNAM(15),NPAGE
1778             COMMON/UNITA1/UDA(3),ULA(3),UVA(3),ULB(3),UHT(9),UDF(6)
1779             COMMON/UNITA2/TU(4),PU(6),HU(3),SU(6),RU(6),UM(3),PUX(6)
1780             COMMON/UNITA3/UARE(3),UVIS(6),UTHC(9),UHPA(3),UVB(3),USG(6)
1781             COMMON/UNITDM/IU1,IU2,IU3,IU21,IU31
1782             EQUIVALENCE(ITCNT(18),N2),(ITCNT(21),NCP),(ITCNT(22),NCPU),
1783            1 (ITCNT(23),NCPT),(ITCNT(24),NCPP),(ITCNT(25),NCPH),
1784            2 (ITCNT(26),NCPS),(ITCNT(27),NCPF),(ITCNT(28),NCPD),
1785            3 (ITCNT(29),NCPN),(ITCNT(30),NCP5),(ITCNT(31),NEL),
1786            4 (ITCNT(60),INTRY),(ITCNT(38),NST),(ITCNT(39),NND)
1787             EQUIVALENCE(IPRC(1),MLCXA),(IPRC(2),MLCY),(IPRC(3),MLCXB),
1788            1 (IPRC( 4),MLTXA),(IPRC(5),MLTY),(IPRC(6),MLTXB),
1789            2 (IPRC(7),MLPXA),(IPRC(8),MLPY),(IPRC(9),MLPXB),
1790            3 (IPRC(10),MLHO),(IPRC(11),MLSO),(IPRC(12),MLCZF),
1791            4 (IPRC(13),MLKVA),(IPRC(14),MLKVB),(IPRC(15),MPHSP),
1792            5 (IPRC(16),MPRC1),(IPRC(17),MPRC2),(IPRC(18),MPRC3),
1793            6 (IPRC(19),MPRC4),(IPRC(20),MPRC5),
1794            7 (IPRC(26),MPRA1),
1795            8 (IPRC(36),MM),
1796            1 (IPRC(62),MECU),(IPRC(63),MECP),(IPRC(64),LOCKP)
1797             COMMON/OUTP/VO
1798             COMMON/CALC2/TO,DF,FF(15),DV
1799             COMMON/EQRXN/NRX(10),GRX(10)
1800             COMMON/EQRXN1/PO
1801             DIMENSION LEFT(10),LRIGHT(10),IRLL(10),RLC(15,10),RC(15,10)
1802             DIMENSION RLC2(15,10),RC2(15,10)
1803             COMMON/INPR2/NNCP,M
1804             COMMON/INPR1/F(10),A(10),ONEX(15,10),STO(15,10),HR(10)
1805             COMMON/SUPP/TPRINT,PPRINT
1806         C
1807         C
1808           1   FORMAT(/'  REAC #  ',I2)
1809           2   FORMAT( '  THE VOLUME INCREMENT=   ',F6.2,'   ',A4)
1810           3   FORMAT(//' THE OPERATION IN THE REACTOR IS ISOTHERMAL ')
1811           4   FORMAT(//' THE OPERATION IN THE REACTOR IS ADIABATIC  ')
1812           5   FORMAT( '  THE  REACTOR VOLUME=  ',F10.2,3X,A4)
1813           6   FORMAT(/'  THE PRODUCTION RATE OF COMP.#  ',I3,'   IS  ',F12.
2
1814              1 ,'       ',A4,'MOLES/HR'/)
1815           7   FORMAT(///'  THE HEAT LOAD ON REACTOR IS ',F12.2,1X,A4,'  per
HR')
1816           8   FORMAT(//'**** THIS IS THE PD FOR THE REACTOR UNIT **** ')
1817           9   FORMAT( '  THE SPECIFIED REACTOR OUTLET TEMPERATURE=  ',F12.3
1818              1 ,'  DEG  ',A4)
1819          10   FORMAT( '  THE SPECIFIED REACTOR VOLUME=  ',F12.3,2X,A4)
1820          12   FORMAT( '  THE OUTLET REACTOR TEMPERATURE= ',F12.3,'  DEG  ',
A1)
1821          13   FORMAT('   THE  INLET PRESSURE TO REACTOR=  ',F12.4,'    ',A4
)
1822          14   FORMAT('   THE OUTLET PRESSURE FROM REACTOR=  ',F12.4,'     '
,A4)
1823          15   FORMAT(//5X,2A4,3X,'->',3X,2A4)
1824
1825          16   FORMAT(//5X,2A4,3X,'=',3X,2A4)
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1826        17  FORMAT(//3X,2A4,2X,'+',2X,2A4,3X,'->',3X,2A4)
1827        18  FORMAT(//3X,2A4,2X,'+',2X,2A4,3X,'=',3X,2A4)
1828        19  FORMAT(//3X,2A4,3X,'->',3X,2A4,2X,'+',2X,2A4)
1829        20  FORMAT(//3X,2A4,3X,'=',3X,2A4,2X,'+',2X,2A4)
1830        21  FORMAT(//1X,2A4,2X,'+',2X,2A4,3X,'->',3X,2A4,2X,'+',2X,2A4)
1831        22  FORMAT(//1X,2A4,2X,'+',2X,2A4,3X,'=',3X,2A4,2X,'+',2X,2A4)
1832        23  FORMAT(///1X,'RXN.',3X,'SEQ.#',3X,'ORDER',3X,'STOCHIO>')
1833        24  FORMAT(/2X,I2,5X,I3,4X,F5.2,5X,F5.2)
1834            IPOS=JPD(NEL)
1835            IF(INTRY.NE.0)GO TO 200
1836            WRITE(NO,1)NEL
1837            NL=IFD(NEL)
1838            NSF=IFDL(NL+1)
1839            NTOP=NSF-1
1840            TPRINT=PD(IPOS+4)
1841            PPRINT=PD(IPOS+364)
1842            WRITE(NO,8)
1843            M=PD(IPOS)
1844            NNCP=NCP
1845            DO 100 J=1,M
1846            NRX(J)=PD(IPOS+41+J)
1847            DO 201 I=1,NNCP
1848            ONEX(I,J)=PD(IPOS+10*J+51+I)
1849            STO(I,J)=PD(IPOS+10*J+201+I)
1850        201 CONTINUE
1851        100 CONTINUE
1852            NOP=PD(IPOS+3)
1853            NCC=PD(IPOS+41)
1854            ROT=CONVRT(1,2,IU1,PD(IPOS+6))
1855            IF(NOP.EQ.0)WRITE(NO,3)
1856            IF(NOP.EQ.1)WRITE(NO,4)
1857            VI=PD(IPOS+1)
1858            WRITE(NO,2)CONVRT(12,1,IU3,VI),UVB(IU3)
1859            NS=PD(IPOS+8)
1860            FP=CONVRT(3,1,IU3,PD(IPOS+9))
1861            RV=PD(IPOS+2)
1862            NPS=PD(IPOS+40)
1863            IF(NPS.EQ.0)ORP=PD(IPOS+5)
1864            IF(NPS.EQ.1)ORP=PPRINT-PD(IPOS+7)
1865            WRITE(NO,13)PPRINT,PU(IU2)
1866            WRITE(NO,14)ORP,PU(IU2)
1867            IF(NCC.EQ.0)WRITE(NO,10)CONVRT(12,1,IU3,RV),UVB(IU3)
1868            IF(NCC.EQ.1)WRITE(NO,9)ROT,TU(IU1)
1869            IF(NCC.EQ.2)WRITE(NO,6)NS,FP,UM(IU3)
1870            DO 30 J=1,M
1871            LEFT(J)=0
1872            LRIGHT(J)=0
1873            DO 40 I=1,NNCP
1874            IF(STO(I,J).EQ.0)GO TO 41
1875            IF(STO(I,J).LT.0)LEFT(J)=LEFT(J)+1
1876            IF(STO(I,J).GT.0)LRIGHT(J)=LRIGHT(J)+1
1877         41 CONTINUE
1878         40 CONTINUE
1879            IRLL(J)=LEFT(J)+LRIGHT(J)
1880         30 CONTINUE
```

```
      DO 50 J=1,M
      LCOUNT=1
      IRCOUNT=1
      DO 60 I=1,NNCP
      ILM=(I-1)*N2+1+MPHSP
      ILN=ILM+1
C     WRITE(NO,*)STO(I,J),LCOUNT,IRCOUNT
      IF(STO(I,J).EQ.0)GO TO 61
      IF(STO(I,J).LT.0)RLC(LCOUNT,J)=PROP(ILN)
      IF(STO(I,J).LT.0)RLC2(LCOUNT,J)=PROP(ILM)
      IF(STO(I,J).LT.0)LCOUNT=LCOUNT+1
      IF(STO(I,J).GT.0)RC(IRCOUNT,J)=PROP(ILN)
      IF(STO(I,J).GT.0)RC2(IRCOUNT,J)=PROP(ILM)
      IF(STO(I,J).GT.0)IRCOUNT=IRCOUNT+1
   61 CONTINUE
   60 CONTINUE
      IF(IRLL(J).NE.2)GO TO 62
      IF(NRX(J).NE.1)WRITE(NO,15)RLC2(1,J),RLC(1,J),RC2(1,J),RC(1,J
)
      IF(NRX(J).EQ.2)WRITE(NO,16)RLC2(1,J),RLC(1,J),RC2(1,J),RC(1,J
)
      GO TO 65
   62 IF(IRLL(J).NE.3)GO TO 63
      IF(LRIGHT(J).NE.2)GO TO 64
      IF(NRX(J).EQ.1)WRITE(NO,19)RLC2(1,J),RLC(1,J),RC2(1,J),RC(1,J
)
     1 ,RC2(2,J),RC(2,J)
      IF(NRX(J).EQ.2)WRITE(NO,20)RLC2(1,J),RLC(1,J),RC2(1,J),RC(1,J
)
     1 ,RC2(2,J),RC(2,J)
      GO TO 65
   64 IF(NRX(J).EQ.1)WRITE(NO,17)RLC2(1,J),RLC(1,J),RLC2(2,J),RLC(2
,J)
     1 ,RC2(1,J),RC(1,J)
      IF(NRX(J).EQ.2)WRITE(NO,18)RLC2(1,J),RLC(1,J),RLC2(2,J),RLC(2
,J)
     1 ,RC2(1,J),RC(1,J)
      GO TO 65
   63  IF(NRX(J).EQ.1)WRITE(NO,21)RLC2(1,J),RLC(1,J),RLC2(2,J),RLC(2
,J)
     1 ,RC2(1,J),RC(1,J),RC2(2,J),RC(2,J)
      IF(NRX(J).EQ.2)WRITE(NO,22)RLC2(1,J),RLC(1,J),RLC2(2,J),RLC(2
,J)
     1 ,RC2(1,J),RC(1,J),RC2(2,J),RC(2,J)
      GO TO 65
   65 CONTINUE
   50 CONTINUE
      WRITE(NO,23)
      DO 70 J=1,M
      DO 80 I=1,NNCP
      ILM=(I-1)*N2+1+MPHSP
      ILN=ILM+1
      WRITE(NO,24)J,I,ONEX(I,J),STO(I,J)
   80 CONTINUE
   70 CONTINUE
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1928            GO TO 11
1929        200 CONTINUE
1930            RXHT=PD(IPOS+362)/1000.0
1931            WRITE(NO,7)CONVRT(4,1,IU3,RXHT),HU(IU3)
1932            IF(NOP.EQ.1)WRITE(NO,12)CONVRT(1,2,IU1,T0),TU(IU1)
1933            WRITE(NO,5)CONVRT(12,1,IU3,V0),UVB(IU3)
1934        11  CONTINUE
1935            RETURN
1936            END
*
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Master of Science

Thesis: INTERACTIVE MODEL OF A HOMOGENEOUS GASEOUS PLUG FLOW REACTOR

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