Copyright Warning & Restrictions

The copyright law of the United States (Title 17, United States Code) governs the making of photocopies or other reproductions of copyrighted material.

Under certain conditions specified in the law, libraries and archives are authorized to furnish a photocopy or other reproduction. One of these specified conditions is that the photocopy or reproduction is not to be "used for any purpose other than private study, scholarship, or research." If a, user makes a request for, or later uses, a photocopy or reproduction for purposes in excess of "fair use" that user may be liable for copyright infringement,

This institution reserves the right to refuse to accept a copying order if, in its judgment, fulfillment of the order would involve violation of copyright law.

Please Note: The author retains the copyright while the New Jersey Institute of Technology reserves the right to distribute this thesis or dissertation

Printing note: If you do not wish to print this page, then select "Pages from: first page # to: last page #" on the print dialog screen

A STUDY OF THE OPTIMIZATION OF ETHYLENE PRODUCTION IN A TUBULAR REACTOR

BY

RICHARD W. J. ROBERTSON

A THESIS

PRESENTED IN PARTIAL FULFILLMENT OF

THE REQUIREMENTS FOR THE DEGREE

OF

MASTER OF SCIENCE IN CHEMICAL ENGINEERING

AT

NEWARK COLLEGE OF ENGINEERING

Newark, New Jersey
1972

APPROVAL OF THESIS

A STUDY OF THE OPTIMIZATION OF ETHYLENE PRODUCTION IN A TUBULAR REACTOR

BY

RICHARD W. J. ROBERTSON

FOR

DEPARTMENT OF CHEMICAL ENGINEERING

NEWARK COLLEGE OF ENGINEERING

BY

FACULTY COMMITTEE

APPROVED:

Newark, New Jersey

May, 1972

Abstract

The pyrolysis of ethane is a complex reaction involving six individual reactions in a reactant mixture of thirteen components. It is further complicated by the deposition of carbon along the reactor walls. The carbon buildup eventually necessitates reactor shutdown. During the intermediate stages the reactor experiences a gradual increase in inlet pressure which affects the reaction conditions. Optimum temperature profiles exist because the yield goes up with increasing temperature, but, consequently, the reactor must be shut down and cleaned out with increasing frequency. The combined effect causes the yearly production of ethylene to go through an optimum.

To find this optimum a computer program was developed with the ability of handling 25 simultaneous reactions involving up to 25 components. It calculates the carbon deposition profile and the changing pressure profiles, as a function of a predetermined reaction gas temperature profile. The reactor will remain in production until the inlet pressure exceeds eight atmospheres. The average yearly production rate is calculated, assessing a reactor shut down penalty of 24 and 48 hours required for the cleaning of the clogged pyrolysis tubes.

The optimum exit temperature for the 24 hour penalty

was 1127°K with a corresponding 57% one pass ethane conversion. The 48 hour penalty lowers the optimum exit temperature to 1124°K and a 50.5% ethane conversion.

The practice of increasing pressure to compensate for carbon buildup results in accelerated carbon deposition and is detrimental to overall production scheme.

The program given here is immediately applicable to any plug flow system, the only additional requirement being the physical and thermodynamic constants for the additional components. The program could, for example, be used to calculate the production of acetylene.

Acknowledgments

The author wishes to take this opportunity to express his gratitude to all the individuals whose cooperation enabled him to bring this thesis to fruition.

He wants to thank his advisor, Dr. Deran Hanesian, for the contribution of his time and effort on the author's behalf. His thanks are also due to the splendid staff at the Computer Center for their indispensable role in processing the necessary data.

The author wants to give a special thanks to his wife, Linda, for her gentle encouragement throughout the period of writing this thesis, as well as her inceasing efforts in preparing this thesis in its final form. He also wishes to thank his son, Donald, for his good behavior.

Table of Contents

List of Figures

List of Tables

Chapter 1

Introduction

Optimization of Ethylene Production

To perform an optimization one needs some sort of plant description to form an objective function such as production rate or profit margin which must be optimized in terms of the independent variables.

Historically, plant data were used in deriving mathematical models by regression analysis. Some plants had even been deliberately disturbed in order to obtain enough data to determine the independent variables into which the plant was being fitted.(47)

This method has many drawbacks such as noise in the plant data causing unreliability in the readings and a limited range of conditions under which the data is collected. Conditions outside of the range of those specifically studied must be calculated by the relatively unreliable method of extrapolation.

An alternative method is to simulate the plant based on the physical and chemical conditions. This simulated model can then be perturbed to determine the effect on the function to be optimized.

In this study, the objective function will be the yearly production rate of ethylene. The temperature profile in the

reactor will be the independent variable.

In order to describe plant conditions as thoroughly and accurately as possible, a model should consider the entire plant, including recycle streams, separators and peripheral equipment as well as the reactor. This is not the intent of this study.

It was decided that the optimization of production rate would be most meaningful and would give optimum conditions close to the optimum based on an overall profit objective function.

Pyrolysis of Ethane Process

Ethylene is a basic raw material used in the manufacture of polyethylene and polyethylene copolymers. Plant sizes range between 50 to 250 million pounds per year. The pyrolysis of ethane is very economically profitable because the raw material, ethane, would have a minimum value as a fuel gas. Ethylene is produced by cracking of feed stock in furnaces at temperatures up to 1250^{o}K.

Almost all larger refineries have several furnaces which operate with different feed stocks, notably various proportions of ethane. propane and butane. The reactor pressure and temperature profiles and feed rates are also varied. The products from these different streams are generally combined into

one stream after quenching to stop the production of unwanted byproducts.

The program PYRO is able to handle each set of feed stocks independently and perform separate optimizations for each furnace. In this study, only the case of pure ethane and steam as feed was considered. The program is also capable of optimizing the production of acetylene by an increase in the residence time. The program is capable of handling any gas or gas solid phase system of reactions. PYRO calculates the changing concentration and pressure profiles as functions of an induced temperature profile.

Carbon Deposition

Carbon is one of the byproducts of the pyrolysis reactions. Carbon is deposited on the wall of the reactor and results in a continuously changing reactor radius. The changing radius results in a change in the inlet pressure because the outlet pressure is maintained at about 2 atmospheres. Eventually the inlet pressure reaches a value which is too high to keep the system operating. When this occurs, the reactor must be shut down for cleaning.

The yearly production rate of ethylene is defined as the total amount of ethylene produced in a year. The yearly production rate is affected by both the yield of ethylene from ethane and the percent of the time the reactor is in production.

An increase in yield causes an increase in the yearly production rate. An increase in the frequency of reactor shutdown causes a drop in the yearly production rate.

An increase in reactor outlet temperature increases both the yield of ethylene and the rate of carbon deposition, hence causing an increase in the frequency of reactor shutdown. Due to these combined effects, the yearly production rate of ethylene will go through an optimum. The yearly production rate will first increase because the increase in yield is the dominant effect. However, the frequency of reactor shutdown first starts to slow down the increase in production rate and then reverses the upward trend. The temperature at which the reversal takes place represents the outlet temperature which will optimize the yearly production rate.

Under extreme conditions, the reactor may be shut down every 40 hours for a 24 - 48 hour cleaning. Under the mildest conditions, the reactor could continue to operate for years between shutdowns with a yield of only 8% ethylene from ethane.

The optimum is also shifted toward the lower end of the temperature range due to the formation of byproducts.

Chemistry of Pyrolysis

The chief products from thermal cracking furnaces vary from feed to feed. For the feed considered in this study,

the chief products were ethane, ethylene, acetylene, methane, hydrogen and coke. Small amounts of aromatics were also formed. As an approximation these were defined to have the properties of C4's and C6's alpha olefins.

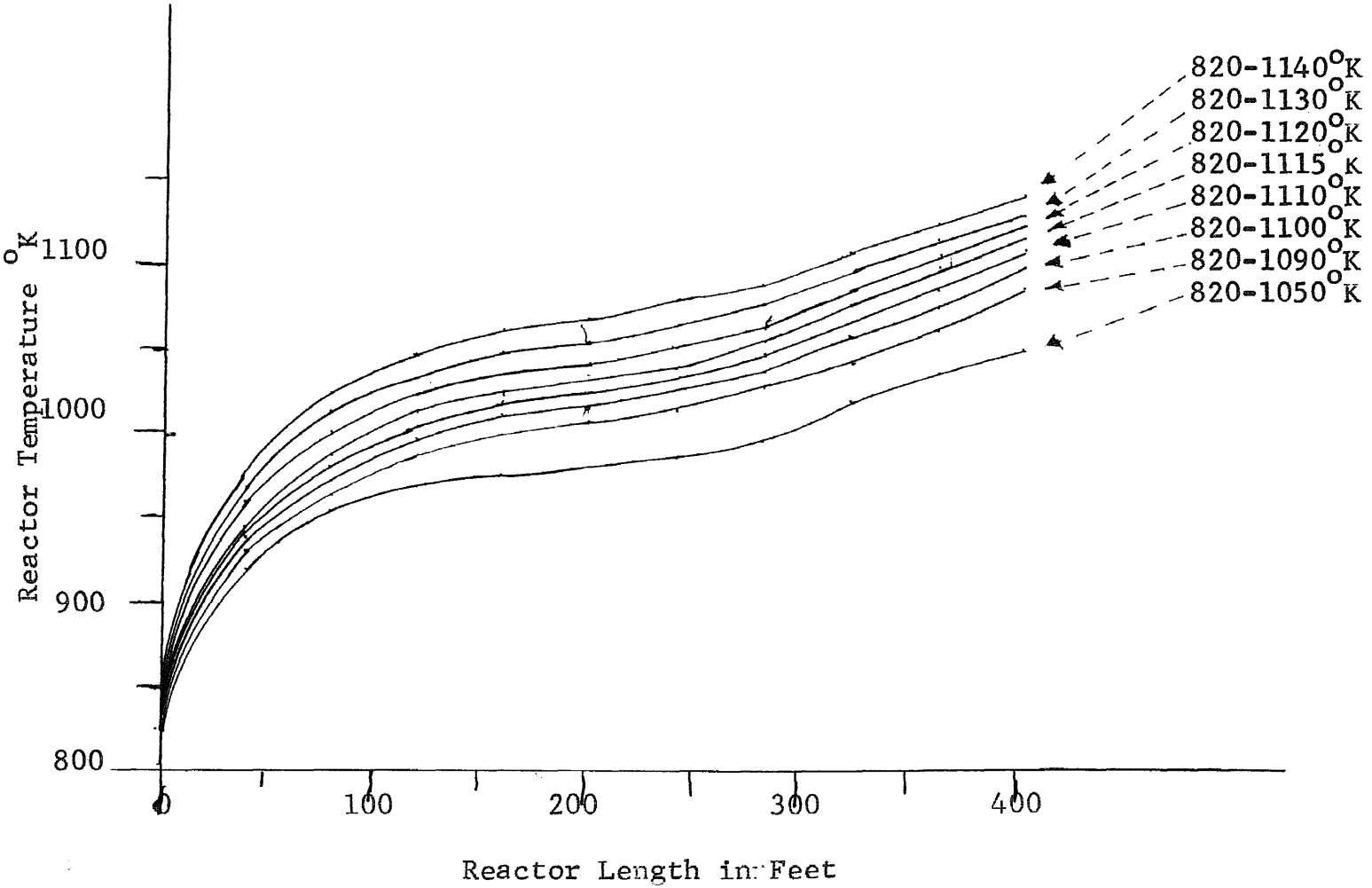
The six equations considered in this study were: (48)

	Order Forward	Order Reverse	
$C_2H_6 \rightarrow C_2H_4 + H_2$	1	1-1	(1)
$C_2H_6 \rightarrow CH_4 + \frac{1}{2}C_2H_4$	1	1-1	(2)
$C_2H_4 \rightarrow C_2H_2 + H_2$	1	1-1	(3)
$C_2H_2 \rightarrow 2C + H_2$	2	1-1	(4)
$2C_2H_2 \rightarrow C_4H_4$ (i.e.) C_4's	1	1	(5)
$C + H_2O \rightarrow CO + H_2$	1-0	1-1	(6)

The temperature profiles were estimated from the published temperature profiles for pyrolysis furnaces. (47) Other profiles were then produced in such a way that the initial temperature remained the same and the increase in temperature along the reactor length was paralleled to the original profile plus an increment proportional to the difference between the final outlet temperature and the distance along the reactor length. In this study, only these temperature profiles were imposed upon the system to determine the optimum.

Figure 1

Temperature Profiles Used in the Optimization of Ethylene Reactor



Chapter 2

Review of the Literature

Use of Computers in Pyrolysis

Shah[46] wrote a computer program to calculate the composition profiles throughout a purolysis furnace. Simultaneous mass and energy balances were used with a forced parabolic pressure profile. The kinetic data were corrected by obtaining data from two furnaces, one cracking ethane and the second cracking primarily propane. The Arrhenius constants were adjusted to make the model agree with the data from the furnaces.

Shah then varied a number of parameters in order to determine their effect of yield. The following was observed:

1. "Increase in the inlet pressure led to increased decomposition of ethane; however the percent of ethane yielding ethylene decreased owing to the increase in the rate of side reactions relative to the conversion rate of ethane to ethylene."
2. The increase in pressure necessary to overcome the pressure drop caused by carbon deposition increased the rate of carbon deposition.
3. As the steam to feed ratio was increased two fold there was a slight increase in ethane decomposition and

ethylene yield. The steam also suppressed the formation of coke and polymerization reactions. The coke had a detrimental effect on the heat transfer through the reactor wall and required additional heat input to maintain the same temperature profile.

4. As the feed rate was increased the percent yield of ethylene dropped off, however the total production rate increased (i.e. the selectivity factor increased). This increase was the result of suppression of side reactions because there was a decrease in gas residence time in the tube with increased feed rate.

5. Feed temperature had little effect on the overall yield, even at a temperature 300^{o}K higher than those first used. This was due to the fact that the initial position of the reactor was used as a preheater and little reaction occurred.

6. The reduction in the overall heat transfer due to carbon buildup decreased ethylene yield by 3%.

7. Reactor temperature profile had a drastic effect on ethane decomposition. However, the higher temperatures were found to reduce ethylene yield due to increase in side reaction.

A second study by Shah[47] showed that it was possible to reduce a complex model to a more simple one. Shah stated that this simplification was necessary despite the advent of third generation high speed computers because of the large number of individual calculations required in the more complex model. The simplified model had the disadvantage that it could not be extrapolated outside of the range of values in which it was derived. This handicap was overcome by using operating data close to the optimum conditions. This method had the further disadvantage that it could not be used with accuracy to predict models with different parameters.

Katz discussed the use of computers in engineering education in a study done at the University of Michigan[40] comparing the efficiency of using finite differential techniques to using Runge-Kuta integral procedures. It was found that reactor length increments 10 to 50 times larger could be used without appreciable loss of accuracy. This enabled a considerable saving in computer time.

Andrews and Pollock[2] used stoichiometric and kinetic data from laboratory data to express the relationship between the main and side reactions in the cracking of butane, propane and ethane feedstock. They used rate expressions which performed a step change at 75% decomposition of the butane.

Andrews and Pollock's computer program took into account the overall rate of reaction coupled with pressure drop and heat transfer calculations.

Andrews and Pollock reported:

> "... composition, temperature, pressure and enthalpy of the gas and skin temperature of the tube are determined for each tube. Average Datatron (computer) time for calculating each tube was less than 2 minutes. This speed makes it possible to investigate and select the tube diameter, length, and number of tubes needed to meet specifications for a given furnace design."

Andrews suggested that for a given furnace design, variation of feed stocks, heat flux pressure, temperature, steam rate and feed rate were readily predictable.

Myers and Watson [36] analyzed data from the literature for the pyrolysis of propane and developed rate equations for ten reactions which contributed significantly in determining the rate and product distribution. The results were in satisfactory agreement with data found in the literature. Myers and Watson used simple stoichiometric equations but with an apparent order of reactions which was empirically evaluated from the effect of pressure on rate.

Myers and Watson reported:

"When using such apparent order of reactions to represent the net results of series or chains of reactions it must be carefully recognized that the treatment is empirical and cannot serve as a reliable basis for extended extrapolation."

Rosier and Watson[42] reported that absolute reaction rate measurements, particularly at high temperatures, were notoriously inconsistent and unreliable largely due to the difficulty of accurately determining the true effective temperature or reactor volume.

Schneider and Frolich[45] did work on the products from propane which was perhaps the most extensively reported in literature. But no report on kinetics was included, nor was there sufficient data from which absolute rates could be calculated.

Frey and Hepp[18] noted in a review of the literature that no data was available which included both detailed product distribution coupled with data necessary to obtain the required absolute reaction rate.

Burk, Laskowski and Lankelma[11] treated the decomposition of pseudo first order reactions and reported the rate in the form $(-r_a)=KC_a$ and used pseudo Arrhenius rate constants $K_c=A\,e^{-E/RT}$ where

r_a = rate of decomposition of reactant A moles/

(volume)(time)

K_c = reaction velocity constant in units 1/time

C_a = concentration of A(moles/volume)

E = apparent energy of activation, calores/gram mole

A = apparent frequency factor, 1/time

Burk et al reported that in spite of the widely varying values of E which are reported in the literature, an average value of 63,000 calories/gram mole is in good agreement with reliable data for all normal paraffins.

Towell and Martin [61] developed a rigorous method to account for non-uniform temperature distribution in the analysis of kinetic data.

Bonner and Honeycutt [8] described the versatile role that the digital computer can play in both on line and off line applications.

Lindsay and Wulzen [32] described the role of the digital computer in off line calculations of product yield and optimization techniques.

Feigin et al [17] used the computer to solve for optimum design. Feigin developed a set of equations with different parameters which the computer adjusted to find optimum operating conditions in a coil tube furnace.

Lindahl [31] used a computer program to calculate unit

operations in a refinery gas recovery process. The results were optimized in terms of equipment efficiency and process variables. The economics of the process operations and equipment changes were reviewed.

Tayyabklan [59] described the use of an on line computer which controlled the values of the pyrolysis stream directly. The computer had also been programmed to obtain operational data of all sorts from the plant and produce reports for various levels of management.

Noguchi et al [37] described a system for optimum control of a refinery. A linear program was discussed in the designing stage as well as the operational phase of a large refinery.

Chemistry of Pyrolysis

Kevorkian [24] gave a complete review of the chemistry of light hydrocarbons at high temperature pyrolysis conditions.

Amano and Uchiyama [1] proposed a mechanism for the formation of propylene which predicted two different reactant zones. At lower temperatures and high propylene concentration the reaction was characterized by the formation of higher boiling materials (polymers) and it obeyed the (3/2) order rate law. At high temperatures and lower pressures the formation of the allene became important and the reaction obeyed first order kinetics. Consistent results were obtained for the

proposed mechanism when existing data was analyzed for both product distribution and reaction rate.

Reaction Rate

Swinbourne [56] developed an extrapolation procedure for obtaining rate constants and final concentrations of the first order reaction. The method was applied to the pyrolysis of cyclohexyl chloride and cyclopentyl chloride and the rate constants from the pressure time data were calculated. The method was both versatile and time saving and was applicable to other pyrolysis reactions.

Szepesy, Simon and Simon [57] developed a method to determine the composition of the product stream from a pyrolysis reaction. This method involved the use of gas chromatography and was able to detect N_2, CH_4, C_2H_2, C_2H_6, C_3H_8, C_4H_{10}. The use of this "fast" analytical method when coupled with the integral rate determination of Otowell should be helpful in determination of plant kinetic data.

Equilibrium Data

Lavrov and Bakilstskii [26] determined the composition of the equilibrium mixture obtained in the pyrolysis of hydrocarbons in the presence of oxygen and water. This was accomplished by solving the simultaneous equations arising from each individual reaction taking place in the system. The equilibrium coefficient for any compound was characteristic

of the compound at the given temperature and pressure and was a constant for all reactions. The equilibrium constant K and the partial pressure can then be calculated from the known value of the equilibrium coefficient.

Heat of Reaction

Stepanov and Stepanova [53] showed how to use total enthalpy of mixture temperature diagrams in determining the amount of heat required during any stage of pyrolysis. It was possible to calculate quickly and show up any errors and inconsistencies in the calculations. The charts were directly applicable to the ethane and propane pyrolysis.

Heat Transfer

Butovski et al [12] gave mathematical equations for heat radiation exchange between coil and furnace based on the Stefan-Boltzman Law.

Stepanov [52] determined the effect of the decomposition of (C_{1-5} and H_2) on the heat transfer coefficient. With studies of the Reynolds number about 50 - 500 experimental results were approximated within 20% by the equation

$$Nu = 0.77\ Re^{.2}\ Pr^{.4}\ Gr^{.1} \qquad (7)$$

where Nu is the Nusselt number

Re is the Reynolds number

Pr is the Prandel number

Gr is the modified Grashoff number

and $$Gr = gd^3 (\delta \Delta X + B \Delta T)/\nu^2 \quad (8)$$

where δ characterizes an increase in the number of moles

ΔX is the difference in conversion between the center and the inside wall

Carbon Deposition

Palmer [39] reviewed the literature and cited references relative to the kinetics and mechanism of carbon deposition during gaseous pyrolysis.

Tamai et al [58] made a study to clarify the phenomenon of the decomposition of carbon on the reactor wall in the thermo decomposition of hydrocarbons. The effect of the wall material on the decomposition of methane was as follows:

1. Iron and nickel plates showed deposition of carbon.
2. Titanium, tungsten and silicon plates caused carbonization of methane.
3. Gold, silver and copper plates showed a thin, non-clinging film similar to graphite.

The differences were attributed to the affinity of carbon to the different materials of the plates.

Cahn et al [13] obtained a U.S. patent describing a decoking method for a pyrolysis tube. The tubes of the

thermo cracking furnace were decoked by cutting out the flow of hydrocarbon feed and passing steam in one of the tubes at a time so as not to completely shut down the furnace. Steam entered at 700°F (645°K) at a rate of 15 lb/sec/ft^2 (tube cross-sectional area). Cleaning took approximately 12 hours per tube and the procedure was carried out in the next tube.

Esso Research and Engineering Company [15] obtained a patent in which the claim was made that carbon would be eliminated by passing free hydrocarbons (e.g. ethane), through the cracking tube. The sulfur content was less than 20 p.p.m. Outlet temperature was 1037°K at a velocity of approximately 1000 ft/sec. The carbon was removed by the mechanical action of the high velocity gas.

Buckley et al [9] described a vertical concentric tubular reactor in which the outer annular section communicates with the central tubular section at the upper end. The reactants were fed together at the lower end of the annular section and were preheated while they flowed up, then reacted in the center tubular section and left at the lower end. Carbon deposition on the walls of the center was avoided by keeping the wall temperature below the point at which the wall metal displays catalysis activity leading to carbon deposition.

This was achieved by maintaining higher gas velocities in the annular preheating section so that the gas to outer wall heat transfer coefficient is lower than the inner wall to gas coefficient maintaining the wall temperature close to gas temperature.

Oliver [37] described a method to clean a pyrolysis tube being fed liquid hydrocarbon feed. By switching to ethane feed every 100 hours and feeding ethane for ½ to 5 hours the pressure drop in the reactor was brought back to normal. This allowed a reactor shut down time to be increased by a factor of six resulting in a greatly increased production rate. No explanation of the phenomenon was offered, although it was most probably due to the mechanical action of a high speed ethane flow.

Tucker [62] described a conical design which minimized coke formation. This served as a purge which kept the tubes clean.

Heicklen et al [20] assumed that the pyrolysis of gas gave an active species (C) that could be added to carbon particles (C_n).

$$C + C_n \rightarrow C_{n+1} \qquad (9)$$

The particle size distribution was a function of pressure and temperature. At high pressures and temperatures the particle size was smaller. The maximum deposition rate of carbon was

achieved soon after reactor start up. At lower pressures and temperatures the maximum rate of deposition occurred after more time had elapsed. The particle size also increased. Carbon deposition was assumed to be linear with the rate of production of (C).

Furnace Construction

Hennig [24] described a vertical furnace which was packed with inert heat exchange solids which were heated to form a hot zone which occupied only a fraction of the total height. When the hot zone was near the bottom, reactants were admitted from the bottom and the hot zone moved up by the heating effect of the reacting mixture. Flow was reversed when the zone reached the top of the furnace and the cycle was repeated. This furnace was successful in eliminating the pre-heat section of the pyrolysis reactor.

Rosendahl [44] discussed the formation of acetylene by the incomplete combustion of methane. Combustion was carried out in an electric arc.

Stepanov et al [54] designed a high pressure reactor consisting of a cylindrical vessel with internal coil as the component in a new pyrolysis process. The reactor used a contact time of .1 to .3 seconds, a pressure of 5. atmospheres and a temperature of 900°C and an outlet temperature on the wall of 1180° C with an outlet pressure of 1.2 atmospheres.

The outlet gas was immediately fed through a series of compressors with interstage brine cooler to bring the mixture to -10°C and 40 atmospheres. A yield of 39.7% ethylene was obtained along with .96 mole percent acetylene.

Chukanov et al [14] received a patent for an improvement of heat transfer in a pyrolysis furnace. The heat was applied via induction currents such as high frequency electric currents. In order to achieve uniform heating of the gas as well as to increase the yield of product, the decomposition was carried out on a fixed attachment made of refractory metal or coke. To decrease radiation losses and improve heat accumulation the reactor was shielded from its immediate environment.

Mamedov et al [34] received a patent describing a furance consisting of a combustion chamber mounted along with a recirculator of the fuel gases and equipment for heating and cracking of hydrocarbons. The continuous circular tubes connected in parallel were placed in jackets lined with fine grained, heat conducting and heat resistant packing and equipped with ribbed heating fins. This system enabled more convenient removal of tubes for decoking.

Smolen et al [50] described the use of heavy oils to heat reactors where the $C_3/C_2 \geq 0.7$. Temperautre up to 1127°K can be achieved. It was recommended for $C_3/C_2 \leq 0.6$ that only horizontal fire heated reactors be used.

Supersonic Oxidative Pyrolysis

Vasil'ev et al [64] carried out the oxidative pyrolysis of hydrocarbons by introducting the hydrocarbons preheated to 500-600°C into oxygen at supersonic rates so that the O_2 was unifromly distributed in the resulting mixture and no zones of extremely high temperature existed in the steel reactor lined with fire brick. Under laboratory conditions they obtained a yield of 58% ethylene from ethane. Propane yielded 57% ethylene and 14% propene. Butane gave 34% ethylene and 16% propene. Gasoline was also successfully pyrolyzed. The yield for butane and gasoline was 50% better than those obtained by conventional cracking.

Carbon black and coke were not produced and losses due to the formation of CO_2 and H_2O amounted to only 1%.

Sub-Sonic Oxidative Pyrolysis

Vasil'ev et al [63] also carried out a study in a full scale plant for three months comparing the thermo pyrolysis with thermo oxidative pyrolysis. The following table compared the results from the two runs:

Conditions	Thermo Cracking	Oxidative Cracking
Exit temperature	1093°C	1053°C
Butane in Kg/Hr	4071	4800
Steam in Kg/Hr	720	390
O_2 in Kg/Hr	-	987
N_2 in Kg/Hr	-	53
Overall Yield of		
Pyrolysis Gas	88.9%	107.3%
CH_4	22.5%	29.0%
C_2H_4	25.5%	34.0%
C_3H_6	15.1%	13.4%
Tars	16.1%	8.5%
Heat Load K Cal		
M Ton Feed	855,000	415,000
Heat Load K Cal		
M Ton C_2H_4	3,340,000	1,240,200

The oxidative cracking was free of soot and coke formation and its efficiency based on C_2H_4 output was stated to be 2.0 to 2.5 times greater than that of the thermal cracking.

Pyrolysis of Heavy Feed Stock

Walker [65] described the history and problems encountered

in pyrolysis of a wide boiling mixture of naptha and gas oil. The system was originally designed for the production of ethylene and propane but has a total of 31 products including higher olefins, diolefins and higher aromatics. The reactor system includes 71 chemical species. To help solve the optimization which lies in the maximization of aromatics, two computer programs were used. One program solved a material balance and a linear program solving for 406 variables and constraints. The other was an extensive computer installation which had been successful in data logging, alarming, stream integration and in control functions but was not used in closed loop optimization or furnace control.

Tmenov et al [60] ran experiments with a paraffin boiling at 250-350°C. The reactor charge was between 3.5 $Kg/cm^2/hr.$ with contact time of 0.1 to 0.5 seconds and using 25 weight percent steam.

The results are illustrated in the following table:

	Weight Percent Product	
	927°K	1098°K
Liquid Products	60.7	27.2
Light Oils	18.8	13.5*
Coke	1.5	7.5
C_2H_4	-	31.5
C_3H_6	16.5	7.0
C_4H	11.5	2.5
$CH_4 + H_2$	16.8	39.1

Tmenov also shows the dependency of unsaturated hydrocarbons and aromatics on temperature and reactor charge.

* The aromatic content increased with increasing temperature.

Chapter 3

Theory

The computer program developed is capable of handling a maximum of twenty five reactions incorporating up to twenty five components. It would therefore be appropriate to discuss the theory incorporated in the program before the handling of the particular topic of this thesis.

Pyrolysis of Ethane

The generalized computer program was adapted to the pyrolysis of ethane. The reactions considered were:

	Order Forward	Order Reverse	
$C_2H_6 \rightarrow C_2H_4 + H_2$	1	1-1	(1)
$C_2H_6 \rightarrow CH_4 + \frac{1}{2}C_2H_4$	1	1-1	(2)
$C_2H_4 \rightarrow C_2H_2 + H_2$	1	1-1	(3)
$C_2H_2 \rightarrow 2C + H_2$	2	1-1	(4)
$2C_2H_2 \rightarrow C_4$'s	1	1	(5)
$C + H_2O \rightarrow CO + H_2$	1-0	1-1	(6)

I Treatment of Initial Data

A. Heat Capacity Data

It is necessary to calculate the delta heat capacity for

each reaction. This quantity will be read in the calculation of equilibrium constants as well as the overall heat balance. Δ CP was calculated from the following relationship:

$$\Delta CP_J = \sum_{I=R+1}^{R+P} (CP_I)_J * B_I - \sum_{I=1}^{R} (CP_I)_J * B_I \qquad (10)$$

where ΔCP_J is the coefficient of the J^{th} temperature term in the Delta heat capacity equation for the reaction Cal./g.mole/^oK.

P is the number of products.

$(CP_I)_J$ is the coefficient of the J^{th} temperature term of the I^{th} component in the heat capacity equation for the component (Cal./g. mole/^oK).

B_I is the stoichiometric coefficient of the I^{th} component.

R is the number of reactants.

In order to get the heat capacity data in the same form it was necessary to curve fit heat capacity data [43] [44] to a third degree polynomial (See Appendix C).

The results of the curve fitting are as follows:

Table 1

Heat Capacity Data of Selected Components

Component	A $\times 10^0$	B $\times 10^2$	C $\times 10^5$	D $\times 10^9$
Acetylene	5.867	1.957	-1.296	3.466
Iso-Butane	-1.901	9.930	-5.475	11.82
N-Butane	0.09114	9.218	-4.761	9.577
Iso-Butene	0.7098	8.209	-4.535	9.837
Ethane	0.9065	4.420	-4.864	2.856
Ethylene	0.9847	3.701	-1.945	4.042
Hydrogen	7.010	-0.05366	0.1006	-0.2453
Methane	4.010	1.493	-0.00173	-1.593
Propane	-1.083	7.314	-3.788	7.672
Propene	0.7342	5.663	-2.838	5.510
Water	7.718	0.01285	0.3151	-1.150
Carbon	-1.356	1.447	-1.101	3.028
Carbon Monoxide	6.863	-0.04085	0.2480	-1.018

Where

$$CP = A + BT + CT^2 + DT^3$$

B. Heat of Reaction Data

It is necessary to calculate the Delta heat of reaction for each reaction per mole of the first component of each reaction. This is used in the overall heat balance. ΔH_T was calculated from the following relationship:

$$\Delta H_T = \sum_{I=R+1}^{R+P} (B_I/B_1)\Delta H_I - \sum_{I=1}^{R} (B_I/B_1)\,\Delta H_I \qquad (11)$$

where ΔH_T is the Delta heat of reaction (Cal/ g mole) at 25^oC.

ΔH_I is the Delta heat of reaction of the I^{th} component of the reaction (Cal/g mole) at 25^o C.

To calculate the heat of reaction, the heat of formation was required. Following are the values of heats of formation.[22]

Table II

Heat of Formation at 25°C

Component	Heat of Formation, Cal/g mole X 10^{-4}
Acetylene	5.4194
Iso-Butane	-3.1452
N-Butane	-2.9812
Iso-Butene	0.0280
Ethane	-2.0236
Ethylene	1.2496
Hydrogen	0.0
Methane	-1.7889
Propane	-2.482
Propene	0.4879
Water	-5.7797
Carbon	0.0
Carbon Monoxide	-2.6416

Using these data the heat of reaction is calculated for each temperature using the data at 25°C and the heat capacity data.

C. Entropy

It is necessary to calculate the delta entropy data for each reaction. ΔS_T is used in the calculation of the equilibrium term for each reaction. ΔS_T is calculated from

the following relationship:

$$\Delta S_T = \sum_{I=R+1}^{R+P} (B_I/B_1)\Delta S_I - \sum_{I=1}^{R} (B_I/B_1)\Delta S_I \qquad (12)$$

where ΔS_T is the Delta entropy for the reaction (Cal/g mole ^{o}K) at $25^{o}C$

ΔS_I is the entropy of the I^{th} component of the reaction (Cal/g mole ^{o}K) at $25^{o}C$

The following values were used:

Table III

Selected Values of Entropy

at 25°C (22)

Component	Entropy of Formation $Cal/g\ mole\ ^{o}K$
Acetylene	47.997
Iso-Butane	70.42
N-Butane	74.10
Iso Butene	72.48
Ethane	54.85
Etyhlene	52.45
Hydrogen	31.21
Methane	44.50
Propane	64.51
Propene	63.80
Water	45.106
Carbon	1.307
Carbon Monoxide	47.301

Entropy data were calculated by the program for each temperature using the data at 25°C and heat capacities.

D. Equilibrium Data

The following are the $Log_{10}(K_f)$ data used to calculate

the equilibrium data:

Table IV

Selected Values of LOG(K) of Formation

Component	LOG(K) (1000°K)
Acetylene	-8.874
Iso-Butane	-14.59
N-Butane	-14.14
Iso-Butene	-13.67
Ethane	-5.701
Ethylene	-6.17
Hydrogen	0.0
Methane	-1.007
Propane	-9.983
Propene	-9.983
Water	10.05
Carbon	0.0
Carbon Monoxide	10.47

E. Calculation of the Equilibrium Constant

All equations are assumed to be reversible. The reverse kinetic rate constants will be calculated from equilibrium data developed from the equation [49]

$$\Delta F = -RT * LN\ (K) \qquad (13)$$

or

$$K = \exp(-\Delta F^{\circ}/RT) \qquad (14)$$

using the relationship that

$$\Delta F = \Delta H - T\Delta S \qquad (15)$$

and

$$\Delta F = -\Delta H_o(I)/RT + \Delta A(I)/R * LN(T) + \Delta B(I)/2R * T + \Delta C(I)/6R * T^2 + \Delta D(I)/12R * T^3 + FI(I) \qquad (16)$$

where FI(I) is a constant of integration evaluated from a known equilibrium constant at a known temperature and using Equation (16) solved for FI(I).

The equilibrium constant for a known temperature was calculated from $Log_{10}(K_f)$. The data were taken from Selected Values of Chmiecal Thermodynamic Properties[44] and are shown in Table IV.

The $Log_{10}(K_f)$ for reaction is calculated below

$$Log_{10}(K_f)_{Reaction} = \sum_{Products} B_K/B_1 * Log_{10}(K_f)_K - \sum_{Reactants} B_K/B_1 * Log_{10}(K_f)_K \qquad (17)$$

The following equilibrium constants were either found in the literature or calculated from entropy and heat of formation data by using Equations (15) and (13):

Table V

Equilibrium Constants

Reaction	Eq. Con.	Temp. ^{o}K	Ref. #
$C_2H_6 \rightarrow C_2H_4+H_2$	5.51	800	(47)
$C_2H_6 \rightarrow CH_4+\frac{1}{2}C_2H_4$	40.45	1000	Eq. (17)
$C_2H_4 \rightarrow C_2H_2+H_2$	0.036	875	(47)
$C_2H_2 \rightarrow 2C+H_2$	7.48×10^7	1000	Eq. (17)
$2C_2H_2 \rightarrow C_4$'s	21843.	1000	Eq. (17)
$C+H_2O \rightarrow CO+H_2$	33.8	900	(47)

$$\Delta F = -RT * LN\ (K) \quad \text{and} \quad (18)$$

$$\Delta F = \Delta H - T\Delta S \quad (19)$$

Shah's data[47] for equilibrium constants used in Table V agreed with Equations (18) and (19) from Rossini's Tables[22] and were used as is.

F. Kinetic Data

The kinetic data used in this study came from two principal sources. They were Shah[47] and Homogenous Reaction Kinetics Pyrolysis of Aliphatic Hydrocarbons[23].

The following kinetic data were used:

Table VI

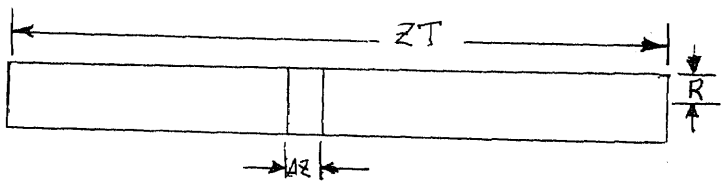
Kinetic Data

Equation	K^o	E* Cal/gm mole
$C_2H_6 \rightarrow C_2H_4 + H_2$	6.04E16	8.20E4
$2C_2H_6 \rightarrow 2CH_4 + C_2H_4$	1.60E12	6.70E4
$C_2H_4 \rightarrow C_2H_2 + H_2$	1.80E13	7.60E4
$C_2H_2 \rightarrow 2C + H_2$	9.70E12	6.20E4
$2C_2H_2 \rightarrow C_4$'s	2.60E13	6.00E4
$C + H_2O \rightarrow CO + H_2$	9.26E3	2.13E4

where $K = K^o \exp(-E^*/RT)$ (20)

II Material Balance

For the material balance the following diagram can be used:



A. Component Balance

IN = OUT + disappearance by reaction + accumulation

expressed in terms of moles of component I.

$$(N_I)_{IN} = (N_I)_{OUT} + \sum_{J=1}^{IT_T} A_{IJ} N_{JO} \Delta X_J + \text{Accumulation} \qquad (21)$$

where IT_i is the total number of reactions in which I is involved.

A_{IJ} is the stoichiometric coefficient of the I^{th} chemical component in the J^{th} reaction.

N_{JO} is the original number of moles of the key component in the J reaction (moles).

ΔX_J is the incremental conversion and can be calculated from the known reaction conditions and kinetic data.

$$\Delta X_J = 2\pi R^2 (-R_J) \Delta Z \qquad (22)$$

$N_{JO}\Delta X_J$ corrected so that the rate was given in terms of

conversion of moles of component per hour was

$$N_{JO}\Delta X_J = 11309.7R^2(-R_J)\ F_O X_{JO}\Delta Z \qquad (23)$$

where F_O was the total molar flow rate (lb moles/hour).

X_{JO} was the mole fraction of the J^{th} component.

ΔZ was the length of the reactor being considered. (feet)

R was the reactor radius (feet).

$(-R_J)$ was the reaction rate of the J^{th} reaction (lb moles/ft^3 sec).

B. The Overall Material Balance

IN = OUT + Change by Reaction + Accumulation

$$\sum_{I=1}^{M} (N_I)_{IN} = \sum_{I=1}^{M} \left[(N_I)_{OUT} + \sum_{J=1}^{IT_I} A_{IJ} N_{JO}\Delta X_J \right] + \text{Accumulation} \qquad (24)$$

Since steady state is assumed, all component accumulation terms are zero in this study with the exception of carbon.

C. Calculation of Conversion

The calculation of an increment of conversion X_A for each reaction is derived from the following: (27)

$$\tau = 1/S = C_{A_0} \int_{X_1}^{X_2} dX_A/-r_A \qquad (25)$$

where $\tau = 1/S$ is the reactor space time (sec.)

dX_A is an increment of conversion of the key component.

$-r_A$ is the rate of reaction (lb moles/ft^3 sec).

C_{A_0} is the initial concentration of the key component (lb moles/ft^3)

This equation is differentiated with respect to X_A.

$$d\tau / dX_A = (C_{A_0} / -r_A) \tag{26}$$

This equation is then solved for dX_A

$$dX_A = (-r_A)\, d\tau / C_{A_0} \tag{27}$$

The following is obtained by considering finite differences:

$$\Delta X_A = (-r_A)\Delta\tau / C_{A_0} \tag{28}$$

Equation (28) will be used to solve for finite difference along the reactor profile. Equation (30) is really the expression for conversion in a back mix reactor. This means the solution is really the solution of a large number of back mix reactors. (i.e.)

$$\Delta X_A \text{ (TOTAL)} = \sum (\Delta X_A)_i \tag{29}$$

By re-evaluating the reaction conditions at hundreds of

positions along the reactor, a good approximation of the total reactor profile can be arrived at. By restricting Max $(\Delta X_A)_i$ to be less than or equal to .01 (and on the average equal to .005 and with a minimum value of .001) the above approximations will be good.

The value of ΔX_A is controlled by controlling the value of τ.

$$\tau = \frac{C_{A_O} V}{F_{A_O}} \tag{30}$$

where C_{A_O} is the original concentration of component A in (lb moles/ft^3).

V is the reactor volume (ft^3).

F_{A_O} is the molar flow rate of component A in (lb moles/hour).

$$V = \pi R^2 L$$

$$\Delta\tau = \frac{C_{A_O} \Delta V}{F_{A_O}} = \pi R^2 \frac{C_{A_O} \Delta L}{F_{A_O}} \tag{31}$$

by combining equations (30) and (31) the following is obtained:

$$\Delta X_A = C_{A_O} (-r_A) \Delta\tau = \pi R^2 / F_{A_O} (-r_A) \Delta L \tag{32}$$

thus the value of ΔX_A can be controlled by the length (ΔL). The procedure to control the value of ΔX_A was to calculate ΔX_A for each reaction and test whether it was larger than .01. If it failed the test, a new value of ΔL was calculated from the equation:

$$\Delta L_{NEW} = ABS(\Delta L_{OLD} * .005)\Delta X_A\ (I)) \qquad (33)$$

The max of $ABS(\Delta X_A)$ was found and compared with .001. If the test failed, a new ΔL was calculated from equation (33).

In both cases the control of the program was returned to the initiation of the reactor design.

If all rates passed both tests then calculation of new reactor conditions was continued.

In order to calculate $\Delta X_A(I)$ the following must first be calculated:

$$\pi R^2/F_{A_O}\Delta L \qquad \text{and}$$

$$(-r_A) = K_o e^{-E^*/RT} \left(C_{F_I}^{N} f_i - C_{R_I}^{N} R_i \right) \qquad (34)$$

or

$$(-r_A) = K_o e^{-E^*/RT} (CF-CR) \qquad (35)$$

where $(-r_A)$ is the rate of the reaction (lb moles/ft^3sec).

K_o is the Arrhenius frequency factor (in appropriate units).

E^* is the Arrhenius energy of activation (BTU/lb mole).

R is the gas constant (1.431 BTU/lb mole ^oK).

T is the temperature in absolute units (^oK).

C_{F_I} is the concentration of the reactants (lb moles/ ft^3).

C_{R_I} is the concentration of the products (lb moles/ ft^3).

N_{F_I} is the order of the I^{th} forward reactant.

N_{R_I} is the order of the I^{th} reverse reactant.

$$CF = \prod_{I=1} C_I^{N_{F_I}} \tag{36}$$

$$CR = \prod_{I=1} C_I^{N_{F_I}} \tag{37}$$

In order to calculate $(-r_A)$, the reaction rate, it is necessary to recalculate the concentration of each chemical species C_I

$$(C_I)_{OUT} = (P)_{OUT} / [(T)_{OUT} * (\text{GAS CONSTANT})] \tag{38}$$

The Pressure Out point was calculated from the momentum balance. The temperature T_{OUT} was fixed by the known temperature profile of the reactor.

$-r_A$, the reaction rate, was calculated from the Arrhenius kinetics (i.e.)

$$-r_A = K_o e^{-E^*/RT} \left(CF - CR/K \right) \qquad (39)$$

where K was the equilibrium constant of the J^{th} reaction. The Arrhenius data and order of reactants has been defined earlier in the chapter.

C. Calculation of Carbon Deposition

Carbon was deposited on the tube wall. The carbon was formed as a result of the decomposition of acetylene (Equation 5). As the carbon was deposited, it reduced the radius of the pyrolysis tube. This in turn reduced the reactor volume, increased the overall heat transfer coefficient, and increased the pressure drop in the reactor. As a result of the increased pressure drop, the inlet pressure needed to be constantly raised. This in turn accelerated the formation of carbon.

In order to duplicate this effect in the model, a changing pressure profile was simulated. This was done by assuming time uniform deposition of carbon for incremental periods of time. A new radius profile was then calculated. This procedure was repeated until an inlet pressure of 8 atmospheres was required to produce an outlet pressure of 2 atmospheres.

1. Calculation of Reactor Radius

The radius was assumed to be smooth. The reactor radius was only calculated at 101 points. The radius between these points was calculated by interpolation between the two closest known reactor positions. The reactor radius was calculated by assuming that all the solid material formed by conversion was deposited evenly over a one percent length of reactor segment. Then all other partial pressures were readjusted so that their sum was equal to the pressure before solid carbon deposition occurred.

To achieve this it was first necessary to calculate the equivalent volume of the solid component.

$$Vol = ((F_a)_{Deposited}\ MW/\varphi\ )*t \qquad (40)$$

where F_a was the molar flow rate of the solid material (lb moles/hr.).

MW was the molecular weight of the material being deposited (lb/ lb mole).

φ was the density of the material being deposited (lb/ft^3).

t was the time during which the material was deposited (hours).

Once the volume was calculated, the new reactor radius was calculated from

$$R_N = \sqrt{R_O^2 - Vol/(.01\ ZT\ )} \qquad (41)$$

where R_N was the new reactor radius in feet.

R_O was the old reactor radius in feet.

ZT was the total reactor radius in feet.

π was 3.14159.

III Momentum Balance

For the momentum balance, Net Flux of Momentum + Net Pressure Force of Element + Resistance to Flow = 0.

Net Flux of Momentum = $(V_2^2 - V_1^2/2gc)\ D_{DN}$ (42)

Resistance to Flow = $((V_2+V_1)/2)^2 F\ Z/R/2gc) D_{DN}$ (43)

Net Pressure Force on Element = $(-\Delta F')$ (44)

$+\ P = DEN(V_A^2 * \Delta F' * DZ/R + (V_2^2 - V_1^2) 2gc)$ (45)

The friction factor is calculated from

$f = 64/Re \qquad Re \leq 3500$ (46)

$f = 0.00560 + .5/Re^{.32} \qquad Re > 3500$ (47)

The calculation of velocity (V_2) was achieved by first assuming velocity V_2 and calculating pressure P_2. Using the new pressure it was possible to calculate a new velocity thus and calculate P_2. This procedure was followed until the velocity V_2 was within a certain tolerance of V_2 guessed.

V_2 is then calculated from the equation

$V_2 = (FA)_{OUT}/2\pi R^2 * (T2/P2)/GC$ (48)

GC is the Gas Constant, 1.413 at. ft^3/lb mole ^oK.

A. Calculation of Viscosity

The viscosity of the solution was determined by calculating the viscosity of each component as though it were a pure component from the equation

$$U_i = 2.6693 * 10^{-5} \; MT/\sigma^2 \Omega_v \qquad (49)$$

where U_i is the viscosity of the I^{th} component Lb ft/sec.

M is the molecular weight.

T is the temperature in ^{o}K.

σ is the collision parameter in Angstroms.

Ω_v is a slowly varying function of the dimensionless temperature KT/ϵ .

Since the function was only given in tabular form, the author decided to curve fit it using a Marquardt non-linear curve fitting subroutine. (See Appendix B). This resulted in the following equation.(4)

$$\Omega_v = \exp(.4398828 - .44245917 \; LN\,(KT/\epsilon) + 0.08640182 \; LN^2\,(KT/\epsilon) - 0.0077884511 \; LN^3\,(KT/\epsilon)) \qquad (50)$$

The viscosity of the gas mixture was then calculated from the equation (66) and (10)

$$U_{mix} = \sqrt{8} \sum_{I=1}^{N} \left(\frac{X(I) \quad U(I)}{\sum_{J=1}^{N} \left[X(J) \left[1+\frac{U(I)}{U(J)} \right]^{1/2} \left[\frac{M(J)}{M(I)} \right]^{1/4} \right]^2 \Big/ \left[1+\frac{M(I)}{M(J)} \right]^{1/2}} \right) \tag{51}$$

where X(I) is the mole fraction of component I.

U(I) is the viscosity of component I Lb/ft/sec.

M(I) is the molecular weight of component I, lb/lb mole.

B. Calculation of Friction Factor

The friction factor is calculated from the correlations between friction factor and Reynold's number. For Reynold's number below 3500 the laminar flow relationship is used.[16]

$$f = 64/N_{Re} \tag{52}$$

and for Reynold's number greater than 3500 the relationship becomes [16]

$$f = 0.00560 + .5/(N_{Re})^{.32} \tag{53}$$

The Reynolds number is recalculated from

$$N_{Re} = 2R*\rho*V/Vis \tag{54}$$

where R is the radius of the reactor in feet.

ρ is the gas density, lb/ft^3.

V is the velocity of the reactor gas, ft/sec.

C. Calculation of Pressure Drop

The pressure drop in the reactor was calculated from the Bernouli equation.(35)

$$P = (VelA^2 * f * L/R + (Vel_2^2 - Vel_1^2)/(62.4*2116.8) \quad (55)$$

where P was the pressure drop in atmospheres

Vel_1 was the velocity at the beginning of the reactor segment, ft/sec.

Vel_2 was the velocity at the end of the reactor segment, ft/sec.

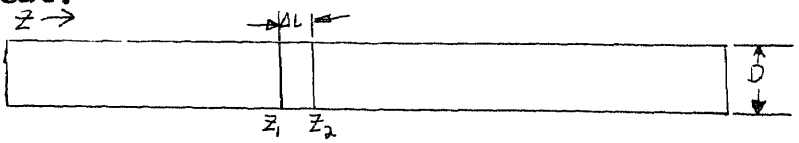
L/R was the length to radius ratio, ft/ft.

VelA was the average velocity in the reactor segment, ft/sec.

f was the friction factor.

IV Heat Balance Equation

The heat supplied by heat transfer throughout the reactor tube must equal the net heat of reaction plus the sensible heat.



Heat in = Heat of Reaction + Sensible Heat

$$UA\Delta T_1 = \sum_{i=1}^{6} (\Delta H)_i (F_J \Delta X_J)_i + \sum_{J=1}^{11} F_J CP_i \Delta T_2 \quad (56)$$

where U is the overall heat transfer coefficient, BTU/hour, ft^2, ^oF

A is the area through which heat is transmitted - $D^2/4\Delta L$, ft^2.

T_1 is the difference between the temperature on the outside tube wall and the mean temperature of the gas stream, ^oK.

H_1 is the heat of reaction of the i equation, BTU/lb mole.

F_J is the molar flow rate of the J^{th} key component of reaction i, Lb moles/hr.

XJ is the extent of reaction of the J^{th} key component of reaction i.

CP_i is the heat capacity of the i^{th} component BTU/ lb moles ^oK.

T_2 is the difference between the temperature at some point Z_1 and $Z_1 + \Delta L$, ^oK.

Sinced forced temperature profiles were used, each small increment of reactor was treated as an isothermal backmix reactor and an energy balance was not necessary.

Chapter 4

Discussion of Results

Using the results set forth in Tables 7, 8, 9 and 10, the production of ethylene in the reactor was optimized.

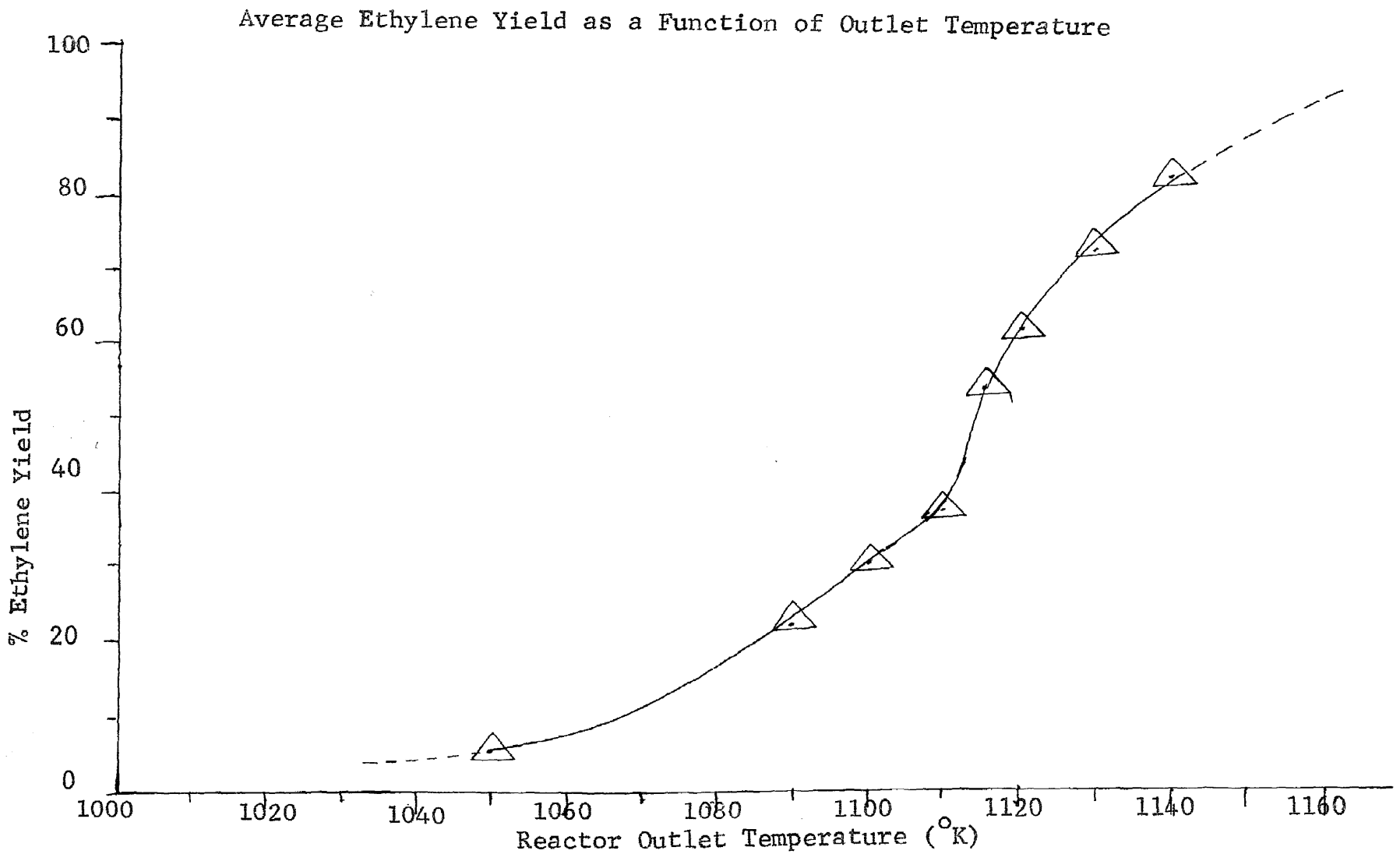
In Table 7 were listed the different temperature profiles which were used, the resulting inlet and outlet pressures in atmospheres, the percent yield, the inlet and outlet velocities and the number of hours the reactor had been run since the last cleaning. Several conclusions were drawn from this table and Figure 2:

1. The yield of ethylene rose sharply with increasing temperature. At the higher temperature the slope of the yield curve approached zero. This curve, called an S curve, is characteristic for endothermic reactions.
2. In System 1, 820-1050°K, the effect of decreasing space time on percent yield became apparent. This effect was best observed by comparing the yield of ethylene with the same initial pressure. It became clear that the computer was able to detect and calculate even small differences in space time and predict a decreasing yield.

The space time was being decreased by two effects:

a) There was physically less room in the reactor due to the carbon build-up.

Figure 2


Average Ethylene Yield as a Function of Outlet Temperature
% Ethylene Yield
100
80
60
40
20
0
1000
1020
1040
1060
1080
1100
1120
1140
1160
Reactor Outlet Temperature (°K)

b) The velocity of the outgoing gases increased due to the increase in pressure drop resulting from carbon build-up.

Of these two effects the second was by far the more important as only a small volume of the reactor was taken up by the carbon build-up.

3. The carbon build-up became much more pronounced as the exit temperature was increased.

This effect was also seen in Table 8 and Figures 3, 4, and 5.

Table 8 showed the effect that the increasing exit temperature had on each of the important components. Appendix G contains the same information as it was derived from the computer, as well as representative plots of pressure, temperature, and reactant and product profiles as a function of reactor position.

Figure 5 showed the effect of reactor exit temperature on the frequency of reactor shut down. The reactor shut down time was calculated from the time the clean reactor first started up until the time the inlet pressure reached 8 atmospheres.

Since the computer was calculating in relatively large increments of reactor run time, the results were represented

graphically (Figures 3 and 4) and extrapolated to a pressure of 8 atmospheres to predict the exact run time.

Table 7. Pressure, Yield and Velocity Conditions as a Function of Reactor Time

System	Press In (At.)	Press. Out (At.)	Percent Yield	Veloc. In Ft/Sec	Veloc. Out Ft/Sec	Time Since Start Up Hours
1 820-1050	5.85	2.00	6.57	209	860	0
	5.85	1.98	6.54	209	877	800
	5.85	1.96	6.52	209	895	1600
	5.85	1.94	6.49	209	913	2400
	5.90	2.11	6.70	207	834	3200
	5.90	2.09	6.68	207	843	4000
	5.90	2.07	6.65	207	852	4800
	5.90	2.04	6.63	207	869	5600
	5.90	2.02	6.60	207	887	6400
	5.90	2.00	6.58	207	926	7200
	5.90	1.97	6.55	207	947	8000
	5.90	1.95	6.33	207	970	8800
	5.95	2.12	6.73	205	840	9600
	5.95	2.10	6.70	205	858	10400
	5.95	1.97	6.57	205	1022	14400
2 820-1090	5.85	2.00	18.9	209	865	0
	5.90	2.01	18.9	206	1040	400
	5.98	2.11	19.3	204	1089	800
	6.18	2.20	20.8	191	928	1200
	6.18	2.20	20.8	191	940	1600
	6.38	2.00	22.2	185	1028	2000
	6.58	2.00	22.4	175	1035	2400
	6.98	2.00	24.6	161	1173	2800
3 820-1100	5.85	1.93	26.1	209	1025	0
	5.95	2.16	26.6	205	991	200
	6.15	2.00	28.9	198	881	400
	6.35	2.00	29.4	192	907	600
	6.55	2.00	30.2	186	1039	800
	6.95	2.00	32.5	175	1068	1000
	7.75	2.00	36.0	153	1099	1200

Table 7 (Cont'd.)

System	Press. In (At.)	Press. Out (At.)	Percent Yield	Veloc. In Ft/Sec	Veloc. Out Ft/Sec	Time Since Start Up Hours
4 820-1110	5.85	2.05	34.1	209	1022	0
	6.05	2.00	35.1	203	852	100
	6.25	2.00	37.2	195	869	200
	6.45	2.00	36.8	189	1085	300
	7.05	2.00	42.0	173	1242	400
5 820-1115	5.88	2.00	47.9	210	1084	0
	6.00	2.00	50.8	203	926	50
	6.20	2.00	52.1	197	964	100
	6.60	2.00	55.6	185	903	150
	7.00	2.00	56.4	174	1208	200
6 820-1120	5.85	2.00	55.5	209	920	0
	6.05	2.00	58.2	202	835	30
	6.25	2.00	59.5	195	881	60
	6.45	2.00	59.8	189	1048	90
	6.85	2.00	62.2	178	1070	120
	7.65	2.00	66.6	159	997	150
8 820-1130	5.85	2.00	67.1	209	971	0
	5.85	2.00	65.1	209	1081	10
	6.05	2.00	69.2	202	865	20
	6.05	2.00	67.3	202	1119	30
	6.25	2.00	69.9	195	978	40
	6.45	2.00	71.3	189	989	50
	6.65	2.00	71.9	189	1051	60
	7.05	2.00	74.7	173	976	70
	7.45	2.00	76.0	163	1090	80
9 820-1140	5.85	2.00	80.1	209	810	0
	5.85	2.00	78.5	209	990	5
	6.05	2.00	81.3	202	959	10
	6.05	2.00	79.6	202	842	15
	6.25	2.00	81.5	195	1125	20
	6.45	2.00	82.6	189	954	25
	6.65	2.00	83.2	183	1017	30
	6.85	2.00	83.4	178	1159	35
	7.25	2.00	85.1	168	1123	40
	7.85	2.00	86.1	155	1082	45

Table 8

System	Acetylene X 10^3	150 Butane X 10^3	Ethane	Ethylene	Hydrogen	Methane	Water	Carbon Monoxide X 10^5	Time Since Start Up Hours
			MOLAR FLOW RATES END OF REACTION LB MOLES/HOUR						
1 820-1050°K	1.538	.0736	121.34	8.531	8.343	.3928	70.133	.0355	0
	1.527	.0727	121.37	8.500	8.312	.3817	70.133	.0349	800
	1.516	.0726	121.41	8.470	8.283	.3805	70.134	.0344	1600
	1.506	.0710	121.44	8.439	8.259	.3794	70.135	.0392	2400
	1.602	.0878	121.15	8.709	8.518	.3905	70.132	.0390	3200
	1.590	.0798	121.19	8.676	8.486	.3893	70.132	.0380	4000
	1.579	.0788	121.12	8.644	8.454	.3881	70.132	.0375	4800
	1.567	.0788	121.25	8.612	8.422	.3869	70.133	.0368	5600
	1.555	.0795	121.29	8.579	8.390	.3857	70.134	.0366	6400
	1.545	.0760	121.33	8.547	8.358	.3845	70.135	.0357	7200
	1.533	.0752	121.36	8.515	8.327	.3833	70.135	.0352	8000
	1.522	.0743	121.39	8.483	8.269	.3821	70.136	.0347	8800
	1.614	.0837	121.13	8.739	8.546	.3926	70.133	.0346	9600
	1.601	.0827	121.16	8.750	8.513	.3914	70.134	.0354	10400
	1.540	.0777	121.30	8.538	8.349	.3851	70.137	.0355	14400
			SYSTEM CONTINUES TO FUNCTION NORMALLY						
2 820-1090°K	11.77	.736	105.38	24.49	24.08	.885	70.33	.791	0
	11.86	.765	105.25	24.58	24.17	.881	70.34	.817	400
	12.29	.843	104.86	25.01	24.59	.907	70.34	.876	800
	16.32	1.522	100.68	28.88	28.39	1.043	70.33	1.532	1600
	16.64	1.752	100.64	29.11	28.63	1.058	70.34	1.711	2000
	19.22	2.43	98.42	31.26	30.74	1.414	70.35	2.361	2400
	22.40	3.47	95.87	33.75	32.20	1.240	70.35	3.362	2800
			REACTOR SHUT DOWN FOR CLEANING (2900 Hrs.)						

Table 8 (Cont'd)

System	Acetylene X 10^3	Iso Butane 10^3	Ethane	Ethylene	Hydrogen	Methane	Water	Carbon Monoxide X 10^5	Time Since Start Up Hours
3 820-1100°K	22.2	1.41	95.90	33.85	33.30	1.15	70.38	1.69	0
	23.2	1.63	95.14	34.58	34.05	1.19	70.37	1.87	200
	27.3	2.31	92.01	37.53	36.97	1.27	70.36	2.43	400
	29.4	2.81	90.67	38.91	38.33	1.32	70.36	2.87	600
	30.0	3.11	90.28	39.28	38.69	1.35	70.35	2.99	800
	34.8	4.30	87.80	42.27	41.65	1.45	70.35	3.82	1000
	42.2	6.91	82.83	46.51	45.81	1.61	70.34	5.63	1200
	Reactor Shut Down For Cleaning (1225 Hours)								
4 820-1110°K	33.3	2.43	88.12	41.44	40.90	1.37	70.40	2.91	0
	40.3	3.51	83.90	45.59	44.97	1.49	70.39	4.04	100
	45.5	4.51	81.03	48.38	47.74	1.58	70.40	5.02	200
	45.4	5.04	81.55	47.83	47.18	1.58	70.36	5.05	300
	58.5	8.61	74.58	54.63	53.93	1.80	70.38	8.46	400
	Reactor Shut Down For Cleaning (460 Hours)								
5 820-1115°K	76.6	5.06	67.10	62.30	61.60	1.90	70.56	9.45	0
	86.6	6.95	62.23	65.94	65.28	2.01	70.51	10.23	50
	91.4	8.13	61.48	67.67	66.90	2.07	70.50	11.40	100
	105.0	11.50	56.74	72.35	71.53	2.22	70.48	14.20	150
	108.0	12.60	55.67	73.28	72.56	2.28	70.49	15.70	200
	Reactor Shut Down For Cleaning (250 Hours)								
6 820-1120°K	105	7.64	56.98	72.17	71.45	2.14	70.54	12.0	0
	116	10.1	53.44	75.59	74.91	2.25	70.53	14.6	30
	121	11.6	51.66	77.30	76.62	2.31	70.53	16.2	60
	124	11.2	51.25	70.70	77.00	2.34	70.53	17.0	90
	134	15.4	48.06	80.77	80.09	2.45	70.53	20.4	120
	157	23.2	42.07	85.56	85.93	2.66	70.55	30.2	150
	Reactor Shut Down For Cleaning (155 Hours)								

Table 8 (Cont'd)

System	Acetylene X 10^3	150 Butane X 10^3	Ethane	Ethylene	Hydrogen	Methane	Water	Carbon Monoxide X 10^5	Time Since Start Up Hours
8 820-1130°K	161	11.9	41.66	87.23	86.63	2.48	70.64	22.0	0
	152	10.3	43.80	85.15	85.54	2.43	70.63	19.3	10
	173	14.5	38.85	89.93	89.39	2.56	70.64	26.0	20
	162	12.2	41.45	87.41	86.83	2.50	70.62	21.9	30
	177	15.6	37.94	90.80	90.26	2.60	70.64	31.5	40
	185	18.1	35.98	92.69	92.18	2.67	70.65	31.5	50
	189	19.6	35.15	93.48	92.98	2.71	70.65	34.1	60
	207	25.1	31.43	97.07	96.64	2.84	70.66	43.0	70
	215	27.8	29.68	98.75	98.36	2.91	70.68	49.9	80
	REACTOR SHUT DOWN FOR CLEANING (90 Hrs.)								
9 820-1140°K	250	18.4	24.44	104.06	103.88	2.85	70.75	38.4	0
	238	16.1	26.95	101.97	101.72	2.81	70.73	35.1	5
	260	21.2	22.85	105.56	105.45	2.91	70.73	45.6	10
	246	18.2	25.11	103.44	103.16	2.86	70.72	38.4	15
	261	22.2	22.52	105.86	105.75	2.94	70.71	44.1	20
	271	25.0	20.99	107.32	107.28	3.00	70.72	49.4	25
	276	26.6	20.09	108.18	108.17	3.04	70.71	51.8	30
	277	27.3	19.86	108.37	108.39	3.07	70.71	54.2	35
	292	32.4	17.61	110.53	110.67	3.15	70.73	64.2	40
	REACTOR SHUT DOWM FOR CLEANING (45 Hrs.)								

Figure 3
Graphical Extrapolation of Reactor Operating Time

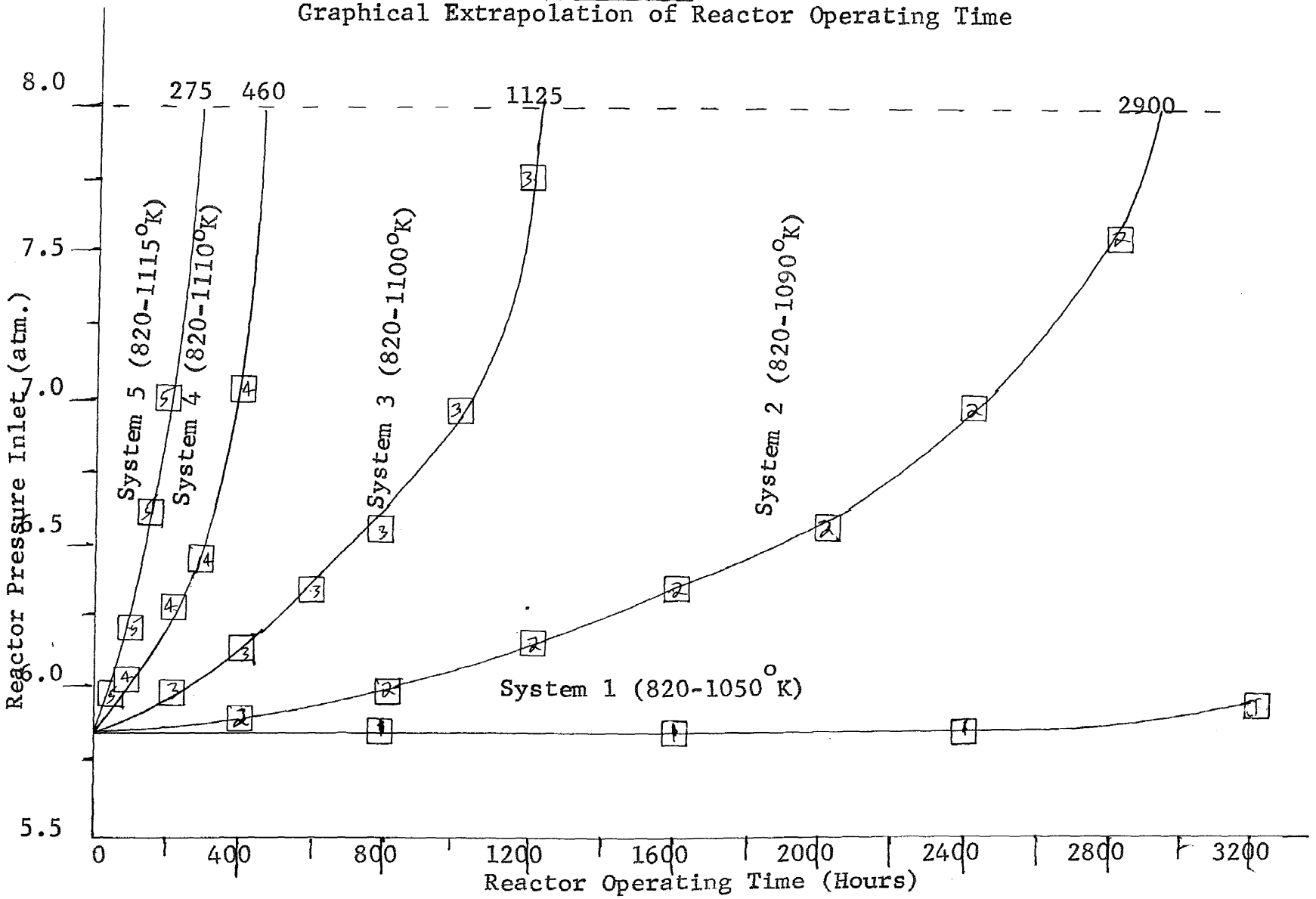


Figure 4

Graphical Extrapolation of Reactor Operating Time

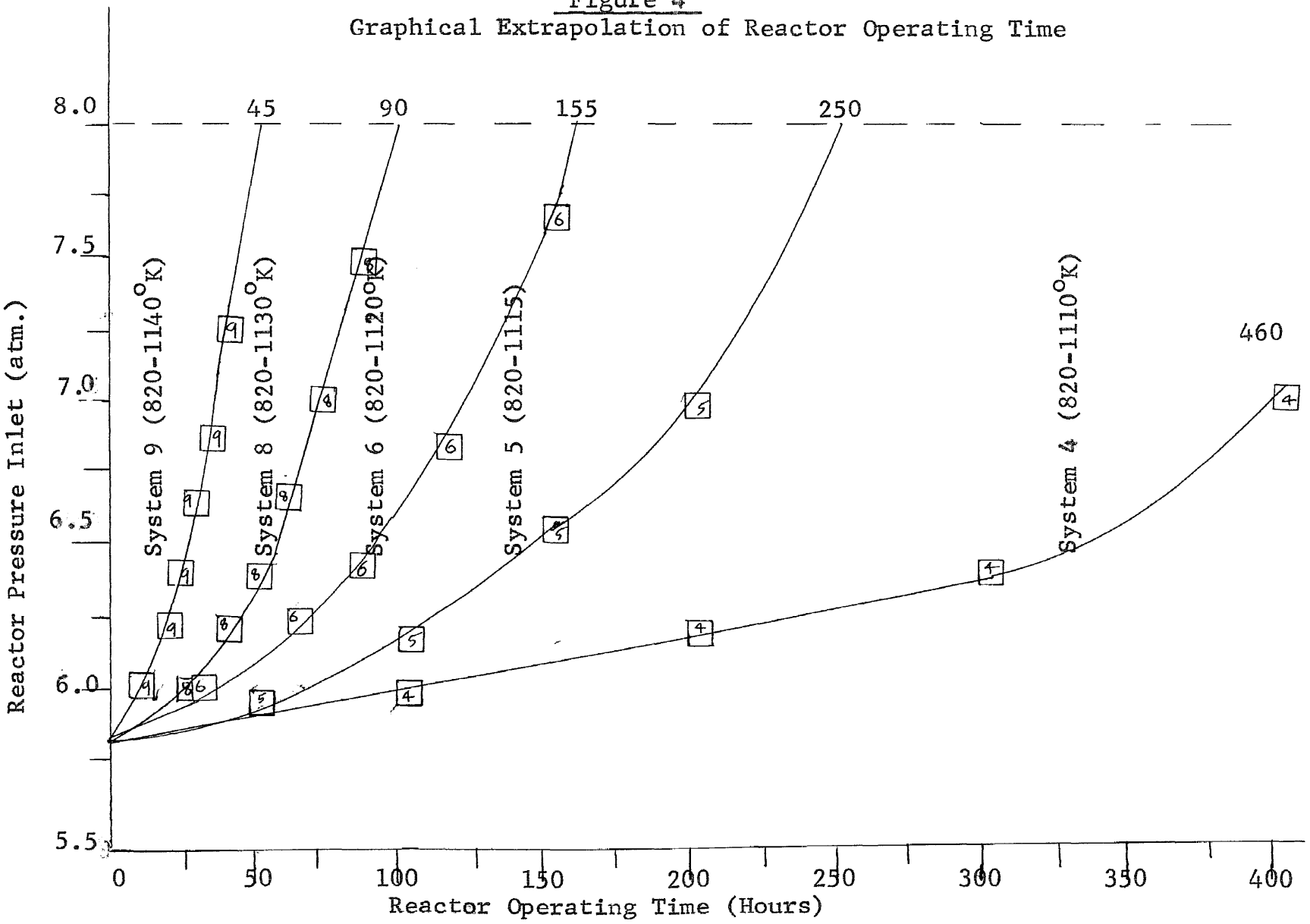


Table 9

Reactor Shut Down Time

Exit Temperature ^{o}K	Reactor Shut Down Time Hours	System Number
1050	(83,100)#	1
1090	2900	2
1100	1125	3
1110	460	4
1115	250	5
1120	155	6
1130	90	8
1140	45	9

#Estimated from regressed curve fit

Plotting the results from the reactor shut down time against reactor exit temperature resulted in a straight line on semi log paper (See Figure 5).

To find a scheme which would optimize the average yearly production rate it was decided to assume two different periods of time required to clean the tubes. An optimum production rate was then calculated for each of these penalty times. The two times chosen were 24 hours and 48 hours.

The average yield for the entire run from start up to shut down was then determined.

$$PAV = \sum_{i=1}^{n} ((\text{percent yield})_i)/n \qquad (57)$$

where $(\text{percent yield})_i$ is the yield for one increment of carbon deposition

n is the number of increments required to raise the inlet pressure to 8 atmospheres.

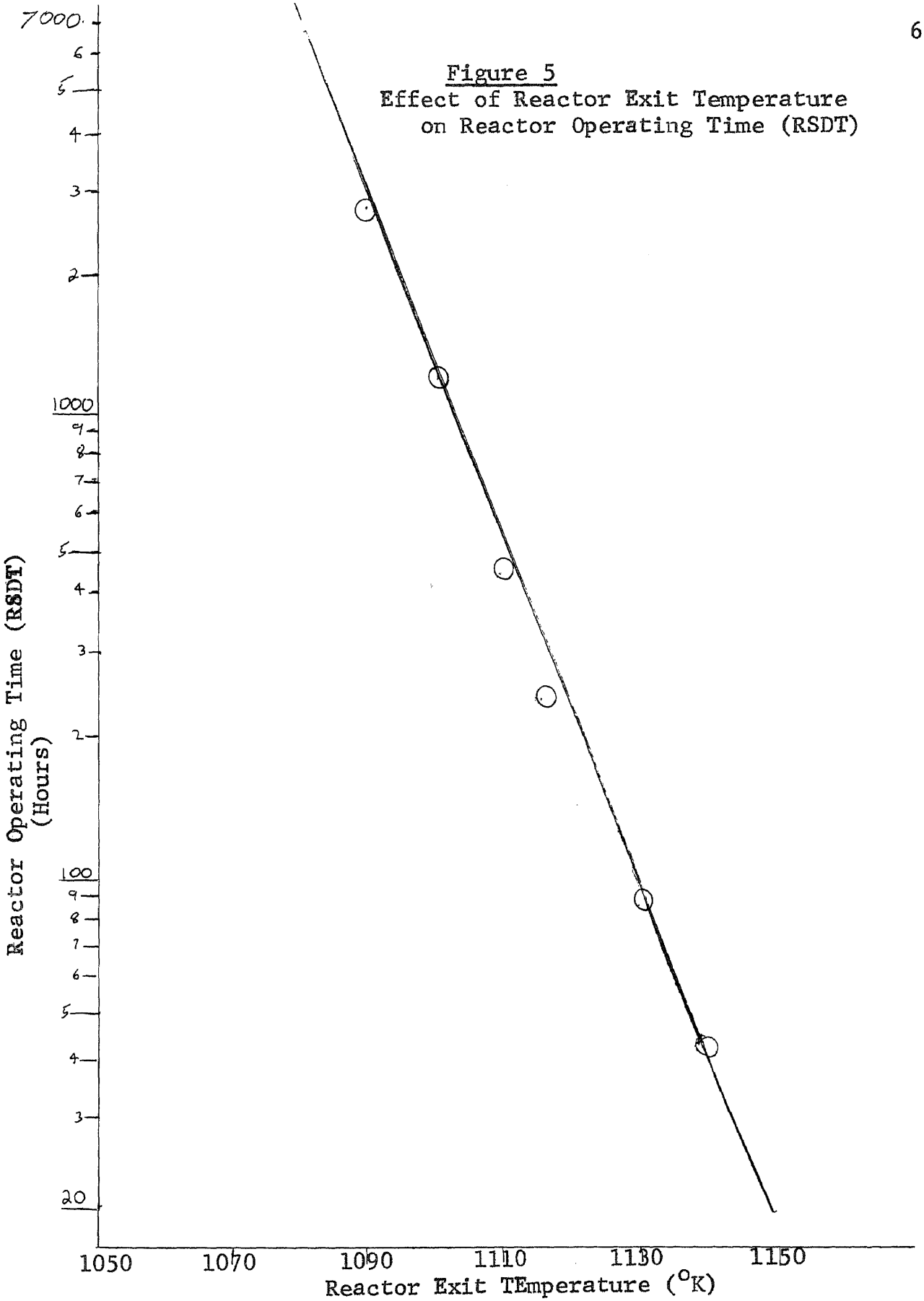
The average yearly production rate (AYPR) becomes

$$AYPR=PAV\left(1 - \frac{P}{RSDT+P}\right) \qquad (58)$$

where P is the assessed penalty for cleaning the reactor, hours.

$RSDT$ is the time the reactor operated between start up and shut down, hours.

Figure 5
Effect of Reactor Exit Temperature
on Reactor Operating Time (RSDT)



The pressure profile presented in Appendix G followed the normal expected results. Since the main reactions increased the number of moles in the reactor, an increase in pressure was expected. This was balanced by the Bernouli pressure drop.

In addition there was a contraction in the reactor walls due to the build-up of carbon which also effects the pressure drop. The pressure at first started to drop off slowly but as the velocity of the gas mixture picked up (due to pressure drop, increasing temperature and increasing number of moles) the pressure drop became much more severe. As a result, the majority of the pressure drop occurred at the end of the reactor.

Under the most severe operating conditions (System 9, 820-1140°K) and after appreciable carbon build-up, there was actually an increase in the pressure in the initial portion of the reactor. Appendix G (System 9, 820-1140°K) at 40 and 45 hours of run time shows this effect most graphically.

In addition the pressure drop at the end of the reactor became so severe that the calculated velocity exceeded the speed of sound. Since this was impossible, the equations being used were no longer applicable under these conditions. To prevent invalid results the program

checked for this limiting case and if found, increased the inlet pressure until the outlet velocity was less than that of sound.

The model also found that the pressure near the end of the reactor went through a critical pressure due to changing reactor radius and that the pressure was not able to fall below this critical pressure without destroying the validity of the equations. When this critical pressure was above desired outlet pressure, it was no longer possible to force a pressure convergence. Since the reacting gases were quenched at the end of the reactor and the pressure was dropped by allowing expansion into a larger container, this effect caused no unreliability and was a predictable result.(25)

Equilibrium

Since the production of ethylene was endothermic, it was expected that the equilibrium would be shifted in favor of product formation with increasing temperature. The equilibrium however was unfavorably affected by high pressure, and product formation was more favorable for lower pressure profiles.

These combined effects were ideally suited to the ethylene reaction because the temperature profile was increasing and the pressure profile was decreasing near

the end of the reactor. The rate of reaction also increased with increasing temperature.

These combined effects resulted in little reaction at the beginning of the reactor, which acted primarily as a preheater section, but near the middle the reaction rate rose sharply. At the extreme end of the reactor the components were near equilibrium as the rate of production of ethylene declines despite the increasing temperature and decreasing pressure.

Temperature

It was necessary to determine whether or not the temperature on the outside of the reactor pipe would melt the reactor tube. In order to determine this, the reaction conditions for the most severe case and at the highest heat flux and maximum carbon deposition were determined. The details of these calculations are given in Appendix I. It was determined that at carbon deposition twice the maximum thickness calculated before reactor shut down, there was a 347°K temperature increase from the temperature of the gas stream to that of the outside tube. This resulted in a skin temperature of 1,467°K. This temperature was still inside the safe operating temperature of 23 or 25% Cr, 70% Ni and 55% Fe steel [19] listed as 2,200°F or

or 1,478°K, although twice the maximum expected amount of carbon was deposited.

Model Verification

The verification of a model with actual plant results was an essential step in justification of simulation results. Exact matching of results was very difficult.

In this case there were not plant data to verify the results, but the results were compared with a second model[47] in work done by Shah. Both authors used the same kinetic data and the temperature profiles in this study were derived from Shah's.

Shah adjusted the original kinetic data to conform with actual plant condiyions. In this study, this refinement in data was not possible. In addition, Shah did not state his reactor diameter. Therefore there was some discrepancy between Shah's results and those herein contained.

A comparison of Shah's results and the author's is given in Table 10. If the author had actual plant conditions it would be relatively easy to adjust the Arrhenius Frequency Factor to conform with the actual results (See Program Logic - Data Input). Shah did not state what his outlet gas pressure was for his model.

Table10 clearly illustrates that there was a discrepancy in the product yields with temperature profiles between Shah's case and this study. The important thing is that the commercially acceptable yield (between 40 - 50%) on both the main and side reaction profiles agree for both studies. No explanation was given for the discrepancy in the exit temperature required to achieve these profiles.. Only comparison with actual plant data could justify either result.

Since the carbon deposits only at the end of the reactor (about the last 25%) it would be possible to make this last section replaceable by the use of a second parallel pipe with appropriate valves. An alternate scheme would be to increase the radius of the last section of the reactor. See Appendix G - Program Output.

Table 10

Comparison of Shah's Results with this Study

	Shah	System - 1 820-1050°K	System - 5 820-1115°K
Total Feed Lb Moles/Hr	170.9	200	200
Steam to Feed Ratio	.363	.350	.350
Inlet Pressure (At.)	4.43	5.85	5.85
Outlet Pressure (At.)	?	2.00	2.00
Reactor Length (Ft.)	394.	400.	400.
Tube Radius (Ft.)	?	.125	.125
Gas Inlet Temperature °K	818.3	820.0	820.0
% Ethylene Yield	45.83%	6.5%	47.9%
$\frac{\text{Moles Methane}}{\text{Moles Ethane Changed}}$	.0177	.00302	.0146
$\frac{\text{Moles Acetylene}}{\text{Moles Ethane Changed}}$	.00053	.00001183	.000589

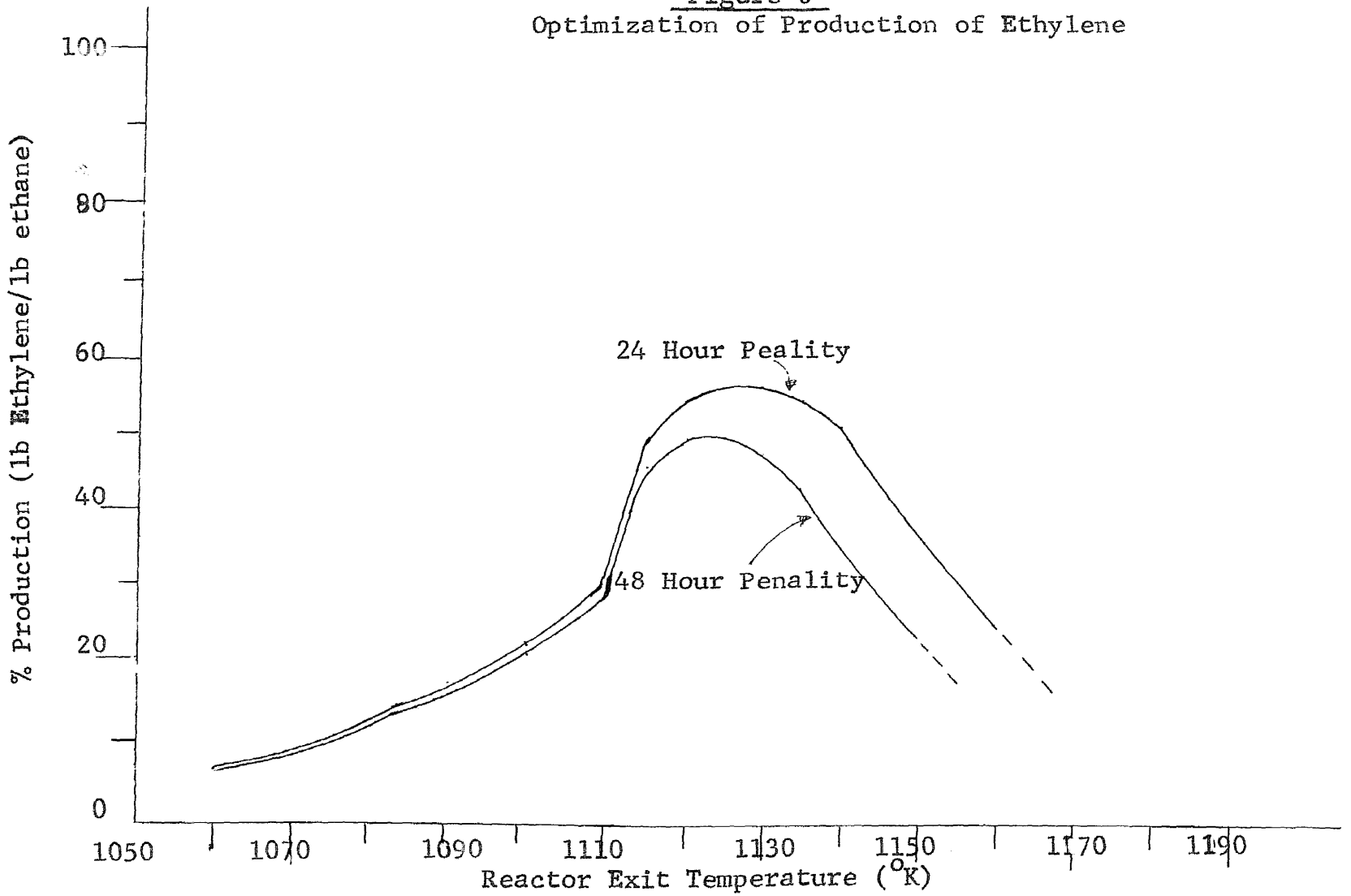
Figure 6 depicts the final graphical optimization of the ethylene reactor. The percent yearly production of ethylene versus reactor exit temperature is depicted. The percent yearly production of ethylene was defined as the ratio of pound moles of ethylene being produced in one year to the pound moles of ethane continuously available for the reactor.

It is important to note that the optimization is being performed on the production of ethylene and not on the overall conversion of ethane to ethylene.

The two parameters being used were a 24 and a 48 hour penalty required to close down the reactor, clean the reactor out, and start up the reactor. It was apparent from Figure 6 that the amount of time required to perform these cleaning operations materially affects the overall yearly production by as much as 7 percent when operating near the optimum. The optimum reaction exit temperature also showed a $3^{o}K$ change due to the different penalty times.

The optimum yearly production rate was relatively flat and allowed a 10 to $15^{o}K$ range of outlet temperatures without materially affecting the overall yearly production rate.

Figure 6
Optimization of Production of Ethylene



Chapter 5

Conclusions

1. Yield

The optimum yearly average of 59 percent conversion of the available ethane to ethylene can be achieved with an outlet temperature of 1127^{o}K.

2. Carbon Deposition

A. The rate of carbon deposition increases with increasing inlet reactor pressure.

B. The practice of increasing inlet reactor pressure to compensate for carbon build-up is detrimental to optimization.

3. Reactor Operating Time

The length of time the reactor could be operated before being shut (RSDT) down for cleaning can be calculated from the following relationship:

$$RSDT = -\exp(TEMP - 1181.4)/11.6 \qquad (59)$$

where RSDT was the reactor run time , Hours.

TEMP was the reactor outlet temperature , ^{o}K

4. Calculation of different feeds could be started to enable optimization of all feed streams which will be

reacted separately. These other feeds may contain propane and butane or combinations of all three.

5. By increasing the reactor residence time, by decreasing feed rates, increasing reactor length and/or reactor radius, this program could be used to calculate the optimum production of acetylene.

6. Since PYRO is completely general and made with provision for easy change in calculating procedures, it could be used for calculation of any gas phase reaction in a plug flow reactor.

7. PYRO is also able to handle any component which settles out as either a liquid or a solid and could therefore be used under conditions near the boiling or sublimation point of one or more of the reactants or products.

8. PYRO is able to make adjustments in the Arrhenius Probability Factor. This makes it suitable in fitting known product distribution and could be used in conjunction with SNOWJO (See Appendix B) to automatically calculate the best factors.

Chapter 6

Recommendations

1. The program PYRO uses fixed temperature profiles. It would be possible to add an energy balance and calculate the gas temperature from the temperature on the skin of the reactor. The skin temperature could either have a fixed temperature profile or be calculated from first principles using the geometry of the furnace and position of the burners, solving the resulting 3 dimensional heat transfer equation.

The calculation of the reactor gas temperature from reactor skin temperature would be more meaningful due to the effect of carbon deposition on the overall heat transfer coefficient.

2. In this study only one feed rate was considered. The production of ethylene could be further optimized by varying the feed rate and finding an optimum of the locus of feed rates.

3. Variation of the amount of steam mixed with the feed should also result in still better optimum. It might even be necessary to increase the steam rate as the carbon deposition necessitates increase in pressure, thus making it possible to keep the same rate of feed of ethane but to increase the proportion of steam to increase the overall pressure.

References

[1]Amano, A. and Uchiyama, M., Journal of Physical Chemistry. Vol. 68, No. 5, 1964, pp. 1133-1137.

[2]Andrews, A. J. and Pollock, L. W., "Tube by Tube Design of Light Hydrocarbon and Cracking Furnaces Using the Digital Computer", Industrial and Engineering Chemistry. Vol. 51, No. 2, Feb., 1959, pp. 125-128.

[3]Aris, R., Introduction to the Analysis of Chemical Reactors. Prentice-Hall, Inc., 1965, pp. 259-313.

[4]Bird, Steward and Lightfoot, Transport Phenomenon. John Wiley & Sons, 1960 p. 23.

[5]Bird, Steward and Lightfoot, Transport Phenomenon. John Wiley & Sons, 1960, p. 746.

[6]Bird, Steward and Lightfoot, Transport Phenomenon. John Wiley & Sons, 1960, p. 257.

[7]Bird, Steward and Lightfoot, Transport Phenomenon. John Wiley & Sons, 1960, pp. 744-745.

[8]Bonner and Honeycutt, "The Use of the Digital Computer in Petroleum Refining", Advanced Petroleum Chemical Refining. Vol. 5, 1962, pp. 83-114.

[9]Buckley, J. W. A., Edge, R. F. and Thompson, B. H., British Patent #1,122,426 (CL-B-01j), Aug. 7, 1968.

[10]Buddenbury, J. W. and Wilke, C. R., Industrial and Engineering Chemistry. Vol. 41, 1947, pp. 1345-1347.

[11]Burk, R. E., Laskowski, Lenoa and Lankelma, H. P., Journal of the American Chemical Society. Vol. 63, 1941, pp. 48-50.

[12]Butovskii, V.A., Feigin, E. A., Girsanov, I. V. and Platonov, V. M., "Mathematical Model of the Pyrolysis Process in Furnaces", Khim. i Tekhnol. Topliv. i Masel 10 (10), 1965, pp. 1-5.

[13]Cahn, R. P., Kevlin, J. A. and Thurlow, D. K., U.S. Patent #3,365,387 (CL 208-48), Jan. 23, 1968.

[14]Chukanov, Z. F. and Kobzev, Y. N., High Speed Thermo Decomposition of Gaseous and Vaporous Hydrocarbons. U.S.S.R. #197,064 (C1.C10g) May 31, 1967.

[15]Esso Research and Engineering, Unsaturated Hydrocarbon Furnaces. U.S. Patent #1,497,055 (C1.C07) Oct. 6, 1967.

[16]Faust et al., Principles of Unit Operations. Corrected Second Edition. John Wiley & Sons, pp. 157, 158.

[17]Feigin, E. A. et al., "Method for the Optimum Design of the Coil in the Pyrolysis Furnace", Klim. Prom. Vol. 5, July, 1963, pp. 19-26.

[18]Frey, F. E. and Hepp, H. J., The Science of Petroleum. Oxford University Press, 1964, p. 1994.

[19]Guy, A.G., Elements of Physical Metallurgy. Second Edition. Addison & Wesley, 1960, p. 386.

[20]Heicklen, J., Hudson, J. L., and Arma, L., "Theory of Carbon Formation in Vapor Phase Pyrolysis - Variable Concentration of Active Species", Carbon Vol. 7 No. 3, 1969, pp. 365-372.

[21]Hennig, H., U.S. Patent #2,885,455, May 5, 1959.

[22]Himmelblau, Basic Principles and Calculations of Chemical Engineering. Prentice Hall.

[23]Homogeneous Reaction Kinetics Pyrolysis of Aliphatic Hydrocarbons. National Bureau of Standards, National Research Council, pp. 507-517.

[24]Kevorkian, V., "High Temperature Chemistry of Light Hydrocarbons", Advanced Petroleum Chemical Refining. Vol. 5, 1962, pp. 369-438.

[25]Lapple, C. E., Fluid and Particle Mechanics. University of Delaware, March, 1966, pp. 51-58.

[26]Lavrov, N. V. and Baklistskii, E. P., "Calculation of the Composition of the Equilibrium Mixture Obtained by the Oxidation Pyrolysis of Hydrocarbons", Dokl. Akad. Nank U.S.S.R. 20(C), 1963, pp. 16-20.

[27]Levenspiel, Chemical Reaction Engineering. John Wiley & Sons, p. 116.

[28]Levenspiel, Chemical Reaction Engineering. John Wiley & Sons, p. 113.

[29]Lichenstein, I., "Design Cracking Furnace by Computer", Chemical Engineering Progress. Vol. 60, No. 12, Dec., 1964, p. 64.

[30]Lichenstein, I. "Design Cracking Furnace by Computer", Chemical Engineering Progress. Vol. 60, No. 12, Dec., 1964, pp. 64-68.

[31]Lindahl, A., "Improved Operation with Process Simulation", Chemical Engineering Progress. Vol. 61, No. 4, 1965, pp. 77-81.

[32]Lindsay, H. F. and Wulzen, R., "Refinery Studies by Digital Computer", World Petroleum Congress, Proc. 5th N.Y. 1959 #3,251-60, 1960.

[33]Lobo, W. W. et al. Transactions of the A.I.Ch.E., Vol. 31, 1939, p. 743.

[34]Mamedov, A. M. Pogorelskii, A. M. and Alizade, N. A., Tubular Furnace. U.S.S.R. Patent #190,867 (CL.B01j) Jan. 14, 1967.

[35]McCabe and Smith, Unit Operations of Chemical Engineering. Second Edition, McGraw-Hill, p. 77.

[36]Myers, P. S. and Watson, K. M., Principles of Reactor Design. Article No. 2 "Pyrolysis of Propane, National Petroleum News" Vol. 38, No. 18, May 1, 1946, pp. 9388-R442.

[37]Noguchi, T., Suzuki, J. and Seki, M. Computer Control of Petroleum Refining, Sekiyu Gakkai, Shi 1969 12 (2) Japan pp. 107-112.

[38]Oliver, G. D. Removal of Coke from a Thermal Cracker by Intermittent Switch to Ethane Feed. U.S. 3,433,731 (LL 208-48;C10g) March 18, 1969.

[39]Palmer, H.B., "Kinetics and Mechanism of Carbon Deposition During Gaseous Pyrolysis", Fuel Society Journal 1962

pp. 13, 7 - 18.

[40]"Pyrolysis of Ethane in a Tubular Reactor", Example Problem No. 116, Symposium University of Wisconsin, Katz, Editor. Use of Computers in Chemical Engineering. pp. 140-144.

[41]Rosendahl, Fritz. Chim and Ind. Paris, 1960 No. 84, pp. 357-374.

[42]Rosier, G. O. and Watson K. M. National Petroleum News, Technical Section, No. 38, April 3, 1946, p. 260.

[43]Selected Values of Chemical Thermodynamic Properties. National Bureau of Standards, March 31, 1947, Series III Table 23.

[44]Selected Values of Chemical Thermodynamic Properties. National Bureau of Standards, June 30, 1946.

[45]Schneider, U. and Frolich, P. K., Industrial and Engineering Chemistry, No. 23, 1931, p. 1405.

[46]Shah, J. Manesh, "An Approach to Model Simplification in Process of Optimization and Control", American Institute of Chemical Engineering - I Chemical Engineering Symposium No. 4, 1965, pp. 4:47-4:52.

[47]Shah, J. Manesh, "Computer Control of Ethylene Production," Industrial and Engineering Chemistry, Vol. 59, No. 5, 1967, pp. 70-87.

[48]Shah, J. Manesh, "Computer Control of Ethylene Production," Industrial and Engineering Chemistry, Vol. 59, No.5, 1967, pp. 74.

[49] Smith and Van Ness, Introduction to Chemical Engineering and Thermodynamics. McGraw-Hill, pp. 410-412.

[50]Smolen, H., "Heating High Severity Pyrolysis Furnaces and Steam Reformers with Gas or Heavy Oil" Erdoel, Kohle, Erdgas, Petrochem 1969, 22(9) (Ger.) pp. 557-561.

[51]Spectra 70 Fortran IV Reference Manual. Radio Corporation of America, Nov. 1967.

[52]Stepanov, A., "Heat Transfer in a Tubular Pyrolysis Reactor", Konvektivryi - Teploobmen 1968 pp. 133-138.

[53]Stepanov, A. A., Stepanova, A. V. and Kostyuk, "Pyrolysis and Gas Compression in a High Pressure Reactor," Neft. i Gaz. Prom. Inform, Mauchn-Tekkn, Sb. 1964 (3) Russian, pp. 56 - 58.

[54]Stepanova, A. V. and Stepanov, A. A., "J-T Diagrams of the Pyrolysis of Ethane and Propane", Khim. i Tekhnol. Topliv i Masel 9 (6), 1964, pp. 10 - 14.

[55]Steacie, E. W. R. et al., Canadian Journal of Research, Vol. 16B 1938, pp. 176, 360, 303, 411.

[56]Swinbourne, E. S., Journal of the Chemical Society, 1960, pp. 231, 232.

[57]Szepesy, F. S. and Simon, P., "The Use of Gas Chromatography in Gas Analysis", Magyar-Kim Folyirat 67, 1961 pp. 27-33.

[58]Tamai, Y., Nishiyama, Y. and Takahashi, "Effects of Solid Substances of the Thermo Decomposition of Hydrocarbons - Effects of Wall on the Carbon Deposition from Methane" Kogyo-Kagaku Zassni 70 (6) 1967, Japan, pp. 889-891.

[59]Tayyabkhan, M. T., "Competitive Development in Computer Applications," Petro/Chem Engineering 38(10) Vol. 58, 1966, pp. 54-56.

[60]Tmenov, D. N. and Mamedov, K. T., "Contract Pyrolysis of a Middle Straight Run Fraction of Petroleum in a Reactor with Rising Flow of Heat Carrier." Izv. Vyash. Ucheb. Zaved., Neft Gaz 15(5), 1969, (Russian) pp. 49-53.

[61]Towell, D. Gordon and Martin, J. Joseph, "Kinetic Data from Nonisothermal Experiments: Thermal Decomposition of Ethane, Ethylene and Acetylene," A.I.Ch.E. Journal, Vol. 7, No. 4, Dec. 1961, pp. 693-698.

[62]Tucker, W., "Conical Joint Between Hydrocarbon Cracking Zone Outlet and Heat Exchange to Minimize Coking," Fr. 1,522.883 (CL.C10g) April 26, 1968.

[63]Vasil'ev, S. F. and Lapides, N. A., "The Oxidative Pyrolysys of N-Butane in Industrial Conditions," Khim. i Tekhnol. Smol Tern, Erabotki Tuerd. Topliv, Akad. Nauk S.S.S.R., Inst. Goryuch. Iskop, 1965 (Russian) pp. 36-56.

[64]Vasil'ev, S. F., Lapides, N. A., and Mosiv, A. M., "Oxidative Pyrolysis," Sintez i Svoistvs, Monomerov Akad. Nauk S.S.S.R. Inst. Neftekhim Sinteza, Sb. Rabot 120i (Dvenadtsatoi) Konf. Po. Vystokomolikuul Soldin, 1962 (Pub. 1964) (Russ.) pp. 12, 13.

[65]Walker, H. M., "Advances in Heavy Liquid Cracking," Chemical Engineering Progress, 1969, 65(8), pp. 53-58.

[66]Wilke, C. R., Journal of Chemical Physics, Volume 18, 1950, pp. 517-554.

Table of Contents for the Appendix

Appendix A

Program Logic and Theory

PYRO consists of four functions and one main program. The main program calls the functions in order to perform certain specific operations. It was found to be more convenient to separate the functions in this manner as it makes the functions more accessible to debugging without unintentionally destroying the logic of the main program. This makes it considerably easier for a later user to make changes in functions without having to understand every nuance of the main program.(51)

The four functions are:

1. Cards 1 - 30 PRR(IS) This is a function designed to calculate the carbon profile along the reactor wall. It is capable of handling up to 25 solid components being thus deposited. It also readjusts the partial pressure of all the components to account for the change of solid to gaseous state (i.e. carbon (g) to carbon (s). The computer first treats the carbon as though it were a gas and PRR removes the gas and treats it as a solid. It is necessary to readjust all the partial pressures so as to make the sum of the pressures equal to the sum of the pressures when each component was considered to be a gas.

2. Cards 31 - 44 REQC(T,I) This is a function designed to calculate the reciprocal of the equilibrium constant at temperature R for Reaction I.

All equations are assumed to be reversible. The reverse rate constants will be calculated from equilibrium data developed from the equation [49]

$$\Delta F = -Rt * LN(K) \quad (1)$$

or $$K = \exp(-\Delta F^{o}/RT) \quad (2)$$

using the relationship that

$$K_c = K_f/K_r \quad \text{or} \quad K_r = K_f/K_c \quad (3)$$

where $$\Delta F = H - T\Delta S \quad (4)$$

$$\Delta F = -\Delta H_o(I)/RT + \Delta A(I)/R * LN(T) + \Delta B(I)/2R * T +$$

$$\Delta C(I)/6R * T^2 + \Delta D(I)/12R * T^3 + FI(I) \quad (5)$$

where FI(I) is a constant of integration evaluated from a known equilibrium constant at a known temperature and using the above equation to solve for FI(I).

The equilibrium constant for a known temperature calculated from $Log_{10}(K_f)$ data taken from Selected Values of Chemical Thermodynamic Properties. [44]

The Log (K_f) for reaction is calculated below:

$$\text{Log}_{10}(K_f)_{\text{Reaction}} = \sum_{\text{Products}} B(K)/B(1) * \text{Log}_{10}(K_{f_K}) -$$

$$\sum_{\text{Reactants}} B(K)/B(1) * \text{Log}_{10}(K_{f_K}) \qquad (6)$$

3. Cards 45 - 150 PRESD(T) This function calculates the pressure drop in the segment of the reactor under consideration. It is subdivided into (a) calculation of viscosity (b) calculation of friction factor (c) calculation of pressure drop.

(a) Cards 45 - 74 Calculation of Viscosity

The viscosity of the solution is determined by calculating the viscosity of each component as though it were a pure component from the equation

$$\mu(I) = 2.6693 * 10^{-5} \sqrt{MT/\sigma^2}\,\Omega_\mu \qquad (7)$$

where μ is the viscosity of the component in grams per centimeter per second raised to the -1 power.

T is the temperature in degrees Kelvin (^{o}K).

σ is the collision parameter in Angstrom units ($\mathring{A}$).

Ω_μ is a slowly varying function of the dimensionless temperature KT/ε .

Since the function is only given in tabular form, the author decided to curve fit it using a Marquardt non-linear curve fitting subroutine. (See Appendix B). This results

in the following equation.[4]

$$\Omega_v = \exp(.4398828 - .44245917\ LN\ (KT/\varepsilon) + 0.08640182\ LN^2\ (KT/\varepsilon) - 0.0077884511\ LN^3\ (KT/\varepsilon)) \quad (8)$$

The viscosity of the gas mixture was then calculated from the equation (66) (10)

$$U\ mix = \sqrt{8} \sum_{I=1}^{N} \frac{X(I)\,U(I)}{\sum_{J=1}^{N} \left(X(J) \left[1+\frac{U(I)}{U(J)}\right]^{\frac{1}{2}} \left[\frac{M(J)}{M(I)}\right]^{\frac{1}{4}} \right)^2 \Big/ \left[1+\frac{M(I)}{M(J)}\right]^{\frac{1}{2}}} \quad (9)$$

where X(I) is the mole fraction of component I

U(I) is the viscosity of component I

M(I) is the molevular weight of component I

Since it is determined that the viscosity is only a slowly changing function going from $2.17 * 10^{-5}$ to $2.76 * 10^{-5}$ lb/ft-sec between extreme reaction conditions (differences between inlet and outlet viscosity.) The viscosity is only calculated at intervals of every 1% of reactor distance. This was found to save considerable computer time, thus making the program more practical.)

(b) Cards 79-94 Calculation of Friction Factor

The friction factor is calculated from the correlations between friction factor and Reynold's number. For Reynold's

below 3000 the laminar flow relationship is used (16)

$$f = 64/N_{Re} \tag{10}$$

and for Reynold's number greater than 300 the relationship becomes

$$f = 0.00560 + .5/(N_{Re})^{.32} \tag{11}$$

The Reynold's number is recalculated from

$$N_{Re} = 2R*\rho*V/Vis \tag{12}$$

where R is the radius of the reactor = f(Z,τ)
i.e. R is a function of its position in the reactor and the length of time the reactor has been in operation. This function is calculated by the main program PYRO.

ρ is the density of the reacting medium = f(C(I) - C(IS), T,P(Z)) (13)

i.e. ρ is a function of the concentration of each component, the temperature of the reactor and the pressure of the reactor segment.

$$\rho = \sum_{I=1}^{IS} P(I)\ SMWT(I)/RT \tag{14}$$

where P is the partial pressure of component I (AT)
SMWT is the molecular weight of component I

R is the gas constant = 1.314. (AT ft^3/Lb mole °K)

T is the temperature of the reactor.(°K)

IS is the total number of components.

(c) Cards 95 - 135 Calculation of Pressure Drop

The pressure drop in the reactor is calculated from the Bernouli equation(35)

$$P = (VelA^2 * F * L/R + Vel2^2 - Vel\ 1^2) /(62.4*2116.8) \quad (15)$$

where P is the pressure drop in atmospheres

VelA is the average velocity in the reactor segment

f is the friction factor

L is the length of the reactor segment under consideration.(ft)

R is the radius of the reactor in feet (See (b) Calculation of Friction Factor)

Vel 2 is the velocity at the end of the reactor segment.

Vel 1 is the velocity at the beginning of the reactor segment.(FT/Sec)

62.4 is twice the gravity constant in foot pounds force per pound mass per second squared (Ft Lb_f/ Lb_m - Sec^2)

2116.8 is the conversion factor to convert from pound feet per square inches to atmospheres.

This function is calculated recurrently as the value of VA and V2 is dependent on the value of the pressure drop. The pressure drop is calculated until the difference between two successive calculations is less than .1%.

4. Cards 136 - 150 HEATR (T2,I)

This function calculates the heat of reaction at Temperature T2 and for Reaction I.

HEATR is calculated by

$$HEATR(T2,I)=HEATR(T1,I)+\int_{T_1}^{T_2} C_P(I)\,dT \qquad (16)$$

Cards 151 - 816 The main program (PYRO) is easily divisible into many subparts which facilitate comprehension of the program. In order to discuss the program, the author will cite the number on the extreme left of the print-out of the program.

Cards 151 - 171 These cards tell the computer how much storage space must be allotted for the different dimension variables. Some of the variables are used in the functions are are linked by named common statements. This makes the storage location for these variables identical for each program, subprogram or function in which they appear. The author has also preset certain variables at specified values and has defined some variables to be literal constants. This

is used in the output to help define the reaction equations and will help any future users in spotting errors in input.

Cards 172 - 261 These cards are used for input of data and initial calculations of constants which will be used by the program.

Input Set 1 Cards 172 - 174 These cards read in factors by which the Arrhenius frequency factor is changed. This allows for adjustment in rate of reaction in order to make the calculated and actual product rates agree.

Input Set 2 Card 175 This card reads in the number of reactions (IR) and the number of chemical species (IS) including inerts.

Input Set 3 Cards 177 - 179 These cards read in computer GO TO instruction IGOW.

IGOW = 1 means read in entirely new data set.

IGOW = 2 means read in new temperature profile only and begin calculations anew.

IGOW = 3 means stop (no more data).

Z(I) is the temperature profile of reactor from beginning to end in 10% increment of reactor length.

Card (I) is the alphanumeric identification of reaction system. (i.e. this card identifies the new temperature profile etc.)

IB, IZZ, IPLOT are three more computer control variables.

IB is the number of hours that constitutes an increment in carbon deposition. IZZ is the total number of increments before the computer goes on to a new case.

IPLOT controls the output from calculations.

IPLOT = 1 means	plot results	do not write out detailed calculation
IPLOT = 2 means	plot results	write out detailed calculation
IPLOT = 3 means	do not plot results	write out detailed calculation
IPLOT = 4 means	do not plot results	do not write out detailed calculation

Input Set 4 Cards 180 - 181

These cards initialize the reactor conditions.

T is the temperature at the inlet of the reactor (^{o}K)

PT is the pressure at the inlet of the reactor (atmospheres)

PRESS is the maximum allowable inlet pressure (atmospheres)

ZT is the total length of the reactor (feet)

DL is the initial reactor increment (feet)

POUT is the minimum outlet pressure (atmospheres)

Input Set 5 Cards 182 - 194 These cards set up reaction equations.

SF(I) and SR(I) are the number of components in the forward reaction and in the reverse direction of the Ith reaction (i.e. if Reaction 5 were $2H_2 + O_2 \rightarrow 2H_2O$) SF(5) = 2 (two components H_2 and O_2 in forward direction), SR(5) = 1 (one component H_2O in reverse direction).

IA(I,M) is the identity of chemical species in reaction I position M. (i.e. in the above example, if water were the second chemical species, hydrogen were the fifth and oxygen the tenth, then

IA(5,1)=5 IA(5,2)=10 IA(5,3)=2

Input Set 6 Cards 195 - 202 These cards read in the initial partial pressure (in atmospheres) of each component. The concentration of each component is then calculated using the ideal gas law C(I)=P(I)/GC/T

Input Set 7 Cards 203 - 205 These cards supply the alphanumeric identity of each component (limit - 20 characters to name). ENAME(20*I) I = 1, IS.

Note: The next four card sets have internal identification to make sure the cards are in proper sequence. This is called Check ID.

Input Set 8 Cards 206 - 208 These cards contain the heat capacity data for each component in the form

$$C_p(J)(\text{Cal/g mole } {}^{o}K)=CP(J,1)+CP(J,2)*T+CP(J,3)*T^2+CP(J,4)*T^3 \quad (17)$$

where C_p is the heat capacity for the J component in calories per gram moles degrees Kelvin (Cal/g mole ^{o}K). See Appendix (H) for methods of evaluating heat capacity.

Input Set 9 Cards 209 - 212 This data set contains the Arrhenius frequency factor EA(I) and activation energy EE(I) for the Ith reaction.

Input Set 10 Cards 213 - 215 This card set contains entropy DS(J), enthalpy DH(J) and $\log(K_F)$ for calculation of equilibrium for the J^{th} component.

Input Set 11 Cards 216 - 219 This data set contains CLJ(J,1), CLJ(J,2) constants of Lennard and Jones, the collision parameter in Angstroms ($\mathring{A}$) and K/ξ (K^{o-1}). If the component is a solid the constant of Lennard and Jones is set equal to zero and the density of the solid is read in as DE(J) Lbs/ft^3 of the J^{th} component.

Cards 220 - 261 These cards set up the remaining constants required for the program. These constants include delta heat capacity, heat of reaction, delta entropy and equilibrium data expressed as a function of temperature for each reaction.

Cards 220 - 233 These cards calculate the Δ CP of reaction by solving the equation

$$DC_P(I,L) = \sum_{M=SF(I)+1}^{SF(I)+SR(I)} C_P(IA(I,M),L)*B(I,M) - \sum_{M=1}^{SF(I)} C_P\ (IA(I,M,L)*$$

$$B(I,M) \qquad (18)$$

which is $\sum_{\text{Products}} C_P$ * (Coefficient) - $\sum_{\text{Reactants}} C_P$ *

(Coefficient)

Cards 234 - 261 The delta heat of reaction, delta Log(K_F) and the delta entropy for each of the reactions was calculated.

$$ST(I) = \sum_{\text{Products}} B(I,M)/B(I,1)\ DS(IA(J,M) - \sum_{\text{Reactants}} B(J,M)/$$

$$B(J,1) * DS(IA(J,M)) = \Delta S^{\circ} \qquad (19)$$

$$HT(I) = \sum_{\text{Products}} B(I,M)/B(I,1)\ DH(IA(J,M)) - \sum_{\text{Reactants}} B(I,M)/$$

$$B(I,1) * DH(IA(J,M)) = \Delta H^{\circ} \qquad (20)$$

$$FT(I) = \sum_{\text{Products}} B(I,M)/B(I,1)\ DF(IA(J,M)) - \sum_{\text{Reactants}} B(I,M)/$$

$$B(I,1) * DF(IA(J,M)) = \Delta \text{ Log}_{10}(K_F) \qquad (21)$$

Cards 262 - 331 This section of the program writes out the reaction system and helps the user to identify any error

he has made on the data input.

The first page of print-out includes the name of each component (a letter and a number computer assigned designation for each component), the heat capacity data for each component, the heat of formation (298°K), the entropy (298°K) and $\log_{10}(K_F)$ at temperature TT.

On the second part of the page the constants of Lennard and Jones, the molecular weight and the initial concentration of each component are written.

On the second page of print-out the reaction system is written in symbolic form with each component assigned a letter designation given on the first page. The Arrhenius frequency factor and activation energies are given. The delta heat capacity is listed.

On the second half of the second page the delta log (K_F) is given, as well as the constant of integration for calculation of the equilibrium constant. The order of reaction by component is listed.

Cards 340 - 422 This section contains all the format statements used in PYRO. It controls the input and output of of all data used and generated by PYRO.

Cards 332 - 339 and 423 - 578 This section is the heart of the program. It is this section in which the actual

calculations of the changing composition and pressure profile takes place.

Card 332 Statement 110 is the card which the computer uses every time it starts a new set of calculations.

Cards 333 - 339 and Cards 423 - 458 The cards initialize values used in the program as computer controls. This section resets values which may have been changed during previous runs, such as the reactor radius profile.

Card 436 This card is used as partial reinitializer in that not all values are reset. It is used in repeat calculations where one or more criterion were not met during the calculation of the reactor profile.

These criteria include:

A. Pressure

1. Maximum pressure at inlet = PRES
2. Pressure at outlet
   a. POUT $\pm$ .2 (atmospheres) and velocity of reactor medium less than the speed of sound.

or

   b. Greater than (POUT $\pm$ .1) atmosphere and velocity of reactor medium less than velocity of sound.

B. Carbon Profile

1. Carbon blocking tube

2. Total number of carbon increments exceeded
3. Convergence on desired outlet pressure not obtainable within 20 complete sets of reactor design.

C. Reaction is so slow that all increments of conversion are less than 10^{-76}.

Cards 453 - 454 These cards set up the number of increments calculated between complete print-out of data.

Card 458 This card sets up initial reactor length increment.

Cards 459 - 460 These cards are the controlling DO loops which allow increments of calculations. Control is returned to these DO loops after each complete calculation is completed.

Card 461 This card calculates the incremental length of convergence.

Card 463 This card calculates the position in the reactor.

Cards 464 - 468 These cards calculate the temperature in the reactor.

Cards 469 - 474 These cards calculate the reactor radius from the previous completed carbon profile. The radius is assumed to be smooth. Since the reactor radius is only defined at 101 points the radius in between these points is

calculated by interpolation between the two closest known reactor positions.

Cards 477 - 510 These cards calculate each individual increment of conversion DXA(I) for each equation (I=I,IR). The calculation of DXA(I) is derived from [27]

$$\tau = \frac{1}{S} = C_{A_0} \int_{X_1}^{X_2} dX_A/-r_A \qquad (22)$$

This equation is solved for the increment of conversion by differentiating with respect to X_A.

$$\frac{d\tau}{dX_A} = \frac{C_{A_0}}{(-r_A)} \qquad (23)$$

This equation is then solved for dX_A

$$dX_A = (-r_A)d\tau/C_{A_0} \qquad (24)$$

The following is obtained by considering finite differences:

$$\Delta X_A = (-r_A)\,\Delta\tau/C_{A_0} \qquad (25)$$

Equation (25) will be used to solve for finite difference along the reactor profile. Equation (25) is really the expression for conversion in a back mix reactor. This means the solution is really the solution of a large number of back mix reactors. (i.e.)

$$\Delta X_A \text{ (TOTAL)} = \Sigma(\Delta X_A)_i \qquad (26)$$

By evaluating the reaction conditions at hundreds of positions along the reactor, a good approximation of the total reactor profile can be arrived at. By restricting Max $(X_A)_i$ to be less than or equal to .01 (and on the average equal to .005 and with a minimum value of .001) the above approximations will be good. Also by using these small increments of conversion we can approximate

$$\varepsilon A = \frac{V_F - V_I}{V_I} = 0 \quad \text{because } V_F \cong V_I \qquad (27)$$

where εA is the volume function of expansion.

V_F is the final volume.

V_I is the initial volume

The value of DX_A is controlled by controlling the value of

τ (=1/space time (sec.)). (28)

$$\tau = \frac{C_{A_0} V}{F_{A_0}} \qquad (28)$$

where C_{A_0} is the original concentration of component A (lb mole/ft^3)

V is the reactor volume in cubic feet

F_{A_0} is the molar flow rate of component A (lb mole/ time)

$$V = \pi R^2 L$$

$$\Delta\tau = \frac{C_{A_0}\Delta V}{F_{A_0}} = \pi R^2 \frac{C_{A_0}\Delta L}{F_{A_0}} \qquad (29)$$

by combining equations (25) and (29) the following is obtained:

$$\Delta X_A = C_{A_0} (-r_A) = \pi R^2/F_{A_0} (-r_A) \Delta L \qquad (30)$$

thus the value of XA can be controlled by the length (Δ L). The procedure to control the value of DXA is to calculate DXA for each reaction and test whether it is larger than .01. If it fails the test a new value of DXA is to calculate DXA for each reaction and test whether it is larger than .01. If it fails the test a new value of ΔL is calculated from the equation:

$$DL = ABS(DL*.005)/DXA(I)) \qquad (31)$$

The max of ABS(DXA) is found and compared with .001. If the test fails, a new DL is calculated from equation (31).

In both cases the control of the program is returned to

the initiation of the reactor design.

If all rates pass both tests then calculation of new reactor conditions is continued.

In order to calculate DXA(I) the following must first be calculated:

$$R^2/F_{A_O}\Delta L \quad \text{and} \quad (-r_A)$$

$$(-r_A) = K_o e^{-E^*/RT} \left(C_{F_I}^{n_{f_i}} - KT\, C_{R_i}^{N_{R_i}} \right) = K_o e^{-E^*/RT}(CF-CR) \tag{32}$$

where

$(-r_A)$ is the rate of the reaction (calculated by Card 493) Lb Moles/ft^3 sec

K_o is the Arrhenius frequency factor

E^* is the Arrhenius energy of activation (cal/g.mole)

R is the gas constant (btu/lb.mole ^oF)

T is the temperature in absolute units (^oF)

C_{F_I} is the concentration of the reactants (lb.mole/ft^3)

C_{R_I} is the concentration of the products (lb.mole/ft^3)

M_{F_I} is the order of the I^{th} forward reactant

M_{R_I} is the order of the I^{th} reverse reactant

$CF=\tilde{\prod}_{I=1} C_{F_I}^{M_{F_I}}$ (Calculated by cards 481 - 485)

$$CR = \prod_{I=1}^{M} R_I \qquad \text{(Calculated by cards 486 - 492)}$$

Since each new reactor segment is considered to be the start of a perfect back mix reactor, F_{A_0} has to be recalculated each time. This calculation is done by a material balance performed later on in the program. The results from the previous material balance are available in the present calculation.

Card 495 This card shows the calculation for DXA(I) the factor 1.13093355E4 comes from the combining of and the conversion factor converting $(-r_A)$ from sec. to hours.

(i.e. 1.13097355E4 = π * 3600)

Cards 512 - 564 These cards calculate the material balance, the pressure drop, the carbon profile and set up the intermediate values which will be saved for output.

Card 513 This card calls the function PRR(IS) which carries with it information on the amount of carbon formed. PRR(IS) then converts this to an equivalent amount of solid carbon which is deposited evenly over a 1% length of reactor segment. PRR then readjusts all other partial pressures so that their sum is equal to the pressure before carbon deposi-

Cards 514 - 535 These cards calculate the material

balance. This calculation is accomplished by summing the increment of conversion (in terms of concentration and pressure) along the reactor segment. This total change in concentration is used to calculate a molar flow rate.

$$TMPH = TMPH(1+\Delta TMPH) \quad \text{when}$$

$$\Delta TMPH = \Delta C * GC * T/P \qquad (32)$$

ΔC is the total change in concentration (lb m/ft^3)

GC is the gas constant $\left(\frac{\text{At. ft}^3}{\text{Lb mole } {}^{o}\text{K}}\right)$

Card 536 This card calculates the pressure drop by calling the function PRESD(T). While the pressure drop is being calculated it also calculates the new partial pressure and concentration of each component.

During the calculations several posibilities occur which must be detected and the appropriate action taken.

Cards 538 - 540 If pressure drop sets the value of MB equal to

Value of MB	Condition	Correction
2000	RENU less than 0 (due to estimated pressure below 0 atmospheres)	Start reactor design again with a higher pressure.

Value of MB	Condition	Correction
3000	Velocity of gas greater than sound	Start reactor design again with a higher pressure
5000	Reactor tube blocked with carbon	Terminate calculation on this data set. Start new temperature profile.

Card 541 If the pressure falls .2 atmospheres below the minimum pressure in the reactor exit (2 atmospheres), the reactor design is started again with a higher pressure.

Cards 542 - 543 These cards calculate the molar flow rate of each component.

Cards 544 - 553 These cards test to see that at least one conversion was greater than the minimum conversion of .1% (otherwise the reactor design will take up unnecessary computer time). Note there is a maximum length of conversion which corresponds to 1% of the reactor length.

Cards 554 - 564 These cards are used to output initial values of concentrated molar flow rates and conversion along the first increment of reactor length.

Cards 565 - 578 These cards are executed only after

every 8 increments of conversion. They are used to prepare data for output after the reactor is totally designed. Control is returned to beginning of DO loop.

Cards 579 - 813 This section of PYRO controls output and is used to converge the pressure so that it falls between the limits set up by the user. It also informs user of any misinformation fed to the computer so that detection and correction of output are made easier.

Cards 579 - 586 These cards write out the final conditions at the end of the reactor.

Cards 590 - 598 These cards test for different final conditions to make sure they meet certain requirements.

Card 590 This card checks to see if $P = P_{OUT} \pm .2$

Card 591 If the condition in Card 590 is not met and if on some previous calculation it was determined that the initial condition giving acceptable outlet conditions was bypassed, then the increment by which the pressure is changed is cut by a factor of 2.

$$(\text{i.e. } P_{IN} = P_{IN_o} + P - P/2 - P/4 + P/8) \qquad (34)$$

where P_{IN} is the pressure at inlet P_{IN_o} is the original guess.

In this case the second increment resulted in a value too

low and the pressure had to be increased by an amount 1/8 P. This convergence technique will always produce an acceptable answer (if one exists) provided that the answer was bracketed because

$$\sum_{M=1}^{L} (\tfrac{1}{2})^M \Delta P = \Delta P \qquad (35)$$

proving that it is possible to reach either extreme of the bracketed answer by allowing one or more terms in the summation to be subtracted. Any intermediate value would eventually be arrived at.

Card 593 If the velocity of sound has been exceeded, the upper limit is removed from the pressure and replaced with the restriction that the speed of sound is not to be exceeded. (i.e.)

$$P \geq P_{OUT} - .2, \text{ and velocity} < \text{velocity of sound} \qquad (36)$$

Cards 595 - 598 These cards decide whether to add or subtract the next pressure increment: ITEST EQUALS 1 if the first time through. ITEST = 2 if last increment was added. ITEST = 3 if last increment was subtracted.

Cards 604 - 628 These cards plot out results if desired.

Cards 629 - 665 These cards write out detailed calculation if desired.

Cards 666 - 684 These cards write out the final reactor condition.

Cards 685 - 697 This section adds pressure increment and starts calculations all over again. (Set values on ITEST = 2)

Cards 698 - 704 This section subtracts pressure increment and starts program over again. (Sets values on ITEST = 3)

Cards 705 - 714 These cards prepare the reactor profile for printing. This section also updates the reactor profile so that the previous profile becomes the working profile used in the next set of reactor design. These cards are only executed if all criteria have been met. Card 714 writes out the reactor profile.

Cards 715 - 721 This section resets initial conditions for the next set of reactor calculations.

Card 722 This card checks to make sure that the maximum number of completed reactor calculations equal to IZZ has not been exceeded. If it hasn't, the program continues. Otherwise, a new temperature profile is read and a new case is started.

Card 723 This card makes sure the inlet pressure is less than the maximum allowable pressure. If it isn't, the program is continued. Otherwise, a new temperature profile is read and a new case is started.

Card 724 This card is a conditional branch to program reinitialization.

Cards 725 - 727 These cards are executed only if the tube is blocked with carbon. These cards print out the information that the tube is blocked, set the value of IZZ so that it will read a new temperature profile and then give control to Cards 705 - 723.

Cards 728 - 756 These cards are only executed at the termination of calculation from a particular temperature profile.

Card 728 This card prints out the information that there was an unstable temperature profile causing ocillation in the calculations which would continue indefinitely if not checked for and handled properly.

Cards 729 - 749 These cards are executed only if the IPLOT variable is either 1 or 2. These cards plot up the reactor profile.

Cards 750 - 751 These cards are used as final identification of the temperature profile.

Cards 752 - 753 These cards reinitialize constants.

Cards 754 - 763 These cards read in the new temperature profile. If the variable IGOW is equal to:

IGOW	Computer Will
1	Read in completely new reaction system.
2	Begin calculation with present system and new temperature profile
3	Stop

Cards 764 - 778 and 807 - 813 These cards are used to terminate the program because of bad data input. The data is identified by variables on the data output. This identity must correspond to an internally generated variable or the computer program is terminated and the location and reason for termination are given.

Cards 779 - 866 These cards are used to generate the equilibrium data, the heat capacity of reaction data and the delta heat of reaction data. The information is put in tabular form and calculations are terminated.

Appendix B

Use of Marquardt's Non-Linear Square Fit Program

I General Description and Limitation

II Requirement to Use Program

III Flexibility

IV Explanation on How to Use Snowjo

V Example One: Heat Capacity of Carbon

Example Two: Heat Capacity of Acetylene

Example Three: Determination of Ω_K (Lennard and Jones Collision Integral) as a function of KT/ε

Appendix B

Use of Marquardt's Non Linear Least Square Fit Program

I. General Description and Limitations

The Marquardt Program works by adjusting the value of a set of components till the value calculated from the adjusted parameter equation minus the observed value (the quantity squared) is equal to a minimum.

(i.e.) $(\text{Observed} - \text{Predicted})^2 = \text{Minimum}$

The program can handle ten independent variables, 500 observation points and 50 adjustable parameters.

II. Requirements

a. The user must supply a set of data with at least as many variables as there are adjustable parameters.

b. The user must supply a set of initial guesses for the values of the adjustable constants.

c. The user must supply three subroutines.

1. Sub Z - This subroutine, called only once during the run of the program, is used to get data into more easily handled form by allowing the user to expand the scale of either the ordinate or the abcissa.

2. F Code - This subroutine is used to define the predicted values and the residue (i.e.) the

difference between the observed and the predicted values.

3. P Code - This subroutine calculates analytical partials of the function with respect to each of the adjustable parameters. This subroutine need not be supplied if the user is weilling to use the somewhat less exact partials: calculated by the program using difference methods (if this latter technique is used, none of the initial guesses for the value of the adjustable parameters may be zero).

III. Flexibility

This program also allows the user to select initial values of the adjustable parameters and let them remain fixed throughout any run of the program. The program has been adapted by the author to allow many runs on the same set of data without reintroducing the entire set of data but simply selecting different sets of initial guesses for the fixed parameters.

It is also possible to enter a set of constants so that the value of any given variable will not fall below (or above) a given value, never turn negative or will not be N times as great as the value of any other adjustable parameter.

IV. Method of Data Input

1. First Card Set Format (2013)

Col. 1 - 3 Number of sets of data or observations ($\leqq 500$)

Col. 4 - 6 Number of variables and fixed parameters ($\leqq 50$)

Col. 7 - 9 Number of fixed parameters ($\leqq 49$)

Col. 10 - 12 Number of independent variables ($\leqq 10$)

Col. 13 - 15 A zero means results not plotted. A one means the results are plotted by computer.

Col. 16 - 18 Number of contraints on variable parameters ($\leqq 50$)

2. Second Card Set Format (2013)

Col. 1 - 3 Not used but nust contain a zero

Col. 4 - 6 A zero means analytical derivatives used (Calculated by P Code). A one means estimated derivative used (Calculated by program).

Col. 7 - 9 A zero means abbreviated form and no plots used. A (one - ninety nine) means the number of detailed printouts and plots used before abbreviated form is used. The last iteration is always detailed.

Col. 10 - 12 A zero means no forced stop (i.e. the program keeps calculating until one of the convergence criterion is met or until the program is cut manually.

A (one - ninety nine) is the number of iterations used before the program is forced off by going to the convergence calculation.

Col. 13 - 15 Not used but must contain a zero

Col. 16 - 18 A zero means non linear confidence region is desired.

A one means non linear confidence region not desired.

3. Third Card Set Format (2F10.0)

Col. 1 - 10 Left side of plot usually smallest value of any observed data point.

Col. 11 - 20 Spread of plot (usually largest minus smallest observed data point.)

4. Fourth Card Set

If Col. 7 - 9 Card 1 equals zero, omit this card. If it equals (1 - 49) list the excluded parameters Format (2513) 25 to the card. (i.e.) This will be a list of the parameters which are fixled. If there are 3 fixed parameters, 1-7-10, then the card would like like: bb1 bb7 b10

5. Fifth Card Set Format (7F10.0)

This card sets the parameters used to calculate confidence and convergence criteria. If set equal to zero the program will supply its own values for details.

6. Sixth Card Set

This card set reads the initial guess for the parameter (both fixed and variable) Format (7F10.0) seven to the card.

7. Seventh Card Set

This card set it used to generate format code for the next set of cards Format (20A4). This card will have an open parenthesis in Col. One followed by the specific format followed by a closed parenthesis. If there are 5 independent variables, Card 7 might look like (6F10.0) or (6E10.0) or any other suitable format.

8. Eighth Card Set

This card set reads in observed data points and the corresponding value of the independent variables. The format is the one generated in card 7. There will be as many cards in Card Set Eight as there are observation points, or if all the data for one set of observation points will not fit on one card, there will be multiple cards,

9. Ninth Card Set

This set contains any information called for by the subroutine supplied by user, using the user's own format.

10. Tenth Card Set

If Col. 1 - 5 is less than zero (the rest of the card being filled in with zeroes) the next set of data read in will be Card Set One and the program will start on a new

problem.

If Col. 1 - 5 is equal to zero (the rest of the card also containing all zeroes) the program will stop.

If Col. 1 - 5 is greater than zero the program will read Card Set Ten as a new set of values as initial guesses for the fixed and variable parameters. The program will be reinitialized (Sub Z will not be recalled) and the program will be run through again. At the end of its run the next card will be read in as Card Set 10.

Subroutine Sub (Z)

Subroutine Sub Z(Y,X,B,PRNT,NPRNT,N) is used to calculate the initial values used in the program. If desired, Subroutine Z can be the following:

```
SUBROUTINE SUB Z (Y,X,B,PRNT,NPRNT,N)
COMMON Y(500),X(500,10)B(50),PRNT(5)
RETURN
END
SUBROUTINE F CODE (Y,X,B,PRNT,F,I,RES)
SUBROUTINE F CODE (Y,X,B,PRNT,F.I.RES)
COMMON Y(500),X(500,10)B(50),PRNT(5)
F-f(X(I,1),X(I,2)...X(I,N),B(1),B(2)...B(M))
  N = Number of independent variables
  M = Number of parameters
RES = Y(I)-F
```

```
      RETURN
      END
```

Note: If you want to brach to next case for any reason just set I=1000 as a result of not meeting some criterion.

(i.e.) If (X(I,2).GE.X(1,3)) I=1000 etc.

This will stop calculations on your program and branch to the next set of input data.

```
      SUBROUTINE P CODE (P,X,B,PRNT,F,I,)
      COMMON Y(500),X(500,10),B(50),PRNT(5)
      DIMENSION P(50)
```

P(N)=dF/dE(N)=f(X(I,1),X(I,2)...X(I,M),B(1),B(2)...B(MM)

Requires that N=(1,MM) one partial for each derivative

P(1) =

P(2) =

$P(3) = f_3(\quad)$

.

.

.

$P(MM) = f_{MM}(\quad)$

Note: MM = total number of parameters

The I in X(I,1) or X(I,3) etc. is the set of data the program is calling for. The I value is supplied by the program.

```
      RETURN
```

```
END
```

HOW TO USE NON LINEAR PROGRAM ON DISK

The non linear least square curve fit is on disk as a subroutine therefore it will be necessary to write a dummy program to use it.

```
// JOB CC 305/0003,RATE F,3600,10000,RICHARD ROBERTSON
// FORTRAN
      PROGRAM RATE F
      CALL SNOWJO
      END
      SUBROUTINE SUB Z(Y,X,B,PRNT,NPRNT,N)
      ------
      ------
      ------
      RETURN END
      SUBROUTINE F CODE (Y,X,B,PRNT,F,I,RES)
      ---------
      ---------
      ---------
      RETURN
      END
      SUBROUTINE P CODE (P,X,B,PRNT,F,I,)
      ------
      ------
```

```
      RETURN
      END

// EXEC
      (DATA
// EXEC RATEF,UTZ
      DATA
// EXEC RATEF,UTZ
      DATA
      ETC.
```

Example

The following program is designed to fit heat capacity data of carbon.

The original data was in the form

$$C_P = 2.673 + 2.617 * 10^{-3} T * 1.169 * 10^5/T**2 \qquad (1)$$

This equation was evaluated at 28 temperatures between 500 and 1175^{o}K using a very simple computer program. The results were punched by the computer in a (2F16.7) format, the heat capacity being the observed value and the temperature being the independent variable.

After being run via the non linear curve fitting program the equation was changed to the following form.

$C_P = 2.673 + 4.4973 * 10^{-2} + 4.6362 * 10^{-6} T**2 - 2.16009 * 10^{-9} * T**3$ (2)

The second form is now consistent with the form of the rest of the heat capacity data.

Sub Z was not used and a very short Sub Z program was written.

F Code defined T as equal to X(I,1) and F = b(1) + b(2)*T + b(3)*T*T* + b(4)*T*T*T. F now becomes the predicted value. RES=Y(I)-F is the difference between the predicted value F and the observed value Y(I).

P Code defined T as equal to X(I,1) and

$\partial F/\partial B(1) = P(1) = 1$

$\partial F/\partial B(2) = P(2) = T$

$\partial F/\partial B(3) = P(3) = T*T$

$\partial F/\partial B(4) = P(4) = T*T*T$.

In this program B(1) was fixed, so that the following data input was used:

Card Set 1

Number of observations = 28

Number of parameters = 4 io B(1)-B(2)-B(3)-B(4)

Number of fixed parameters = 1 only B(1) fixed

Number of independent variables = 1 only temperature

Results of be plotted = 1

Number of constraints = 0

Card Set 2

Col. 1 - 3 = 0

Number of detailed printouts = 20

Number of iterations before forced off = 20

Col. 13 - 15

Non linear confidence region = 0 is desired

Card Set 3

Lowest value = 3.000

(Highest value - 10)

10 - 3 = 7.000

Card Set 4

The first parameter is fixed = 1

Card Set 5

7 zeroes. Space 10 spaces apart, allowing computer to fix the values.

Card Set 6

The initial guesses for B(1) = 2.673

B(2) = .002617

B(3) = .000009

B(4) = .000000002

Card Set 7

The format for the rest of the data is (2F16.7)

Card Set 8

The data heat capacity = 3.5139

temperature = 500.0

is repeated for all 28 observations.

Card Set 9

This card set is not used (none of the subroutines have any cards to read).

Card Set 10

0.00 0. 0. 0.

This is what the computer is desired to do. The first value is 0. so that the computer will stop when it gets to this point.

```
// JOB CC 305/003,RROB,1800,10000 RICHARD ROBERTSON
// PARAM LIST=YES,DEBUG=YES,MAP=YES,CODE=1
// FORTRAN
      PROGRAM IBWTT
      CALL SNOWJO
      STOP
      END

      SUBROUTINE SUB Z(Y,X,B,PRNT,NPRNT,N)
      COMMON Y(500),X(500,10),B(50),PRNT(5)
      NPRNT=0
      RETURN
      END

      SUBROUTINE FCODE (Y,X,B,PRNT,F,I,RES)
      COMMON Y(500)X(500,10),B(50),PRMT(5)
      T=X(I,1)
      F=B(1)+B(2)*T+B(3)*T*T+B(4)*T*T*T
      RES=Y(I)-F
      RETURN
      END

      SUBROUTINE PCODE (P,X,B,PRNT,F,I)
      COMMON Y(500),X(500,10),B(50),PRNT(5)
      DIMENSION P(50)
```

```
P(1)=1

P(2)=T

P(3)=T*T

P(4)=T*T*T

RETURN

END
```

DATA SET

Card Set 1
```
 28  4  1  1  1  0
```
Card Set 2
```
  0  0 20 20  0  0
```
Card Set 3
```
3.       7.
```
Card Set 4
```
  1
```
Card Set 5
```
0.       0.       0.       0.       0.       0.       0.
```
Card Set 6
```
2.673    .002617  .000009  .000000002
```
Card Set 7
```
(2F16.0)
```
Card Set 8
```
   3.5139000     500.00000
   3.6227981     525.00000
   3.7259038     550.00000
   3.8242023     575.00000
   3.9184778     600.00000
   4.0093610     625.00000
   4.0973637     650.00000
   4.1829044     675.00000
   4.2663286     700.00000
   4.3479231     725.00000
   4.4279278     750.00000
   4.5065445     775.00000
   4.5839438     800.00000
   4.6602711     825.00000
   4.7356507     850.00000
   4.8101893     875.00000
   4.8839791     900.00000
   4.9570998     925.00000
   5.0296210     950.00000
   5.1016033     975.00000
   5.1730000     1000.0000
   5.2441579     1025.0000
   5.3148183     1050.0000
   5.3851177     1075.0000
   5.4550885     1100.0000
   5.5247596     1125.0000
   5.5941569     1150.0000
   5.6633033     1175.0000
```
Card Set 9 - not used
Card Set 10
```
0.00 0.0  0.0  0.0
```

Example 1

Heat Capacity of Carbon

In this example the heat capacity of carbon was not available in the standard form. It was available as:

$$C_P \text{ Carbon} = A + BT + C/T^2 \qquad (3)$$

The heat capacity of carbon was fit to the form:

$$C_P \text{ Carbon} = A + BT + CT^2 + DT^3 \qquad (4)$$

The value of A was fixed as a constant.

All of the heat capacity data used in this study were obtained from Selected Values of Chemical Thermodynamic Properties.(43) (44)

The result of this curve fitting is found on page 118.

Example 2

Heat Capacity of Acetylene

The heat capacity of acetylene was fit between 300 and 1500°K. Data was in 100° increments. The standard error for this range was found to be .0941. The percent average standard error became .0941/15.45 * 100 ≅ .6%

The final equation became

$$C_{P\ CH\equiv CH} = 5.867 + 1.957 * 10^{-2}T - 1.296 * 10^{-5}T^2 + 3.466 * 10^{-9}T^3 \qquad (5)$$

where T is °K.

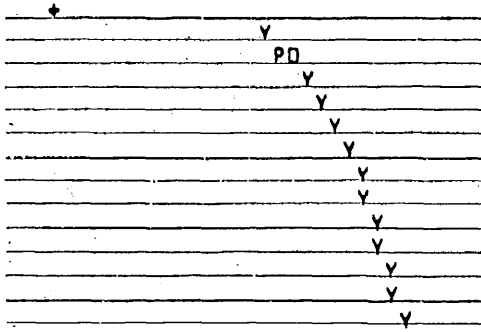
The values of the heat capacity for each component are listed in Appendix C.

ACETYLENE HEAT CAPACITY EPSILON TEST

N = 13 K = 4 P = 0 M = 1
FF = 0.400E 01 T = 0.200E 01 E = 0.500E-04 TAU = 0.100E-02

(5) PARAMETERS 0.58672009E 01 0.19574307E-01 -0.12957129E-04 0.34664522E-08

0.00E 00 0.70E 02



(5) PARAMETERS 0.58672009E 01 0.19574307E-01 -0.12957129E-04 0.34664522E-08

DBS	PRED	DIFF
0.10532000E 02	0.10666945E 02	-0.13494492E 00
0.11973000E 02	0.11845635E 02	0.12736416E 00
0.12967000E 02	0.12848379E 02	0.11862087E 00
0.13728000E 02	0.13695959E 02	0.32040596E-01
0.14336000E 02	0.14409216E 02	-0.73215485E-01
0.14933000E 02	0.15008903E 02	-0.75902939E-01
0.15449000E 02	0.15515825E 02	-0.66824913E-01
0.15922000E 02	0.15950808E 02	-0.28807640E-01
0.16352997E 02	0.16334625E 02	0.18371582E-01
0.16744003E 02	0.16688126E 02	0.55877686E-01
0.17098999E 02	0.17032028E 02	0.66970825E-01
0.17417999E 02	0.17387177E 02	0.30822754E-01
0.17703995E 02	0.17774368E 02	-0.70373535E-01

PHI	S E	LAMBDA	ANALYTIC PARTIALS USED
0.79793751E-01	0.94159245E-01	0.100E-06	

PTP INVERSE

1	0.15125728E 02	-0.59988748E-01	0.69572809E-04	-0.24528543E-07
2	-0.59988689E-01	0.24802075E-03	-0.29545390E-06	0.10609866E-09
3	0.69572707E-04	-0.29545379E-06	0.35979486E-09	-0.13140883E-12
4	-0.24528489E-07	0.10609855E-09	-0.13140866E-12	0.48670381E-16

PARAMETER CORRELATION MATRIX

1	1.0000	-0.9794	0.9431	-0.9040
2	-0.9794	1.0000	-0.9891	0.9657
3	0.9431	-0.9891	1.0000	-0.9930
4	-0.9040	0.9657	-0.9930	1.0000

	STD	ONE - PARAMETER		SUPPORT PLANE	
B	ERROR	LOWER	UPPER	LOWER	UPPER
1	0.36620224E 00	0.51347961E 01	0.65996046E 01	0.44023924E 01	0.73320093E 01
2	0.14828830E-02	0.16608540E-01	0.22540070E-01	0.13642777E-01	0.25505837E-01
3	0.17860357E-05	-0.16529200E-04	-0.93850576E-05	-0.20101259E-04	-0.58129863E-05
4	0.65689387E-09	0.21526645E-08	0.47802367E-08	0.83887675E-09	0.60940266E-08

3	0.17860357E-05	-0.16529200E-04	-0.93850576E-05	-0.20101229E-04	-0.38129869E-05
4	0.65629307E-09	0.21526645E-08	0.47802367E-08	0.83887675E-09	0.60940266E-08

NONLINEAR CONFIDENCE LIMITS

PHI CRITICAL = 0.22164929E 00

PARA	LOWER B	LOWER PHI	UPPER B	UPPER PHI
1	NONE FOUND			
2	NONE FOUND			
3	NONE FOUND			
4	NONE FOUND			

ETHYNE, ACETYLENE HEAT CAPACITY

Example 3

Determination of Lennard and Jones Collision Intergral

In the subroutine Pressure Drop (see Program Logic) it was necessary to determine the viscosity of the reactor components. This was done by calculating the viscosity of each component from the equation [#]

$$\mu = 2.6693 * 10^{-5} \sqrt{MT/\Omega_\mu^2} \qquad (6)$$

This made it necessary to calculate the value of Previous to this the values were only available in table form requiring linear interpolation between values.

It was decided that the program would be more flexible if this data could be curve fitted. Plotting the values on log-log paper gave a slowly curving line when lent itself to a polynomial fit.

The values of the Lennard and Jones parameter were fed into SNOWJO with the corresponding values of KT/ε .[(5)] The log of each value was taken (in SUBZ) and SNOWJO proceded to curve fit the data in the identical way that the heat capacity data was curve fitted.

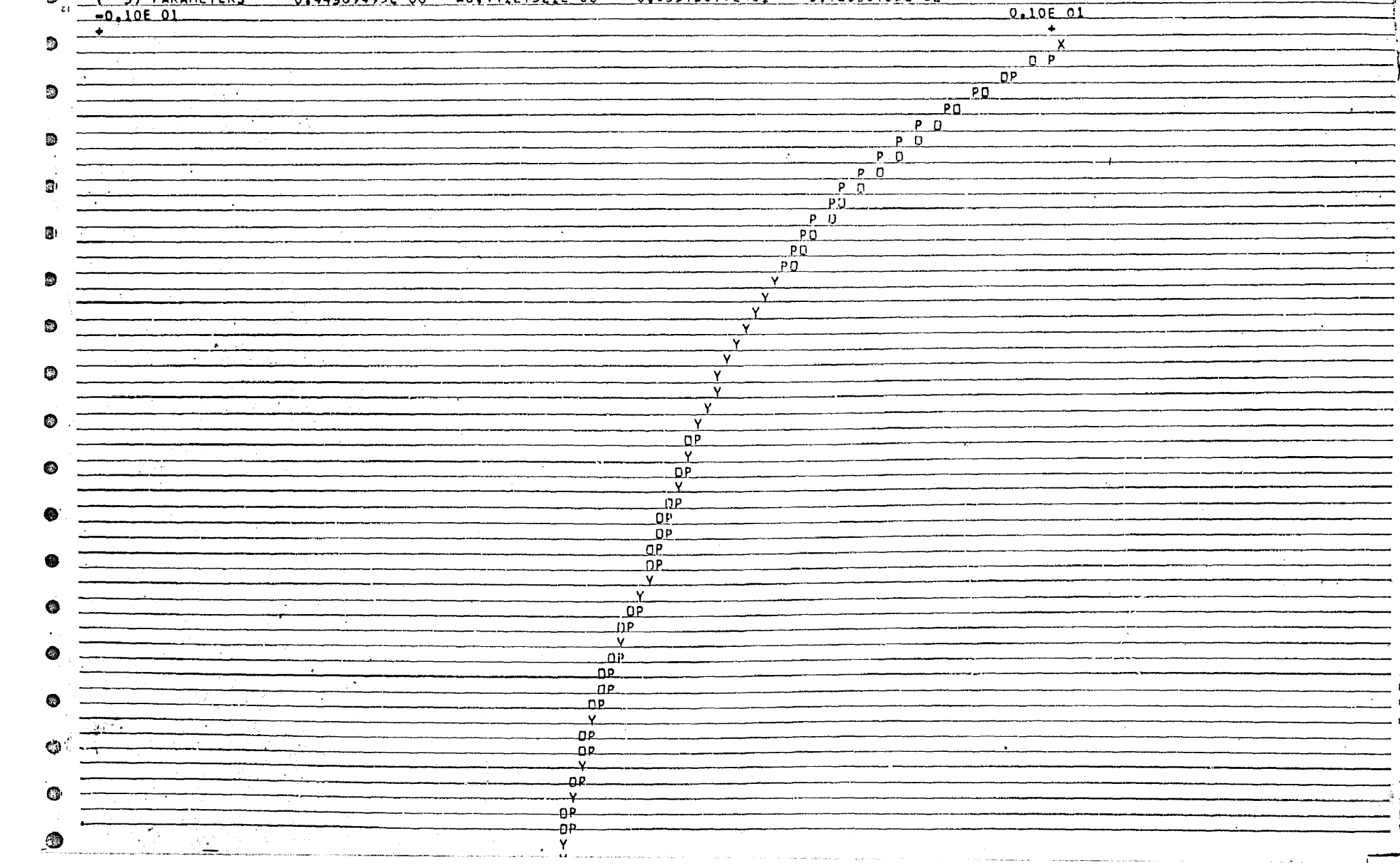
[#]See Pressure Drop in Program Logic to get details.

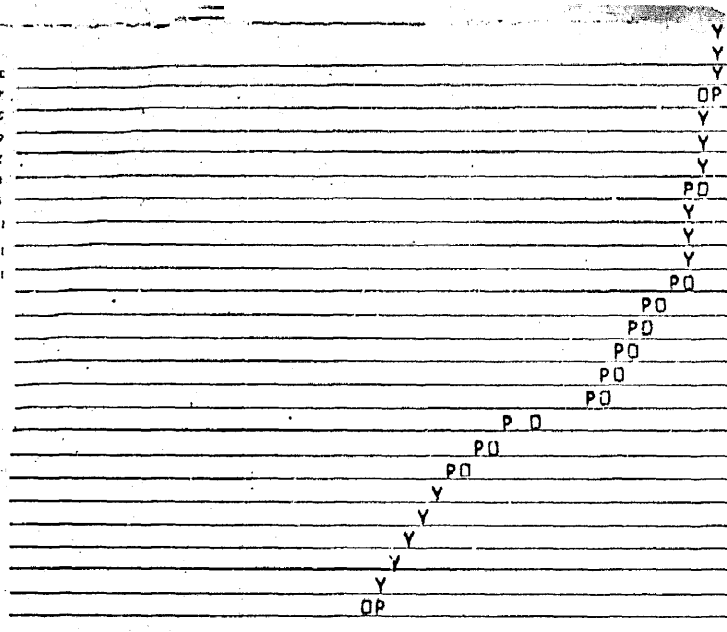
CURVE FIT OF
ΔK AS A FUNCTION OF $K_{T/E}$

EPSILON TEST

N = 79 K = 4 P = 0 M = 1
FF = 0.400E 01 T = 0.200E 01 E = 0.500E-04 TAU = 0.100E-02

(3) PARAMETERS 0.44369495E 00 -0.44127321E 00 0.83573699E-01 -0.72000735E-02





(3) PARAMETERS 0.44369495E 00 -0.44127321E 00 0.83573699E-01 -0.72000735E-02

OBS	PRED	DIFF	X(1,1)	% DIFF
0.10242472E 01	0.11086845E 01	-0.84437370E-01	-1.20397	-8.81%
0.96622318E 00	0.10073919E 01	-0.41168749E-01	-0.91629	-4.20%
0.91308546E 00	0.92373604E 00	-0.10650575E-01	-0.79851	0.90%
0.86204571E 00	0.85300851E 00	0.90371966E-02	-0.69315	2.17%
0.81403649E 00	0.79211318E 00	0.21923304E-01	-0.59784	2.89%
0.76825470E 00	0.73891276E 00	0.29341936E-01	-0.51083	3.27%
0.72513002E 00	0.69187611E 00	0.33253908E-01	-0.43078	3.37%
0.68410659E 00	0.64987248E 00	0.34234107E-01	-0.35667	3.34%
0.64605552E 00	0.61204469E 00	0.34010828E-01	-0.28768	3.21%
0.61030865E 00	0.57772928E 00	0.32579362E-01	-0.22314	2.98%
0.57661319E 00	0.54640353E 00	0.30209661E-01	-0.16252	2.72%
0.54522723E 00	0.51764834E 00	0.27578890E-01	-0.10536	2.44%
0.51581323E 00	0.49112380E 00	0.24689436E-01	-0.05129	2.12%
0.48796612E 00	0.46655011E 00	0.21416008E-01	0.00000	1.80%
0.46184534E 00	0.44369495E 00	0.18150389E-01	0.04879	1.51%
0.43760937E 00	0.42236310E 00	0.15246272E-01	0.09531	1.23%
0.41475511E 00	0.40238988E 00	0.12365222E-01	0.13976	0.97%
0.39339274E 00	0.38363469E 00	0.97580552E-02	0.18232	0.69%
0.37294167E 00	0.36597580E 00	0.69658756E-02	0.22314	0.42%
0.35346961E 00	0.34930903E 00	0.41605830E-02	0.26236	0.22%
0.33575779E 00	0.33354330E 00	0.22144914E-02	0.30010	-1.34%
0.30527663E 00	0.31859899E 00	-0.13322353E-01	0.33647	-0.21%
0.30232412E 00	0.30440629E 00	-0.20821691E-02	0.37156	-0.35%
0.28743213E 00	0.29090273E 00	-0.34705997E-02	0.40547	-0.50%
0.27307600E 00	0.27803373E 00	-0.49577355E-02	0.43826	-0.65%
0.25928217E 00	0.26575047E 00	-0.64682961E-02	0.47000	-0.80%
0.24607873E 00	0.25400901E 00	-0.79302788E-02	0.50078	-0.85%
0.23428124E 00	0.24277043E 00	-0.84891915E-02	0.53063	-1.05%
0.22154236E 00	0.23199874E 00	-0.10456383E-01	0.55962	-1.15%
0.21026111E 00	0.22166240E 00	-0.11401296E-01	0.58779	-1.21%
0.19966996E 00	0.21173239E 00	-0.12062430E-01	0.61519	-1.25%
0. 00	0.20218235E 00	-0.12389123E-01	0.64185	-1.33%
0.	0.19298851E 00	-0.13170481E-01	0.66783	-1.36%

0.19966996E 00	0.21173239E 00	-0.11200[illegible]E-01	0.64[illegible]	-1.33%
0.18979323E 00	0.20218295E 00	-0.12387120E-01	0.66783	-1.36%
0.17981803E 00	0.19298851E 00	-0.13170481E-01	0.69315	-1.44%
0.17058617E 00	0.18412876E 00	-0.13542593E-01	0.74194	-1.45%
0.16126829E 00	0.17558306E 00	-0.14314771E-01	0.78846	-1.50%
0.14496589E 00	0.15936208E 00	-0.14396191E-01	0.83291	-1.50%
0.12927192E 00	0.14419544E 00	-0.14923513E-01	0.87547	-1.51%
0.11511254E 00	0.12997228E 00	-0.14859736E-01	0.91629	-1.52%
0.10165393E 00	0.11659753E 00	-0.14943602E-01	0.95551	-1.43%
0.88926554E-01	0.10398883E 00	-0.15062273E-01	0.99325	-1.42%
0.77886820E-01	0.92074990E-01	-0.14188170E-01	1.02962	-1.36%
0.66723824E-01	0.80793738E-01	-0.14069915E-01	1.06471	-1.31%
0.56379993E-01	0.70090353E-01	-0.13710361E-01	1.09861	-1.20%
0.46883907E-01	0.59916530E-01	-0.13032623E-01	1.13140	-1.15%
0.38258268E-01	0.50229009E-01	-0.11970721E-01	1.16315	-1.05%
0.29558558E-01	0.40990096E-01	-0.11431538E-01	1.19392	-0.99%
0.21761809E-01	0.32165952E-01	-0.10404143E-01	1.22377	-0.87%
0.13902843E-01	0.23725528E-01	-0.98226853E-02	1.25276	-0.80%
0.69755837E-02	0.15641946E-01	-0.86663626E-02	1.28093	-0.73%
-0.10002159E-03	0.78900009E-02	-0.79900213E-02	1.30833	-0.64%
-0.68232194E-02	0.44753775E-03	-0.72707571E-02	1.33500	-0.55%
-0.13085250E-01	-0.67058951E-02	-0.63793547E-02	1.36098	-0.46%
-0.19080866E-01	-0.13588827E-01	-0.54920390E-02	1.38629	-0.39%
-0.24805132E-01	-0.20217992E-01	-0.45871399E-02	1.41099	-0.39%
-0.30459180E-01	-0.26609089E-01	-0.38500912E-02	1.43508	-0.21%
-0.36663998E-01	-0.32776088E-01	-0.38879104E-02	1.45861	-0.27%
-0.40822014E-01	-0.38731933E-01	-0.20900816E-02	1.48160	-0.05%
-0.47196459E-01	-0.44488713E-01	-0.27077459E-02	1.50408	0.04%
-0.50556742E-01	-0.50057437E-01	-0.49930438E-03	1.52606	0.11%
-0.55089977E-01	-0.55448513E-01	0.35853684E-03	1.54756	0.19%
-0.59537705E-01	-0.60671106E-01	0.11334009E-02	1.56862	0.27%
-0.63792109E-01	-0.65733790E-01	0.19416809E-02	1.58923	0.34%
-0.67957640E-01	-0.70645392E-01	0.26877522E-02	1.60944	0.41%
-0.72033226E-01	-0.75412512E-01	0.33792853E-02	1.79176	1.05%
-0.75909555E-01	-0.80042958E-01	0.41334033E-02	1.94591	1.53%
-0.10948002E 00	-0.12007189E 00	0.10591865E-01	2.07944	1.90%
-0.13616341E 00	-0.15157807E 00	0.15414655E-01	2.19722	2.17%
-0.15805829E 00	-0.17726833E 00	0.19210041E-01	2.30258	2.35%
-0.17685652E 00	-0.19878101E 00	0.21924496E-01	2.99573	2.47%
-0.19334209E 00	-0.21717340E 00	0.23831308E-01	3.40120	1.75%
-0.29679006E 00	-0.32178968E 00	0.24999619E-01	3.68888	1.04%
-0.35596085E 00	-0.37365979E 00	0.17698944E-01	3.91202	0.45%
-0.39779454E 00	-0.40827864E 00	0.10484099E-01	4.09434	-0.03%
-0.43016773E 00	-0.43463361E 00	0.44658780E-02	4.24850	-0.42%
-0.45649529E 00	-0.45621389E 00	-0.28139353E-03	4.38203	-0.72%
-0.47900391E 00	-0.47470230E 00	-0.43016076E-02	4.49981	-0.96%
-0.49823850E 00	-0.49102551E 00	-0.72129965E-02	4.60517	-1.15%
-0.51533574E 00	-0.50574875E 00	-0.95869899E-02		

SUM OF SQUARES= 0.25807E-01

-0.53068829E 00 -0.51923728E 00 -0.11451006E-01

PHI	S E	LAMBDA	ANALYTIC PARTIALS USED
0.25806993E-01	0.18549748E-01	0.100E-04	

PTP INVERSE

1	0.29627133E-01	-0.60996935E-02	-0.13612781E-01	0.31657408E-02
2	-0.60996711E-02	0.44309102E-01	-0.26053179E-01	0.37040554E-02
3	-0.13612799E-01	-0.26053175E-01	0.36333051E-01	-0.69516972E-02
4	0.31657459E-02	0.37040552E-02	-0.69517009E-02	0.14202138E-02

PARAMETER CORRELATION MATRIX

1	1.0000	-0.1684	-0.4149	0.4880
2	-0.1684	1.0000	-0.6493	0.4669
3	-0.4149	-0.6493	1.0000	-0.9678
4	0.4880	0.4669	-0.9678	1.0000

ONE - PARAMETER		SUPPORT PLANE	
LOWER	UPPER	LOWER	UPPER

The results were:

$$LN(\Lambda_K) = .4437 - .4413\ LN\left(\frac{KT}{\varepsilon}\right) + .08357\ LN^2\left(\frac{KT}{\varepsilon}\right) - .007200\ LN^3\left(\frac{KT}{\varepsilon}\right) \quad (7)$$

$$\Lambda K = \Lambda_\mu = EXP\left(.4437 - .4413\ LN\left(\frac{KT}{\varepsilon}\right) + .8357\ LN^2\left(\frac{KT}{\varepsilon}\right) - .0072\ LN^3\left(\frac{KT}{\varepsilon}\right)\right)$$

The results from this regression analysis are given in the preceding 3 pages.

Appendix C

Heat Capacity

Component Number	Component
1	Acetylene
2	Iso-Butane
3	Normal Butane
4	Iso-Butene
5	Ethane
6	Ethylene
7	Hydrogen
8	Methane
9	Propane
10	Propene
11	Water
12	Carbon
13	Carbon Monoxide

Heat Capacity BTU/Lb Mole ^{o}K

Temp.	1	2	3	4	5	6	7	8	9	10	11	12	13
800	15.009	48.550	48.268	42.394	25.799	20.217	7.099	15.031	37.118	30.697	9.249	4.727	7.603
810	15.063	48.892	48.609	42.676	25.996	20.352	7.105	15.146	37.389	30.913	9.279	4.753	7.619
820	15.117	49.228	48.946	42.954	26.191	20.486	7.111	15.261	37.656	31.127	9.308	4.779	7.635
830	15.170	49.559	49.277	43.227	26.384	20.618	7.117	15.375	37.919	31.337	9.338	4.803	7.651
840	15.222	49.885	49.604	43.497	26.574	20.748	7.123	15.488	38.178	31.545	9.368	4.828	7.667
850	15.273	50.206	49.927	43.762	26.763	20.876	7.130	15.600	38.434	31.750	9.398	4.851	7.683
860	15.323	50.521	50.244	44.023	26.948	21.002	7.136	15.712	38.686	31.952	9.428	4.874	7.699
870	15.372	50.833	50.558	44.280	27.132	21.126	7.143	15.823	38.934	32.151	9.458	4.896	7.715
880	15.421	51.139	50.866	44.533	27.314	21.249	7.149	15.932	39.179	32.347	9.488	4.918	7.731
890	15.469	51.441	51.170	44.783	27.493	21.370	7.156	16.041	39.420	32.540	9.518	4.939	7.747
900	15.516	51.738	51.470	45.028	27.670	21.489	7.163	16.149	39.658	32.731	9.548	4.959	7.763
910	15.562	52.030	51.765	45.270	27.844	21.606	7.170	16.256	39.892	32.919	9.578	4.979	7.778
920	15.608	52.318	52.056	45.508	28.017	21.722	7.176	16.362	40.123	33.104	9.608	4.998	7.794
930	15.653	52.601	52.343	45.743	28.188	21.836	7.183	16.468	40.351	33.287	9.638	5.017	7.810
940	15.697	52.881	52.626	45.973	28.356	21.949	7.190	16.572	40.575	33.467	9.668	5.035	7.825
950	15.741	53.155	52.904	46.201	28.522	22.059	7.197	16.675	40.796	33.645	9.698	5.053	7.841
960	15.784	53.426	53.179	46.425	28.686	22.169	7.205	16.778	41.014	33.820	9.728	5.071	7.856
970	15.827	53.693	53.449	46.645	28.848	22.276	7.212	16.879	41.229	33.992	9.758	5.087	7.872
980	15.869	53.955	53.716	46.862	29.008	22.382	7.219	16.980	41.441	34.162	9.788	5.104	7.887
990	15.910	54.213	53.978	47.076	29.166	22.487	7.226	17.079	41.649	34.330	9.818	5.120	7.902
1000	15.951	54.468	54.237	47.287	29.322	22.590	7.234	17.178	41.855	34.495	9.848	5.135	7.917
1010	15.991	54.719	54.492	47.494	29.476	22.692	7.241	17.276	42.057	34.658	9.878	5.151	7.932
1020	16.031	54.965	54.744	47.698	29.628	22.792	7.249	17.372	42.257	34.818	9.907	5.165	7.947
1030	16.070	55.209	54.991	47.900	29.778	22.891	7.256	17.468	42.454	34.977	9.937	5.180	7.962
1040	16.109	55.448	55.235	48.098	29.926	22.988	7.264	17.562	42.648	35.133	9.966	5.194	7.976
1050	16.148	55.684	55.476	48.293	30.072	23.084	7.271	17.656	42.839	35.286	9.996	5.208	7.991
1060	16.186	55.916	55.713	48.486	30.216	23.179	7.279	17.748	43.027	35.438	10.025	5.221	8.005
1070	16.224	56.145	55.946	48.675	30.358	23.273	7.287	17.840	43.213	35.587	10.054	5.235	8.019
1080	16.261	56.371	56.177	48.862	30.498	23.365	7.294	17.930	43.396	35.734	10.084	5.248	8.033
1090	16.298	56.593	56.403	49.047	30.637	23.455	7.302	18.020	43.577	35.879	10.113	5.260	8.047
1100	16.335	56.812	56.627	49.228	30.773	23.545	7.310	18.108	43.754	36.022	10.142	5.273	8.060
1110	16.371	57.028	56.847	49.407	30.908	23.633	7.318	18.195	43.930	36.163	10.170	5.285	8.074
1120	16.407	57.241	57.065	49.584	31.041	23.721	7.326	18.281	44.103	36.302	10.199	5.297	8.087
1130	16.443	57.451	57.279	49.758	31.172	23.807	7.334	18.366	44.273	36.439	10.228	5.309	8.100
1140	16.479	57.658	57.490	49.929	31.301	23.891	7.342	18.450	44.441	36.574	10.256	5.321	8.113
1150	16.514	57.862	57.698	50.099	31.429	23.975	7.350	18.533	44.607	36.707	10.284	5.333	8.126
1160	16.549	58.063	57.904	50.266	31.554	24.058	7.358	18.614	44.771	36.838	10.312	5.344	8.138
1170	16.584	58.262	58.106	50.430	31.678	24.139	7.366	18.695	44.932	36.968	10.340	5.356	8.151
1180	16.619	58.458	58.306	50.593	31.801	24.220	7.374	18.774	45.091	37.095	10.368	5.367	8.163
1190	16.654	58.651	58.502	50.753	31.921	24.299	7.382	18.852	45.248	37.221	10.395	5.379	8.174
1200	16.688	58.842	58.697	50.912	32.040	24.378	7.390	18.929	45.403	37.345	10.423	5.390	8.186

**FORTRAN ** STOP 00099

03RT 00:01:06

Appendix D

Equilibrium Constants

Equation No.	Equation
1	$C_2H_6 \longrightarrow C_2H_4 + H_2$
2	$C_2H_6 \longrightarrow CH_4 + \frac{1}{2}C_2H_4$
3	$C_2H_4 \longrightarrow C_2H_2 + H_2$
4	$2C_2H_2 \longrightarrow C_4$'s
5	$C + H_2O \longrightarrow CO + H_2$
6	$C + H_2O \longrightarrow CO + H_2$

TEMP EQUILIBRUM CONSTANTS (KP)

	EQUATION(S) NUMBER							
	1	2	3	4	5	6	7	8
800	5.9610E-02	1.9785E 02	1.8067E-06	6.5951E 08	1.8549E-01	6.8955E 01	1.5820E 00	1.4906E 03
810	6.6285E-02	1.7956E 02	2.7817E-06	6.6394E 08	1.8711E-01	5.6326E 01	1.6491E 00	1.4160E 03
820	7.3523E-02	1.6333E 02	4.2387E-06	6.6837E 08	1.8874E-01	4.6241E 01	1.7173E 00	1.3466E 03
830	8.1359E-02	1.4890E 02	6.3943E-06	6.7279E 08	1.9037E-01	3.8175E 01	1.7866E 00	1.2819E 03
840	8.9822E-02	1.3603E 02	9.5535E-06	6.7722E 08	1.9200E-01	3.1612E 01	1.8571E 00	1.2217E 03
850	9.8941E-02	1.2452E 02	1.4141E-05	6.8165E 08	1.9363E-01	2.6314E 01	1.9287E 00	1.1654E 03
860	1.0875E-01	1.1421E 02	2.0743E-05	6.8607E 08	1.9526E-01	2.1999E 01	2.0014E 00	1.1128E 03
870	1.1929E-01	1.0495E 02	3.0164E-05	6.9050E 08	1.9690E-01	1.8469E 01	2.0751E 00	1.0636E 03
880	1.3058E-01	9.6614E 01	4.3495E-05	6.9491E 08	1.9854E-01	1.5547E 01	2.1497E 00	1.0174E 03
890	1.4266E-01	8.9100E 01	6.2211E-05	6.9933E 08	2.0019E-01	1.3172E 01	2.2254E 00	9.7414E 02
900	1.5556E-01	8.2309E 01	8.8280E-05	7.0375E 08	2.0183E-01	1.1187E 01	2.3019E 00	9.3345E 02
910	1.6931E-01	7.6163E 01	1.2433E-04	7.0817E 08	2.0348E-01	9.5359E 00	2.3794E 00	8.9519E 02
920	1.8396E-01	7.0587E 01	1.7380E-04	7.1258E 08	2.0513E-01	8.1568E 00	2.4577E 00	8.5922E 02
930	1.9952E-01	6.5520E 01	2.4124E-04	7.1698E 08	2.0678E-01	7.0007E 00	2.5369E 00	8.2527E 02
940	2.1603E-01	6.0909E 01	3.3253E-04	7.2140E 08	2.0844E-01	6.0283E 00	2.6168E 00	7.9328E 02
950	2.3354E-01	5.6701E 01	4.5531E-04	7.2580E 08	2.1010E-01	5.2073E 00	2.6976E 00	7.6305E 02
960	2.5206E-01	5.2861E 01	6.1937E-04	7.3020E 08	2.1176E-01	4.5120E 00	2.7791E 00	7.3450E 02
970	2.7164E-01	4.9346E 01	8.3728E-04	7.3460E 08	2.1342E-01	3.9211E 00	2.8612E 00	7.0749E 02
980	2.9229E-01	4.6127E 01	1.1250E-03	7.3900E 08	2.1509E-01	3.4175E 00	2.9441E 00	6.8193E 02
990	3.1406E-01	4.3173E 01	1.5025E-03	7.4340E 08	2.1675E-01	2.9868E 00	3.0276E 00	6.5771E 02
1000	3.3698E-01	4.0458E 01	1.9953E-03	7.4779E 08	2.1842E-01	2.6175E 00	3.1117E 00	6.3473E 02
1010	3.6107E-01	3.7958E 01	2.6349E-03	7.5217E 08	2.2010E-01	2.2999E 00	3.1964E 00	6.1293E 02
1020	3.8638E-01	3.5656E 01	3.4607E-03	7.5656E 08	2.2177E-01	2.0259E 00	3.2816E 00	5.9222E 02
1030	4.1292E-01	3.3530E 01	4.5215E-03	7.6093E 08	2.2345E-01	1.7890E 00	3.3674E 00	5.7254E 02
1040	4.4072E-01	3.1566E 01	5.8772E-03	7.6531E 08	2.2513E-01	1.5836E 00	3.4536E 00	5.5380E 02
1050	4.6983E-01	2.9749E 01	7.6015E-03	7.6968E 08	2.2682E-01	1.4050E 00	3.5404E 00	5.3599E 02
1060	5.0026E-01	2.8066E 01	9.7843E-03	7.7405E 08	2.2850E-01	1.2495E 00	3.6275E 00	5.1901E 02
1070	5.3205E-01	2.6504E 01	1.2535E-02	7.7841E 08	2.3019E-01	1.1135E 00	3.7151E 00	5.0282E 02
1080	5.6519E-01	2.5055E 01	1.5985E-02	7.8277E 08	2.3188E-01	9.9452E-01	3.8030E 00	4.8737E 02
1090	5.9976E-01	2.3707E 01	2.0294E-02	7.8712E 08	2.3357E-01	8.9004E-01	3.8913E 00	4.7264E 02
1100	6.3575E-01	2.2452E 01	2.5654E-02	7.9146E 08	2.3527E-01	7.9816E-01	3.9799E 00	4.5857E 02
1110	6.7319E-01	2.1284E 01	3.2292E-02	7.9581E 08	2.3697E-01	7.1719E-01	4.0688E 00	4.4510E 02
1120	7.1213E-01	2.0193E 01	4.0482E-02	8.0015E 08	2.3867E-01	6.4565E-01	4.1580E 00	4.3224E 02
1130	7.5256E-01	1.9175E 01	5.0547E-02	8.0448E 08	2.4037E-01	5.8233E-01	4.2473E 00	4.1993E 02
1140	7.9453E-01	1.8224E 01	6.2867E-02	8.0880E 08	2.4207E-01	5.2616E-01	4.3370E 00	4.0814E 02
1150	8.3802E-01	1.7334E 01	7.7896E-02	8.1313E 08	2.4378E-01	4.7625E-01	4.4269E 00	3.9685E 02
1160	8.8308E-01	1.6501E 01	9.6159E-02	8.1744E 08	2.4549E-01	4.3182E-01	4.5169E 00	3.8602E 02
1170	9.2975E-01	1.5720E 01	1.1827E-01	8.2175E 08	2.4720E-01	3.9218E-01	4.6070E 00	3.7564E 02
1180	9.7800E-01	1.4987E 01	1.4497E-01	8.2605E 08	2.4891E-01	3.5676E-01	4.6973E 00	3.6568E 02
1190	1.0279E 00	1.4299E 01	1.7709E-01	8.3035E 08	2.5063E-01	3.2505E-01	4.7877E 00	3.5612E 02
1200	1.0794E 00	1.3652E 01	2.1559E-01	8.3464E 08	2.5236E-01	2.9663E-01	4.8781E 00	3.4694E 02

Appendix E

Enthalpy of Reaction

Reaction No.	Reaction
1	$C_2H_6 \rightarrow C_2H_4 + H_2$
2	$C_2H_6 \rightarrow CH_4 + \frac{1}{2}C_2H_4$
3	$C_2H_4 \rightarrow C_2H_2 + H_2$
4	$C_2H_2 \rightarrow 2C + H_2$
5	$2C_2H_2 \rightarrow C_4$'s
6	$C + H_2O \rightarrow CO + H_2$

Enthalpy of Reaction

Temp °K	1	2	3	4	5	6	7	8
800	1.1885E 04	-1.3812E 04	5.2747E 04	9.9585E 02	1.1828E 03	-2.7691E 04	3.3780E 03	-7.6240E 03
810	1.1900E 04	-1.3825E 04	5.2766E 04	1.0113E 03	1.2024E 03	-2.7684E 04	3.3845E 03	-7.6428E 03
820	1.1915E 04	-1.3839E 04	5.2784E 04	1.0268E 03	1.2222E 03	-2.7677E 04	3.3906E 03	-7.6618E 03
830	1.1928E 04	-1.3853E 04	5.2801E 04	1.0423E 03	1.2421E 03	-2.7671E 04	3.3962E 03	-7.6809E 03
840	1.1942E 04	-1.3867E 04	5.2817E 04	1.0579E 03	1.2620E 03	-2.7665E 04	3.4013E 03	-7.7003E 03
850	1.1954E 04	-1.3881E 04	5.2833E 04	1.0735E 03	1.2821E 03	-2.7659E 04	3.4060E 03	-7.7198E 03
860	1.1967E 04	-1.3896E 04	5.2848E 04	1.0891E 03	1.3022E 03	-2.7653E 04	3.4102E 03	-7.7394E 03
870	1.1978E 04	-1.3911E 04	5.2862E 04	1.1047E 03	1.3225E 03	-2.7648E 04	3.4140E 03	-7.7592E 03
880	1.1989E 04	-1.3926E 04	5.2875E 04	1.1203E 03	1.3428E 03	-2.7643E 04	3.4174E 03	-7.7791E 03
890	1.2000E 04	-1.3941E 04	5.2888E 04	1.1360E 03	1.3632E 03	-2.7639E 04	3.4204E 03	-7.7992E 03
900	1.2010E 04	-1.3956E 04	5.2900E 04	1.1516E 03	1.3837E 03	-2.7634E 04	3.4229E 03	-7.8193E 03
910	1.2020E 04	-1.3972E 04	5.2912E 04	1.1673E 03	1.4042E 03	-2.7630E 04	3.4251E 03	-7.8396E 03
920	1.2029E 04	-1.3988E 04	5.2923E 04	1.1829E 03	1.4248E 03	-2.7626E 04	3.4269E 03	-7.8599E 03
930	1.2037E 04	-1.4004E 04	5.2933E 04	1.1986E 03	1.4455E 03	-2.7623E 04	3.4283E 03	-7.8803E 03
940	1.2045E 04	-1.4020E 04	5.2943E 04	1.2142E 03	1.4662E 03	-2.7620E 04	3.4293E 03	-7.9009E 03
950	1.2053E 04	-1.4036E 04	5.2952E 04	1.2299E 03	1.4870E 03	-2.7617E 04	3.4299E 03	-7.9214E 03
960	1.2060E 04	-1.4052E 04	5.2961E 04	1.2455E 03	1.5078E 03	-2.7614E 04	3.4302E 03	-7.9421E 03
970	1.2067E 04	-1.4069E 04	5.2968E 04	1.2611E 03	1.5287E 03	-2.7611E 04	3.4301E 03	-7.9628E 03
980	1.2073E 04	-1.4086E 04	5.2976E 04	1.2767E 03	1.5497E 03	-2.7609E 04	3.4297E 03	-7.9836E 03
990	1.2078E 04	-1.4102E 04	5.2983E 04	1.2923E 03	1.5707E 03	-2.7607E 04	3.4289E 03	-8.0044E 03
1000	1.2084E 04	-1.4119E 04	5.2989E 04	1.3078E 03	1.5917E 03	-2.7605E 04	3.4278E 03	-8.0252E 03
1010	1.2088E 04	-1.4136E 04	5.2994E 04	1.3233E 03	1.6128E 03	-2.7604E 04	3.4264E 03	-8.0461E 03
1020	1.2093E 04	-1.4154E 04	5.3000E 04	1.3388E 03	1.6339E 03	-2.7602E 04	3.4247E 03	-8.0670E 03
1030	1.2097E 04	-1.4171E 04	5.3004E 04	1.3543E 03	1.6551E 03	-2.7601E 04	3.4226E 03	-8.0879E 03
1040	1.2100E 04	-1.4188E 04	5.3008E 04	1.3697E 03	1.6763E 03	-2.7600E 04	3.4202E 03	-8.1089E 03
1050	1.2103E 04	-1.4206E 04	5.3012E 04	1.3851E 03	1.6975E 03	-2.7600E 04	3.4176E 03	-8.1299E 03
1060	1.2106E 04	-1.4223E 04	5.3015E 04	1.4005E 03	1.7188E 03	-2.7599E 04	3.4146E 03	-8.1509E 03
1070	1.2108E 04	-1.4241E 04	5.3018E 04	1.4159E 03	1.7401E 03	-2.7599E 04	3.4114E 03	-8.1719E 03
1080	1.2110E 04	-1.4258E 04	5.3020E 04	1.4312E 03	1.7614E 03	-2.7599E 04	3.4078E 03	-8.1929E 03
1090	1.2111E 04	-1.4276E 04	5.3021E 04	1.4464E 03	1.7827E 03	-2.7599E 04	3.4040E 03	-8.2139E 03
1100	1.2112E 04	-1.4294E 04	5.3023E 04	1.4617E 03	1.8041E 03	-2.7599E 04	3.3999E 03	-8.2349E 03
1110	1.2113E 04	-1.4312E 04	5.3023E 04	1.4768E 03	1.8255E 03	-2.7600E 04	3.3956E 03	-8.2559E 03
1120	1.2113E 04	-1.4330E 04	5.3024E 04	1.4920E 03	1.8469E 03	-2.7601E 04	3.3910E 03	-8.2769E 03
1130	1.2113E 04	-1.4348E 04	5.3024E 04	1.5071E 03	1.8683E 03	-2.7602E 04	3.3861E 03	-8.2979E 03
1140	1.2113E 04	-1.4366E 04	5.3023E 04	1.5222E 03	1.8898E 03	-2.7603E 04	3.3810E 03	-8.3189E 03
1150	1.2112E 04	-1.4384E 04	5.3022E 04	1.5372E 03	1.9113E 03	-2.7604E 04	3.3756E 03	-8.3399E 03
1160	1.2111E 04	-1.4402E 04	5.3021E 04	1.5522E 03	1.9328E 03	-2.7606E 04	3.3699E 03	-8.3609E 03
1170	1.2109E 04	-1.4420E 04	5.3019E 04	1.5672E 03	1.9543E 03	-2.7607E 04	3.3641E 03	-8.3819E 03
1180	1.2107E 04	-1.4439E 04	5.3017E 04	1.5821E 03	1.9758E 03	-2.7609E 04	3.3580E 03	-8.4029E 03
1190	1.2105E 04	-1.4457E 04	5.3015E 04	1.5970E 03	1.9973E 03	-2.7611E 04	3.3517E 03	-8.4238E 03
1200	1.2102E 04	-1.4476E 04	5.3012E 04	1.6118E 03	2.0189E 03	-2.7614E 04	3.3451E 03	-8.4448E 03

Appendix F

Computer Program

```
      FUNCTION PRR(IS)                                                  10
      COMMON/PD/RAD,P(25),DN,SMWT(25),CLJ(25,2),IS,VI(25),AMWT,VEL1,DL  20
      COMMON/TM/TMPH,RADI(100),DE(25),ZIC,ZTT                           30
      COMMON/SET/MY,MZ,IB                                               40
      PT=0.                                                             50
      PT2=0.                                                            60
      HRS=IB
      DO 1 I=1,IS                                                       80
      IF(CLJ(I,2).NE.0.)PT2=PT2+P(I)                                    90
    1  PT=PT+P(I)                                                       100
      DO 2 I=1,IS                                                       110
      IF(CLJ(I,2).EQ.0.)GO TO 5                                         120
      GO TO 2                                                           130
    5 IJ=100.001-(ZTT-ZIC)/ZTT*99.                                      140
      VOL=TMPH*SMWT(I)*P(I)/PT/DE(I)*HRS                                150
      PI=3.14159                                                        160
      DLR=ZTT/100.                                                      170
      IF((RADI(IJ)**2-VOL/DLR/PI).LE.0.)MZ=5000
      IF(MZ.EQ.5000)RETURN
      RADI(IJ)=SQRT(RADI(IJ)**2-VOL/DLR/PI)                             180
      IF(CLJ(I,2).EQ.0.)P(I)=0.                                         190
    2 P(I)=P(I)*PT/PT2                                                  200
      PRR=PT                                                            210
      IF((MY.EQ.1).AND.(MZ.EQ.1))GO TO 1001                             220
      RETURN                                                            230
 1001  WRITE(6,9001)PRR,RADI(1),VOL                                     240
 9001 FORMAT(' FUNCTION PRR(IS)'/' PR='1PE14.5,5X'RADI(1)='1PE14.5,5X'  250
     1VOL='1PE14.5)                                                     260
      RETURN                                                            270
      END                                                               280
```

```
      FUNCTION REQC(T,I)                                                290
      COMMON/FE/DCP(25,4),HO(25),SO(25),FD(25),FI(25)                   300
      COMMON/SET/MY,MZ                                                  310
      R=1.987                                                           320
      RR=1.3143                                                         330
      ELNK=-HO(I)/R/T+DCP(I,1)/R*LOG(T)+DCP(I,2)/(2.*R)*T+DCP(I,3)/(6.*R 340
     1)*T*T+DCP(I,4)/(12.*R)*T**3+FI(I)                                 350
      REQC=EXP(-ELNK)                                                   360
      IF((MY.EQ.1).AND.(MZ.EQ.1))GO TO 1001                             370
      RETURN                                                            380
 1001  WRITE(6,9001)REQC,T,I                                            390
 9001 FORMAT(' FUNCTION REQC(T,I)'/' REQC(T,I)=',DPE14.5,'('F7.2',I2')') 400
      RETURN                                                            410
      END                                                               420
```

```
      FUNCTION PRESD(T)                                                 430
      COMMON/PD/RAD,P(25),DN,SMWT(25),CLJ(25,2),IS,VI(25),AMWT,VEL1,DL  440
      COMMON/PT2/TT,RN1,RN2,VIS
      COMMON/SET/MY,MZ                                                  460
      PT=PRR(IS)                                                        470
      IF(MZ.EQ.5000)RETURN
C THIS SUBROUTINE CALULATES PRESSURE DROP FROM BERNOULIE LAW            480
C MODIFIED TO TAKE FRICTION LOSS INTO CONSIDERATION                     490
      IF(MY.NE.1)GO TO 1
      IF(MZ.NE.1)GO TO 11
      A=0.4398818                                                       510
      B=-0.44245917                                                     520
      C=0.086401820                                                     530
      D=-0.0077484511                                                   540
      PRESDT=0.                                                         550
11    DO 2 I=1,IS
      IF(CLJ(I,2).EQ.0) GO TO 2                                         570
      E=LOG(T/CLJ(I,2))                                                 580
      VI(I)=2.66D3E-5*SQRT(SMWT(I)*T)/(CLJ(I,1)**2*EXP(A+B*E+C*E**2+D*E* 590
     1*3))                                                              600
2     CONTINUE                                                          610
      VIS=0.                                                            620
      DO 3 I=1,IS                                                       630
      IF(CLJ(I,1).EQ.0.)GO TO 3                                         640
      V=P(I)/PT*VI (I)                                                  650
      U=0.                                                              660
      DO 4 J=1,IS                                                       670
      IF(CLJ(J,1).EQ.0.)GO TO 4                                         680
      U=U+P(J)/PT*1./SQRT(8.)/(1.+SMWT(I)/SMWT(J))*(1.+(VI(I)/VI(J))**.5 690
     1*(SMWT(J)/SMWT(I))**.25)**2                                       700
4     CONTINUE                                                          710
      VIS=VIS+V/U                                                       720
3     CONTINUE                                                          730
      VIS=VIS*.0672                                                     740
1     AMWT=0.                                                           750
      VEL2=1.1620929E-4*T/(PT-PRESDT)/RAD**2*DN
      DO 5 I=1,IS                                                       760
5     AMWT=P(I)/PT*SMWT(I)+AMWT                                         770
C     GC IN AT.*FT**3  /(OK LB.MOLES)                                   780
      GC=1.3143                                                         790
      DEN=PT/(GC*T)*AMWT                                                800
      IF(DEN.LE.0.)GO TO 21                                             810
6     VELA=(VEL1+VEL2)/2.                                               820
      RENU=2.*RAD*DEN*VELA/VIS                                          830
      IF(RENU.LE.0.)GO TO 19                                            840
      IF(RENU.LE.3500.)GO TO 20                                         850
      GO TO 10                                                          860
20    F=64./RENU                                                        870
      GO TO 100                                                         880
10    F=0.00560+.5/(RENU**.32)                                          890
```

```
      95 100  PRESD=DEN*(VELA**2*F*DL/RAD+VEL2**2-VEL1**2)/62.4/2116.8                900
      96      PRESD=ABS(PRESD)                                                        910
      97      P2=PT-PRESD                                                             920
      98      IF(P2.LE.0.)GO TO 21
      99      VEL2=1.1620929E-04*T/P2/RAD**2*DN                                       930
     100      IF(PRESD.EQ.0.)GO TO 7                                                  940
     101      IF(ABS((PRESDT-PRESD)/PRESD).LE..001)GO TO 7                            950
     102      PRESDT=PRESD                                                            960
     103      DEN=(P2+PT)/(2.*GC*T)*AMWT                                              970
     104      GO TO 6                                                                 980
     105 7    PT2=0.                                                                  990
     106      DO 9 I=1,IS                                                            1000
     107 9    PT2=PT2+P(I)                                                           1010
     108      DO 8 I=1,IS                                                            1020
     109 8    P(I)=P(I)*(PT2-PRESD)/PT2                                              1030
     110      IF((MY.EQ.1).AND.(MZ.EQ.1))GO TO 1001                                  1040
     111      VEL1=VEL2                                                              1050
     112      IF(VEL1.GE.1214.5)GO TO 22
     113      IF(VEL1.GE.SQRT(7.37495E4*P2/DEN))GO TO 22
     114      RETURN                                                                 1060
     115 22   MZ=3000
     116      PT=.5
     117      RETURN
     118 1001  WRITE(6,9001)RENU, VIS,DEN,F,VEL1,VEL2,VELA,T ,PRESD                  1070
     119      VEL1=VEL2                                                              1080
     120      RETURN                                                                 1090
     121 19   WRITE(6,900)RAD,DEN,VELA,VIS,RENU                                      1100
     122      WRITE(6,902)T,PT,(P(I),I=1,IS),GC,AMWT,P2
     123      MZ=2000
     124      RETURN                                                                 1110
     125 21   WRITE(6,902)T,PT,(P(I),I=1,IS),GC,AMWT,P2
     126      MZ=2000
     127      RETURN
     128 900  FORMAT(' RAD='1PE12.5'DEM,VELA,VIS,RENU'4(2X,1PE12.5))                 1140
     129 901  FORMAT(' PRESSURE DROP ='1PE12.5'DEN,VELA,DL,VEL1,VEL2'5(2X,1PE12.,   1150
     130      15))                                                                   1160
     131 902  FORMAT(' T PT P(1)-&(12), GC AMWT '10(1X,F8.2))
     132 9001 FORMAT(' FUNCTION PRESD(T)'/' RENU='1PE14.5,5X'VIS='1PE14.5,5X'DEN    1180
     133     1='1PE14.5,/' FRICTION FACTOR= '1PE14.5,5X'V1,V2,VA='3(1PE14.5,5X)/    1190
     134     1' TEMPERTURE='0PF8.2,'PRESSURE D='1PE14.5)                            1200
     135      END                                                                    1210
```

```
      FUNCTION HEATR(T2,I)                                              1220
      COMMON/FE/DCP(25,4),HT(25),ST(25)                                 1230
      COMMON/SET/MY,MZ                                                  1240
      TI=T2                                                             1250
      HEATR=HT(I)                                                       1260
      T1=298.15                                                         1270
      DO 1 L=1,4                                                        1280
      X=L                                                               1290
    1 HEATR=HEATR+DCP(I,L)*(T2**L/X-T1**L/X)
      IF((MY.EQ.1).AND.(MZ.EQ.1))GO TO 1001                             1310
      RETURN                                                            1320
 1001  WRITE(6,9001)HEATR,T2,I                                          1330
      RETURN                                                            1340
 9001 FORMAT(' HEATR(T,I)'/  (PE14.5'('OPF8.2','I2')'))                 1350
      END                                                               1360
```

```
      PROGRAM PYRO                                                          1380
      COMMON IA(25,10),SF(25),Z(11),SR(25),B(25,10),C(25),ENAME(500),       1420
     1CP(25,4),EA(25),EE(25),IDATB(44),DH(25),DS(25),      DF(25),BB(25,    1400
     2 10)                                                                  1410
      COMMON/FE/DCP(25,4),HT(25),ST(25),FT(25),FI(25)                       1420
      COMMON/PD/RAD,P(25),DN,SMWT(25),CLJ(25,2),IS,VI(25),AMWT,VEL1,DL
      COMMON/PT2/TT,RN1,RN2,VIS                                             1440
      COMMON/TM/TMPH,RADI(100),DE(25),ZIC,ZTT                               1450
          COMMON/SET/MY,MB,IB                                               1460
      DIMENSION DXA(25),TM(25),PPI(25),RADF(100),CARD(80)
      DIMENSION WZIC(50),WT(50),WTMPH(50),WPT(50),WVEL1(50),WC(25,50),WT
     1M(25,50),WDXA(25,50),F(25)
      DIMENSION RADD(100,25)
      DATA DXA/25*0./,F/25*1./
       INTEGER IDATA(43)/'A','B','C','D','E','F','G','H','I','J','K','L'   1860
     1,'M','N','O','P','Q','R','S','T','U','V','W','X','Y','Z','->','+'    1870
     2,' ','1','2','3','4','5','6','7','8','9','0','<','=','>'/            1880
      INTEGER IDATP(9)/'1N','2N','3N','4N','5N','6N','7N','8N','9N'/
      IDATP(1)=IDATP(1)
      IB=1                                                                  1480
      IGUTO=1                                                               1490
  107 READ(5,953),ID,F(ID)
      IF(ID.EQ.25)GO TO 100
      GO TO 107
  100 READ(5,900,END=99)IR,IS                                               1500
C IR=TOTAL NUMBER OF REACTIONS,IS=TOTAL NUMBER OF CHEMICAL SPECIES          1510
      READ(5,943)IGOW,(Z(II),II=1,11)                                       1520
      READ(5,950)CARD                                                       1530
      READ(5,958)IB,IZZ,IPLOT
      READ(5,919)T,PT,PRES,ZT,DL,POUT                                       1540
      TIN=T                                                                 1550
C IA(I,M)=IDENTITY OF CHEMICAL SPECIES IN CHEMICAL REACTION POSITION M      1560
      INTEGER SF,SR                                                         1570
      GC=1.3143                                                             1580
      READ(5,901)(SF(I),SR(I),I=1,IR)                                       1590
      DO 1 I=1,IR                                                           1600
      IT=SF(I)+SR(I)                                                        1610
      READ(5,901)ID,(IA(I,M),M=1,IT)                                        1620
    1 IF (ID.NE.I)GO TO 101                                                 1630
C B(I,M)COEFFICIENT OF M CHEMICAL SPECIES IN REACTION I                     1640
      DO 2 I=1,IR                                                           1650
      IT=SF(I)+SR(I)                                                        1660
      READ(5,903)ID,(B(I,M),M=1,IT),(BB(I,M),M=1,IT)                        1670
    2 IF(ID.NE.I)GO TO  102                                                 1680
C C(J) IS THE INITIAL CONCENTRATION OF THE J COMPONENT (8 PER CARD)         1690
      READ(5,904)(C(J),J=1,IS)                                              1700
      CT=0.                                                                 1710
      DO 18 I=1,IS                                                          1720
      P(I)=C(I)                                                             1730
      PPI(I)=C(I)                                                           1740
```

```
      PT=CT+P(I)                                                        1750
   18 C(I)=P(I)/GC/T                                                    1760
    C ENAME(I)IS THE NAME OF EACH COMPONENT (MAX 20 LETTERS) 4 PER CARD) 1770
      IT=IS*20                                                          1780
      READ(5,905)(ENAME(J),J=1,IT)                                      1790
      DO 3 J=1,IS                                                       1800
      READ(5,906) (CP(J,M),M=1,4),ID                                    1810
    3 IF(ID.NE.J)GO TO 103                                              1820
      DO 4 I=1,IR                                                       1830
      READ(5,907)ID,EA(I),EE(I)                                         1840
      EA(I)=EA(I)*F(I)
    4 IF (ID.NE.I)GO TO 104                                             1850
      DO5 J=1,IS                                                        1890
      READ(5,908) ID,DS(J),DH(J),DF(J)                                  1900
    5 IF(ID.NE.J) GO TO 105                                             1910
      DO 21 J=1,IS                                                      1920
      READ(5,911) ID,(CLJ(J,M),M=1,2),SMWT(J)                           1930
      IF(CLJ(J,2).EQ.0.)READ(5,940)DE(J)                                1940
   21 IF(ID.NE.J)GO TO 106                                              1950
      DO 6 I=1,IR                                                       1960
      DO 7 L=1,4                                                        1970
    7 DCP(I,L)=0.                                                       1980
      I1=SF(I)+1                                                        1990
      I2=SR(I)+SF(I)                                                    2000
      DO 8 M=I1,I2                                                      2010
      J=IA(I,M)                                                         2020
      DO 8 L=1,4                                                        2030
    8 DCP(I,L)=DCP(I,L)+B(I,M)*CP(J,L)/B(I,1)
      I2=SF(I)                                                          2050
      DO 6 M =1,I2                                                      2060
      J=IA(I,M)                                                         2070
      DO 6 L=1,4                                                        2080
    6 DCP(I,L)=DCP(I,L)-B(I,M)*CP(J,L)/B(I,1)
    C TEMPERATURE                                                       2100
      R1=1.987                                                          2110
      DO 9 I=1,IR                                                       2120
      FT(I)=0.                                                          2130
      ST(I)=0                                                           2140
      HT(I)=0                                                           2150
      I1=SF(I)+1                                                        2160
      I2=SR(I)+SF(I)                                                    2170
      DO 10 M=I1,I2                                                     2180
      J=IA(I,M)                                                         2190
      ST(I)=ST(I) +B(I,M)*DS(J)/B(I,1)                                  2200
      FT(I)=FT(I)+B(I,M)*DF(J)/B(I,1)                                   2210
   10 HT(I)=HT(I)+B(I,M)*DH(J)/B(I,1)                                   2220
      I2=SF(I)                                                          2230
      DO 9 M=1,I2                                                       2240
      J=IA(I,M)                                                         2250
      FT(I)=FT(I)-B(I,M)*DF(J)/B(I,1)                                   2260
```

```
  251          ST(I)=ST(I)-B(I,M)*DS(J)/B(I,1)                                  2270
  252 9        HT(I)=HT(I)-B(I,M)*DS(J)/B(I,1)                                  2280
  253          DO19  I=1,IR                                                     2290
  254          TT=298.15                                                        2300
  255          DO 29 M=1,4                                                      2310
  256          X=M                                                              2320
  257 29       HT(I)=HT(I)-DCP(I,M)/X*TT*M                                      2330
  258          READ(5,908)IJ,TT,FI(I)
  259          IF(FI(I).GT.0.)FI(I)=LOG(FI(I))
  260 19       FI(I)=HEATR(TT,I)/R1/TT+FI(I)-DCP(I,1)/R1*LOG(TT)-DCP(I,2)/2./R1*T
  261         1T-DCP(I,3)/6./R1*TT**2-DCP(I,4)/12./R1*TT**3
  262 C  NOW WE HAVE THE REACTION SYSTEM, IT WILL BE PRINTED OUT.               2380
  263 C COMPONENT IDENTIFICATION                                                2390
  264          WRITE(6,909)                                                     2400
  265          WRITE(6,910)                                                     2410
  266          DO 11 J=1,IS                                                     2420
  267          JJ1=1+20*(J-1)                                                   2430
  268           JJ2=20*J                                                        2440
  269 11       WRITE(6,912)(ENAME(JJ),JJ=JJ1,JJ2),IDATA(J),J,(CP(J,M),M=1,4),DH(J  2450
  270         1),DS(J),DF(J)                                                   2460
  271          IGOTO=1                                                          2470
  272          WRITE(6,920)                                                     2480
  273          DO 17 J=1,IS                                                     2490
  274          JJ1=1+20*(J-1)                                                   2500
  275           JJ2=20*J                                                        2510
  276 17       WRITE(6,917)(ENAME(JJ),JJ=JJ1,JJ2),IDATA(J),J,(CLJ(J,M),M=1,2),SMW  2520
  277         1T(J),C(J)                                                       2530
  278          WRITE(6,913)                                                     2540
  279          DO 12 I=1,IR                                                     2550
  280          II=2                                                             2560
  281          IF (EE(I).EQ.0.)II=1                                             2570
  282          I2=SE(I)                                                         2580
  283          DO 14 M=1,I2                                                     2590
  284          J=IA(I,M)                                                        2600
  285          MM=M*3-1                                                         2610
  286          IDATB(MM)=IDATA(J)                                               2620
  287          J=B(I,M)+29.01                                                   2630
  288          MM=M*3-2                                                         2640
  289          IDATB(MM)=IDATA(J)                                               2650
  290          MM=M*3                                                           2660
  291 14       IDATB(MM)=IDATA(28)                                              2670
  292          MM=SF(I)*3                                                       2680
  293          KK=40                                                            2690
  294          GO TO (122,121),II                                               2700
  295 121      IDATB(MM)=IDATA(KK)                                              2710
  296          MM=MM+1                                                          2720
  297 122      KK=KK+1                                                          2730
  298          IDATB(MM)=IDATA(KK)                                              2740
  299          MM=MM+1                                                          2750
  300          KK=KK+1                                                          2760
```

```
      IDATB(MM)=IDATA(KK)                                                2770
      I1=SF(I)+1                                                         2780
      I2=SF(I)+SR(I)                                                     2790
      DO 15 M=I1,I2                                                      2800
      J=IA(I,M)                                                          2810
      MM=M*3-1 +II                                                       2820
      IDATB(MM)=IDATA(J)                                                 2830
      J=B(I,M)+29.01                                                     2840
      MM=M*3-2+II                                                        2850
      IDATB(MM)=IDATA(J)                                                 2860
      MM=M*3+II                                                          2870
   15 IDATB(MM)=IDATA(28)                                                2880
      DO 16 J=MM,44                                                      2890
   16 IDATB(J)=IDATA(29)                                                 2900
   12 WRITE(6,915)I,(IDATB(M),M=1,40),EA(I),EE(I),(DCP(I,M),M=1,4)       2910
      WRITE(6,927)                                                       2920
      DO 28 J=1,IR                                                       2930
      I2=SF(J)+SR(J)                                                     2940
      DO 32 I=1,I2                                                       2950
      I3=IA(J,1)                                                         2960
   32 IDATB(I)=IDATA(I3)                                                 2970
   28 WRITE(6,926)J,FT(J),FI(J),(IDATB(I),BB(J,I),I=1,I2)                2980
      READ(5,902),RAD,TMPH                                               2990
      READ(5,900)KEYR,KEYP                                               3000
      TMPHI=TMPH                                                         3010
      RADU=RAD                                                           3020
      ZTT=ZT                                                             3030
      IGOTO=1                                                            3040
      PDP=.2
      PSAVE=5.85
      IF(KEYR.EQ.0)GO TO 92
  110 WRITE(6,918)                                                       3050
      HR=0.
      MAZE=1
      KK=1
C T=GAS TEMPERATURE AT ENTRANCE, PRES=PRESSURE OF GAS, ZT=LENGTH OF REAC 3060
      HR=0.                                                              3070
C DZ=INCREMENTAL CHANGE IN REACTOR,CI=CONCENTRATION OF INERTS, A=T=A(1)+  3090
C A(2)Z + A(3) Z**L + A(4)*Z**3                                          3100
  900 FORMAT(2I2)                                                        3110
  901 FORMAT(40I2)                                                       3120
  902 FORMAT(2F10.5)                                                     3130
  903 FORMAT(I2,25F3.2)                                                  3140
  904 FORMAT(12F6.5)                                                     3150
  905 FORMAT(80A1)                                                       3160
  906 FORMAT(4E16.8,I7)                                                  3170
  907 FORMAT(I2,E7.1,F10.4)                                              3180
  908 FORMAT(I2,3F9.2)                                                   3190
  909 FORMAT('1  PROGRAM PYRO'/' PROGRAMMER RICHARD ROBERTSON'/' DR. HAN 3200
     1ESIAN ADVISOR'/' AS MASTER THESIS REQUIREMENT')                    3210
```

```
      910  FORMAT (1H1'IDENTIFICATION OF REACTION SYSTEM!/T5'COMPONENT'T22'CO      3220
      1 NO.'T44'HEAT CAPACITY DATA'T81'DELTA-H'T98'DELTA-S'T116'LOG(K) '/        3230
     1T29'A',T43'B',T56'C',T68,'D')                                              3240
      911  FORMAT(I2,3X,3F5.0)                                                    3250
      912  FORMAT(' ',20A1,1A1 ,I2,4(2X,1PE10.3),3(3X,1PE15.8))                  3260
      913  FORMAT(1H1,'REACTION SYSTEM!/' EQUATION',T45,'ARRHENIUS  RATE CONS     3270
     1TANT',T75,'DELTA HEAT CAPACITY  DATA FOR REACTION'/1H T71'DELTA A          3280
     2',T83,'DELTA B'T95,'DELTA C',T107'DELTA D',T51'K(0)',T61'E')               3290
      915  FORMAT(1H ,I2,2X,40A1,6(1PE10.3,2X))                                   3300
      916  FORMAT(1H )                                                            3310
      917  FORMAT(' ',21A1,I2,5X,F5.3,5X,F5.1,5X,F7.2,1PE12.4)                    3320
      918  FORMAT(1H1)                                                            3330
      919  FORMAT(6E12.5)                                                         3340
      920  FORMAT('0  COMPONET',T19,'CO NO',T36,'LENNARD-JONES  MOL. WT.',T62     3350
     1'INITAL CONCENTRATION'/T36'PARAMETERS'/T31'(A)     (DEG-K)')               3360
      921  FORMAT('1COMPONENT     IDENTIFICATION'I2' OUT OF PLACE 'I5,' ID')
      924  FORMAT('1ARRHENIUS     IDENTIFICATION'I2' OUT OF PLACE 'I5,' ID')
      925  FORMAT('1ENTHALPHY     IDENTIFICATION'I2' OUT OF PLACE 'I5,' ID')
      926  FORMAT(' 'I2,2(5X,1PE12.5),5X,6(5X,1A1,'**('0PF3.1')'))                3420
      927  FORMAT('0','EQ',T13'LOG(K) REACTION  CONSTANT OF INTEGERATION '
     110X,'ORDER  OF REACTION BY CONPONENT')                                     3440
      928  FORMAT(' 'I2,1PE14.4,E14.4,E14.4)                                      3450
      929  FORMAT(' ITERATION NUMBER='I3,/' NO CONCENTRATION      TMPH           3460
     1   DXA')                                                                   3470
      930  FORMAT('0 DL CHANGED  TO'1PE15.5,5X,'ZIC='1PE14.5)                     3480
      931  FORMAT('1  ALL DXA= 0, SYSTEM MUST BE CHANGED TO ALLOW REACTION')      3490
      932  FORMAT (' I='I2,2X'RA='1PE14.5,2X'DXA(I)='1PE14.5,2X'CF,CR='2E14.5     3500
     1,2X'REQC='1PE14.5,/5HORATE'='1PE14.5)                                      3510
      933  FORMAT(' ' 25(1PE14.5,5X,I2/' '))                                      3520
      934  FORMAT(' 'I2,1PE12.5)                                                  3530
      935  FORMAT('1',' LENNARD JONES CONSTANTS',I2,'CARD ID',I2,'INTERNAL')      3540
      936  FORMAT('0',3(5X,1PE16.7))                                              3550
      937  FORMAT('1REACTOR IS 'F10.2' FEET LONG AND 'F6.3' FEET IN RADIUS'/'     3560
     1 TOTAL MOLES  / HOUR ARE'F6.1'POUND MOLES  AT PRESSURE'F8.3'A  VEL        3570
     2OCITY OF '1PE12.5' AT TEMPERATURE'0PF8.1'DEG K'/' INITIAL REACTOR          3580
     3INCREMENT(DL'1PE12.5'FEET')                                                3590
      938  FORMAT(' 'I2,14X,1PE14.4)                                              3600
      939  FORMAT(' ',I2,1PE14.5,E14.5)                                           3610
      940  FORMAT(F10.0)                                                          3620
      942  FORMAT(' PRESSURE IS'1PE14.5'    VELOCITY'1PE14.4'FEET/SEC.')          3630
      943  FORMAT(I3,11F7.2)                                                      3640
      944  FORMAT(' '10(F9.6,2X))                                                 3650
      945  FORMAT('1',T25,'REACTOR RADIUS PROFILE AFTER  'F9.2,'  HOURS'//)
      946  FORMAT(' 'I2,'=',1A1,2X,20A1,1PE14.5,5X,E14.5)                         3670
      948  FORMAT(' 'I2,1PE14.4,E14.4)                                            3680
      949  FORMAT('; UNSTABLE TEMPERATURE PROFILE NEW CASE')                       369
      950  FORMAT(80A1)                                                           3700
      951  FORMAT(' '80A1)                                                        3710
      952  FORMAT('0VELOCITY OF GAS GREATER THAN SOUND')
      953  FORMAT(I2,E8.2)
```

```
401 954   FORMAT(!0 REACTOR TUBE COMPLETELY BLOCKED WITH CARBON!)
402 955   FORMAT(! REACTOR RADIUS PROFILE FROM START TO CLOSE DOWN!)
403 956   FORMAT(T20,'TEMPERATURE REACTANT PRODUCT PROFILES!)
404 958   FORMAT(313)
405 960   FORMAT(T9'0%'T29'20%'T49'40%'T69'60%'T89'80'T109'100%!)
406 961   FORMAT(! !F4.0,'FT!)
407 922   FORMAT(!1COEFFICIENT IDENTIFICATION!I2! OUT OF PLACE !I5,! ID!)
408 923   FORMAT(!1CP(HEAT CAP) IDENTIFICATION!I2! OUT OF PLACE !I5,! ID!)
409 962   FORMAT(T15'|!T25'|!T35'|!T45'|!T55'|!T65'|!T75'|!T85'|!T95'|!T105!
410       1|!T115'|!)
411 963   FORMAT(!0 REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(
412       1P) AFTER!F8.0!HOURS OF RUN!)
413 965   FORMAT(!0CONVERSION OF !20A1!TO !20A1!IS!F6.2!%!)
414 966   FORMAT(! 0. FT!T60!|/T59!CL!)
415 967   FORMAT(///,25X,80A1)
416 968   FORMAT(! 'F8.2! FT!T59!CL!/T60!|!)
417 969   FORMAT(! !I4,3X,3(! ',1PE11.4,9E11.4,/))
418 970   FORMAT(!1TEMP EQUILIBRUM CONSTANTS!/!0!T30!EQUATION S NUMBER!
419       1/,5X,10(5X,I2,4X))
420 973   FORMAT(! ',I5,4X,13(F7.3,2X))
421 9934  FORMAT(! REACTOR POSITION!1PE14.5!FEET!/' TEMPERTURE!0PF8.2!DEGREE   3720
422       1=K MOLAR FLOW RATE!1PE14.5!POUND MOLES PER HOUR!)                  3730
423 C     DENC= DENSITY OF CARBON AT UI 1200DEG. F                            3740
424 C TEMPERTURE ON OUTSIDE WALL OF REACTOR WILL BE ASSUMED CONSTANT           3750
425 CC  RAD=RADIUS OFPIPE IN FEET                                             3760
426       ISS=MAXO(IR,IS)
427       IM=MINO(IR,IS)                                                      3770
428       IGO=1                                                               3780
429       IF(IR.EQ.IS)IGO=3                                                   3790
430       IF(IR.LT.IS)IGO=2                                                   3800
431       RAD=RADU                                                            3810
432       DO 48 I=1,100                                                       3820
433       RADF(I)=RAD                                                         3830
434 48    RADI(I)=RAD                                                         3840
435       ITEST=1                                                             3850
436 58    MA=1                                                                3860
437       TMPH=TMPHI                                                          3870
438       PT=PI                                                               3880
439       PT=0.                                                               3890
440       DO 57 I=1,IS                                                        3900
441 57    PT=PT+P(I)                                                          3910
442       DO 60 I=1,100                                                       3920
443 60    RADI(I)=RADF(I)                                                     3930
444       RAD=RADF(1)                                                         3940
445       T=TIN
446       PI=PT                                                               3950
447       VEL1=1.162029600E-4*TMPH*T/PT/RAD**2                                3960
448       WRITE(6,937)ZT,RAD,TMPH,PT,VEL1,T,DL                               3970
449       R=1.987                                                             3980
450       ZT=ZTT                                                              3990
```

```
      MT=ZT/DL                                                          4000
      ZIC=0.                                                            4010
      MI=8                                                              4020
      M10=MT*1000                                                       4030
      MMM=1                                                             4040
      MZ=0.
      ZICI=0.
      DL=ZTT*.01001
      DO 30 MB=1,M10
      DO 30 MY=1,MI
25    DLL=MI*(MZ-1)+MY                                                  4070
      IF(MA.GT.9)GO TO 55                                               4080
      ZIC=ZIC+DL                                                        4090
      IF(ZIC.GE.ZTT)GO TO 33
      XN=ZIC/ZTT*10.+1.
      IIN=XN
      XXN=IIN
      TR=Z(IIN)+(Z(IIN+1)-Z(IIN))*(XN-XXN)
      RAF=RAD                                                           4120
      IJ=100.001-(ZTT-ZIC)/ZTT*99.                                      4130
      RIJ=IJ                                                            4140
      RJ=100.000-(ZTT-ZIC)/ZTT*99.                                      4150
      IF(IJ.LE.99)RAD=RADF(IJ)+(RADF(IJ+1)-RADF(IJ))*(RIJ-RJ)           4160
      IF(IJ.GE.100)RAD=RADF(100)                                        4170
      TT=T                                                              4180
      T=TR                                                              4190
      DO34 I=1,IR                                                       4200
      ND=0                                                              4210
      I1=1                                                              4220
      I2=SF(I)                                                          4230
      K=IA(I,1)                                                         4240
      CF=1.                                                             4250
      DO 35 M=I1,I2                                                     4260
      J=IA(I,M)                                                         4270
       IF(CLJ(J,2).EQ.0.)ND=I                                           4280
35    IF(BB(I,M).NE.0.)CF=CF*C(J)**BB(I,M)                              4290
      CR=1                                                              4300
      I1=SF(I)+1                                                        4310
      I2=SR(I)+SF(I)                                                    4320
      DO 36 M=I1,I2                                                     4330
      J=IA(I,M)                                                         4340
       IF(CLJ(J,2).EQ.0.)ND=I                                           4350
36    IF(BB(I,M).NE.0.)CR=CR*C(J)**BB(I,M)                              4360
      RA=EA(I)*EXP(-EE(I)/R/T)*(CF-CR*REQC(T,I))                        4370
      IF(P(K).NE.0.)DXA(I)=1.130973355E4*DL*RA*RAD**2/TMPH*PT/P(K)      4380
      IF(P(K).EQ.0.)DXA(I)=0.                                           4390
      IF(ND.NE.0)GO TO 54                                               4400
      GO TO 68
54    IF(DXA(ND).LE.0.)DXA(ND)=0.                                       4420
68    IF((ABS(DXA(I)).GE.1.E-2).AND.(F(I).LE.9.))GO TO 20
```

```
      IF(DXA(I),GE,.1)DXA(I)=DXA(I)*.1
   34 IF(DXA(I),GE,.1)GO TO 20                                          4440
      GO TO 23                                                          4450
   20 ZIC=ZIC-DL
      DL=ABS(DL*.005/DXA(I))
      REQ=REQC(T,I)                                                     4470
      RATE=EA(I)*EXP(-EE(I)/R/T)                                        4480
      WRITE(6,930)DL,ZIC                                                4490
      WRITE(6,932)I,RA,DXA(I),CF,CR,REQ,RATE                            4500
      MA=MA+1                                                           4510
      GO TO 25                                                          4520
   23 DN=0.                                                             4530
      PT2=PRR(IS)                                                       4540
      DO 39 I=1,IR                                                      4550
      K=IA(I,1)                                                         4560
      I1=1                                                              4570
      I2=SE(I)                                                          4580
      DO 38 M=I1,I2                                                     4590
      J=IA(I,M)                                                         4600
      DN=DN-B(I,M)/B(I,1)*C(K)*DXA(I)                                   4610
   38 P(J)=P(J)-B(I,M)/B(I,1)*P(K)*DXA(I)                               4620
      I1=SE(I)+1                                                        4630
      I2=SR(I)+SE(I)                                                    4640
      DO 39 M=I1,I2                                                     4650
      J=IA(I,M)                                                         4660
      DN=DN+B(I,M)/B(I,1)*C(K)*DXA(I)                                   4670
   39 P(J)=P(J)+B(I,M)/B(I,1)*P(K)*DXA(I)                               4680
      CT=0.                                                             4690
      DO 37 I=1,IS                                                      4700
      C(I)=P(I)/T/GC                                                    4710
   37 CT=CT+C(I)                                                        4720
      RN1=CT                                                            4730
      RN2=CT-DN                                                         4740
      TMPH=TMPH*DN*GC*T/PT+TMPH                                         4750
      DN=TMPH                                                           4760
      PD=PRESD(T)                                                       4770
      PT=PRR(IS)                                                        4780
      IF(MB,EQ,5000)GO TO 72
      IF(MB,EQ,3000)GO TO 71
      IF(MB,EQ,2000)PT=.5
      IF(PT,LE,(POUT-.2))GO TO 69
      DO 40 J=1,IS                                                      4800
   40 TM(J)=TMPH*P(J)/PT                                                4810
      D=0.                                                              4820
   44 DO 43 IX=1,IR                                                     4830
   43 D=AMAX1(ABS(DXA(IX)),D)                                           4840
      IF(D,EQ,0,)GO TO 26                                               4850
      IF(D,GE,.0010)GO TO 24                                            4860
   27 IF(DL,GE,.01*ZTT)GO TO 24                                         4870
      DL=ABS(DL*.005/D)
```

```
      IF(DL.GE..01*ZTT)DL=.01001*ZTT                                    4890
      WRITE(6,930)DL,ZIC                                                4900
      WRITE(6,933)(DXA(I),I,I=1,IR)                                     4910
24    IF(MR.NE.1)GO TO 31
      IF(MY.GE.2)GO TO31                                                4930
      WRITE(6,942)PT,VEL1                                               4940
      WRITE(6,928)(J,C(J),TM(J),DXA(J),J=1,IM)                          4950
      GO TO(46,47,31),IGO                                               4960
46    II=IS+1                                                           4970
      WRITE(6,938)(J,DXA(J),J=II,IR)                                    4980
      GO TO 31                                                          4990
47    II=IR+1                                                           5000
      WRITE(6,939)(J,C(J),TM(J),J=II,IS)                                5010
31    CONTINUE
      ZICI=ZICI+DL
      IF(ZICI.LE.(ZTT/25.))GO TO 30
      ZICI=0.
      MZ=MZ+1
      WZIC(MZ)=ZIC
      WT(MZ)=T
      WTMPH(MZ)=TMPH
      WPT(MZ)=PT
      WVEL1(MZ)=VEL1
      DO 70 J=1,ISS
      WC(J,MZ)=C(J)
      WTM(J,MZ)=TM(J)
70    WOXA(J,MZ)=DXA(J)
30    CONTINUE
33    PT=PT2                                                            5190
69    IWMZ=MZ
      WRITE(6,918)                                                      5200
      WRITE(6,951)CARD                                                  5210
      WRITE(6,9934)ZIC,T,TMPH                                           5220
      PTTE=PT
      IF(MAZE.EQ.2)PT=2.
      WRITE(6,942)PT,VEL1                                               5230
      PT=PTTE
      DO 64 I=1,IS                                                      5240
64    P(I)=PPI(I)                                                       5250
      IF((PT.GE.(POUT-.2)).AND.(PT.LE.(POUT+.2)))GO TO 65               5260
      IF(KK.EQ.2)PDP=PDP/2
      IF(KK.EQ.2)GO TO 63
      IF((PT.GE.POUT+.2).AND.(ITEST.EQ.2))PDP=PDP/2.                    5260
      IF((MAZE.EQ.2).AND.(PT.GE.(POUT-.2)))GO TO 65
      IF(MAZE.EQ.2)GO TO 63
      IF((PT.LE.POUT-.2).AND.(ITEST.EQ.3))PDP=PDP/2.                    5280
      IF((PT.GE.POUT+.2).AND.(ITEST.EQ.2))KK=2
      IF((PT.LE.POUT-.2).AND.(ITEST.EQ.3))KK=2
      GO TO 63                                                          5290
71    MAZE=2
```

```
      PT=.5
      WRITE(6,952)
      GO TO 69
   65 IF(IPLOT.GT.2)GO TO 91
      WRITE(6,918)
      WRITE(6,916)
      WRITE(6,916)
      WRITE(6,962)
      DO 81 I=14,116
   81 CALL PLOT(I,'*N')
      CALL PLOT(1,'  ')
      DO 82 I=1,IWMZ
      J1=WTM(KEYP,I)/WTM(KEYR,1)*100.+15.
      J2=WTM(KEYR,I)/WTM(KEYR,1)*100.+15.
      J3=(WT(I)-Z(1))/(Z(11)-Z(1))*100.+15.
      J4=(WPT(I)-2.)/6.*100.+15
   82 CALL PLOT(14,'*N',J1,'EN',J2,'RN',J3,'TN',J4,'PN',116,'*O')
      J1=TM(KEYP)/WTM(KEYR,1)*100.+15.
      J2=TM(KEYR)/WTM(KEYR,1)*100.+15.
      J3=115
      J4=15
      CALL PLOT(14,'*N',J1,'EN',J2,'RN',J3,'TN',J4,'PN',116,'*O')
      DO 83 I=14,116
   83 CALL PLOT(I,'*N')
      CALL PLOT(1,'  ')
      WRITE(6,951)CARD
      WRITE(6,963)HR
      WRITE(6,918)
   91 KK=1
      IF((IPLOT.GT.3).OR.(IPLOT.LT.2))GO TO 90
      MMM=2
      DO 75 I=1,IWMZ
      PT=WPT(I)
      VEL1=WVEL1(I)
      ZIC=WZIC(I)
      T=WT(I)
      TMPH=WTMPH(I)
      DO 76 J=1,ISS
      C(J)=WC(J,I)
      TM(J)=WTM(J,I)
   76 DXA(J)=WDXA(J,I)
      MMM=MMM+1
      IF(MMM.LE.1)GO TO 41
      MMM=0
      WRITE(6,918)
      WRITE(6,951)CARD
   41 WRITE(6,9934)ZIC,T,TMPH
      YIELD=TM(KEYP)/TMPHI/PPI(KEYR)*PI*100.
      J2=KEYR*20
      J1=J2-19
```

```
      J4=KEYP*20                                                        
      J3=J4-19                                                          
      WRITE(6,965)(ENAME(L),L=J1,J2),(ENAME(L),L=J3,J4),YIELD           
      WRITE(6,942)PT,VEL1                                               
      WRITE(6,929)I                                                     
      WRITE(6,928)(J,C(J),TM(J),DXA(J),J=1,IM)                          
      GO TO(42,45,75),IGO                                               
   42 II=IS+1                                                           
      WRITE(6,938)(J,DXA(J),J=II,IR)                                    
      GO TO 75                                                          
   45 II=IR+1                                                           
      WRITE(6,939)(J,C(J),TM(J),J=II,IS)                                
   75 WRITE(6,916)                                                      
      WRITE(6,918)                                                      
   90 WRITE(6,951)CARD.                                                 5310
      MB=1                                                              
      MY=1                                                              5320
      MZ=1                                                              5330
      WRITE(6,916)                                                      5340
      DO 59 I=1,IR                                                      5350
   59 REQTT=REQC(T,I)                                                   5360
      WRITE(6,916)                                                      5370
      PRETT=PRESD(T)                                                    5380
      DO 51 I=1,IS                                                      5390
      I1=1+(I-1)*20                                                     5400
      I2=I*20                                                           5410
   51 WRITE(6,946)I,IDATA(I),(ENAME(J),J=I1,I2),C(I),TM(I)              5420
      YIELD=TM(KEYP)/TMPHI/PPI(KEYR)*PI*100.                            
      J2=KEYR*20                                                        
      J1=J2-19                                                          
      J4=KEYP*20                                                        
      J3=J4-19                                                          
      WRITE(6,965)(ENAME(I),I=J1,J2),(ENAME(I),I=J3,J4),YIELD           
      GO TO 50                                                          5430
   63 PTI=PI                                                            5440
      IF(PT.LT.PDUT)GO TO 49                                            5450
      GO TO 61                                                          5460
   49 PDIR=PI-PT                                                        5470
   67 PTI=PI                                                            5490
      PI=PI+PDP                                                         
      IF(PI.GE.8.1)GO TO  56                                            5510
      DO 53 I=1,IS                                                      5520
      PPI(I)=PPI(I)*PI/PTI                                              5530
      P(I)=PPI(I)                                                       5540
   53 C(I)=P(I)/T/GC                                                    5550
      ITEST=2                                                           5560
      GO TO 58                                                          5570
   61 PTI=PI                                                            5580
      PI=PI-PDP                                                         
      DO 62 I=1,IS                                                      5610
```

```
      PPI(I)=PPI(I)*PI/PTI                                                    5620
   62 P(I)=PPI(I)                                                             5630
      ITEST=3                                                                 5640
      GO TO 58                                                                5650
   50 T=TIN                                                                   5660
      TMPH=TMPHI                                                              5670
      HR=HR+18
      IGOTO=IGOTO+1                                                           5720
      WRITE(6,945)HR                                                          5730
      RADI(100)=RADI(99)
      DO 52 I=1,100                                                           5740
      RADD(I,IGOTO)=RADI(I)
   52 RADE(I)=RADI(I)                                                         5750
      WRITE(6,944)RADI                                                        5760
      HAZE=1
      POP=.2
      DO 66 I=1,IS                                                            5770
      P(I)=PPI(I)
   66 C(I)=P(I)/GC/820.
      ITEST=1                                                                 5790
      MA=1                                                                    5800
      IF(IGOTO.GE.IZZ)GO TO 56
      IF(PT.LT.PRES)GO TO 58                                                  5820
      GO TO 56                                                                5830
   72 WRITE(6,954)
      IGOTO=IZZ
      GO TO 50
   55 WRITE(6,949)                                                            5840
   56 WRITE(6,918)
      IF(IPLOT.GT.2)GO TO 95
      WRITE(6,955)
      WRITE(6,968)ZTT
      IGOTO=IGOTO-1
      DO 77 J=9,111
   77 CALL PLOT(J,'*N')
      CALL PLOT(1,'  ')
      DO 78 J=2,100,2
      J1=102-J
      IJK=0.
      DO 79 I=1,IGOTO
      IJK=IJK+1
      IF(IJK.GT.9)IJK=1
      J2=RADD(J1,I)/RADI(1)*50.+60.
      J3=120-J2
   79 CALL PLOT(9,'*N',J2,IDATP(IJK),J3,IDATP(IJK),111,'*N')
   78 CALL PLOT(60,1+ ')
      DO 80 J=9,111
   80 CALL PLOT(J,'*N')
   95 CALL PLOT(1,'  ')
      WRITE(6,966)
```

```
      WRITE(6,967)CARD
      IGOTO=1
      MA=1                                                          5860
      READ(5,943)IGOW,(Z(II),II=1,11)
      READ(5,950)CARD                                               5880
      READ(5,958)IB,IZZ,IPLOT
      PT=0.
      DO 73 I=1,IS
   73 PT=PT+PP1(I)
      DO 74 I=1,IS
      PP1(I)=PP1(I)*PSAVE/PT
   74 P(I)=PP1(I)
      GO TO(100,110,111),IGOW                                       5890
  101 CONTINUE                                                      5900
      WRITE(6,921)I,ID                                              5910
      STOP111                                                       5920
  102 CONTINUE                                                      5930
      WRITE(6,922)I,ID                                              5940
      STOP112                                                       5950
  103 CONTINUE                                                      5960
      WRITE(6,923)J,ID                                              5970
      STOP113                                                       5980
  104 CONTINUE                                                      5990
      WRITE(6,924)I,ID                                              6000
      STOP114                                                       6010
  105 CONTINUE                                                      6020
      WRITE(6,925)J,ID                                              6030
      STOP115                                                       6040
  111 CONTINUE                                                      6050
      WRITE(6,918)
   92 WRITE(6,970)(I,I=1,IR)
      DO 84 IT=800,1200,10
      J=(IT-800)/10+1
      T=IT
      DO 85 N=1,IR
   85 WC(J,N)=1./REQC(T,N)
   84 WRITE(6,969)IT,(WC(J,N),N=1,IR)
      WRITE(6,918)
      WRITE(6,916)
      WRITE(6,916)
      DO 86 IT=800,1200,10
      J=(IT-800)/10+1
      T=IT
      DO 87 N=1,IR
   87 WC(J,N)=HEATR(T,N)
   86 WRITE(6,969)IT,(WC(J,N),N=1,IR)
      WRITE(6,918)
      WRITE(6,916)
      WRITE(6,916)
      WRITE(6,916)
```

```
      DO 88 IT=800,1200,10                                              6060
      J=(IT-800)/10+1                                                   6070
      T=IT                                                              6080
      DO 89 N=1,IS                                                      6090
   89 WC(J,N)=CP(N,2)*T+CP(N,1)+CP(N,3)*T**2+CP(N,4)*T**3               6100
   88 WRITE(6,973)IT,(WC(J,N),N=1,IS)                                   6110
   99 STOP99                                                            6120
  106 WRITE(6,935) ID,J
      STOP116
   26 WRITE(6,931)
      WRITE(6,940)(J,C(J),DXA(J),J=1,IS)
      STOP26
      END
```

Appendix G

Program Output

```
PROGRAM PYRO
PROGRAMMER RICHARD ROBERTSON
DR. HANESIAN ADVISOR
AS MASTER THESIS REQUIREMENT
```

IDENTIFICATION OF REACTION SYSTEM

COMPONENT	CO NO.	HEAT CAPACITY DATA A	B	C	D	DELTA-H	DELTA-S	LOG(K)
ACETYLENE	A 1	5.867E 00	1.957E-02	-1.296E-05	3.466E-09	5.41940000E 04	4.79969940E 01	-8.87480020E 00
ISO BUTANE	B 2	-1.901E 00	9.930E-02	-5.475E-05	1.182E-08	-3.14520000E 04	7.04199980E 01	-1.45972990E 01
N-BUTANE	C 3	9.114E-02	9.218E-02	-4.761E-05	9.577E-09	-2.98120000E 04	7.41900060E 01	-1.41027000E 01
ISO-BUTENE	D 4	7.098E-01	8.209E-02	-4.535E-05	9.837E-09	2.80000000E 02	7.24799950E 01	-1.36880990E 01
ETHANE	E 5	9.065E-01	4.320E-02	-1.864E-05	2.856E-09	-2.02360000E 04	5.48500060E 01	-5.70139280E 00
ETHYLENE	F 6	9.847E-01	3.701E-02	-1.345E-05	4.042E-09	1.24960000E 04	5.24499960E 01	-6.17380040E 00
HYDROGEN	G 7	7.010E 00	-5.366E-04	1.006E-06	-2.453E-10	0.00000000E-01	3.12109980E 01	0.00000000E-01
METHANE	H 8	4.010E 00	1.493E-02	-1.477E-07	-1.593E-09	-1.78000000E 04	4.45000000E 01	-1.00149960E 00
PROPANE	I 9	-1.053E 00	7.314E-02	-3.788E-05	7.672E-09	-2.48200000E 04	6.45099940E 01	-9.98399980E 00
PROPENE	J10	7.342E-01	5.663E-02	-2.838E-05	5.510E-09	4.87900000E 03	6.38000030E 01	-9.49799990E 00
WATER	K11	7.716E 00	1.285E-04	3.151E-06	-1.150E-09	-5.7797898UE 04	4.51060020E 01	1.00597290E 01
CARBON	L12	-1.356E 00	1.447E-02	-1.101E-05	4.029E-09	0.00000000E-01	1.30690000E 00	0.00000000E-01
CARBON MONOXIDE	M13	6.863E 00	-4.085E-04	2.480E-06	-1.018E-09	-2.64156990E 04	4.73009940E 01	1.04 76090E 01

COMPONET	CO NO	LENNARD-JONES PARAMETERS (A)	(DEG-K)	MOL. WT.	INITAL CONCENTRATION
ACETYLENE	A 1	4.221	185.0	26.04	0.0000E-01
ISO BUTANE	B 2	5.341	313.0	58.12	0.0000E-01
N-BUTANE	C 3	5.333	327.4	58.12	0.0000E-01
ISO-BUTENE	D 4	5.389	314.0	56.12	0.0000E-01
ETHANE	E 5	4.418	230.0	30.07	3.5262E-03
ETHYLENE	F 6	4.221	185.0	28.05	0.0000E-01
HYDROGEN	G 7	2.915	38.0	2.02	0.0000E-01
METHANE	H 8	3.822	137.0	16.04	0.0000E-01
PROPANE	I 9	5.061	254.0	44.09	0.0000E-01
PROPENE	J10	4.757	281.0	42.08	0.0000E-01
WATER	K11	3.218	499.0	18.02	1.9012E-03
CARBON	L12	0.000	0.0	12.00	0.0000E-01
CARBON MONOXIDE	M13	3.590	110.0	28.01	0.0000E-01

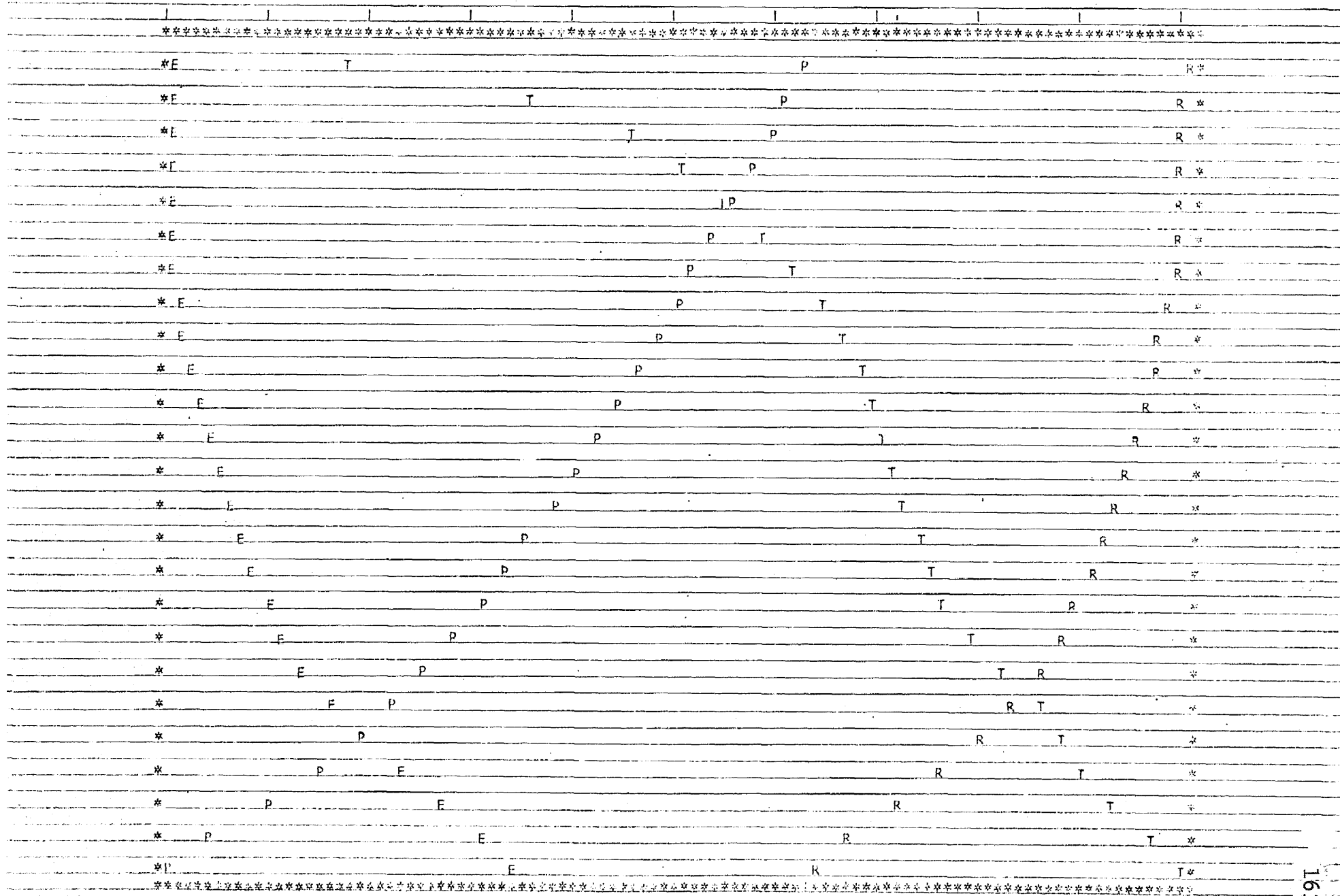
REACTION SYSTEM

EQUATION	ARRHENIUS RATE CONSTANT K(Q)	E	DELTA HEAT CAPACITY DATA FOR REACTION DELTA A	DELTA B	DELTA C	DELTA D
1 1E<->1B+1G	6.040E 16	8.200E 04	7.088E 00	-7.723E-03	1.966E-07	9.400E-10
2 2E<->2H+1F	1.600E 12	6.700E 04	7.191E 00	-2.152E-02	1.748E-05	-4.856E-09
3 1F<->1A+1G	1.800E 13	7.600E 04	1.189E 01	-1.797E-02	7.497E-06	-8.204E-10
4 1A<->2L+1G	9.700E 12	6.200E 04	-1.569E 00	8.835E-03	-8.056E-06	2.364E-09
5 2F<=>1D	2.600E 13	6.000E 04	-1.260E 00	8.065E-03	-6.453E-06	1.754E-09
6 1K+1L<->1M+1G	9.255E 03	2.130E 04	7.511E 00	-1.555E-02	1.134E-05	-3.141E-09
7 1I<->1J+1G	2.900E 13	6.330E 04	8.827E 00	-1.705E-02	1.050E-05	-2.407E-09
8 1I<=>1H+1F	3.200E 13	6.300E 04	6.077E 00	-2.119E-02	1.825E-05	-5.223E-09

EQ	LOG(K) REACTION	CONSTANT OF INTEGERATION	ORDER OF REACTION BY COMPONENT			
1	-4.72401E-01	-1.86429E 01	E**(1.0)	F**(1.0)	G**(1.0)	
2	1.60700E 00	-2.41095E 01	E**(1.0)	H**(1.0)	F**(0.5)	
3	-2.70000E 00	-1.81660E 01	F**(1.0)	A**(1.0)	G**(1.0)	
4	8.87380E 00	2.44518E 01	A**(1.0)	L**(1.0)	G**(1.0)	
5	-6.60699E-01	1.52761E 00	F**(2.0)	D**(1.0)		
6	4.17886E-01	-3.64982E 01	K**(0.0)	L**(1.0)	M**(1.0)	G**(1.0)
7	4.93000E-01	-2.49397E 01	I**(1.0)	J**(1.0)	G**(1.0)	
8	2.80260E 00	-1.43070E 01	I**(1.0)	H**(1.0)	F**(1.0)	

```
 REACTOR IS      400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES  AT PRESSURE    5.849A  VELOCITY OF   2.08526E 02 AT TEMPERATURE    820.0DEG R
 INITIAL REACTOR INCREMENT(DL 5.00000E-01FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.68841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14312E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14237E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
 FUNCTION PRR(IS)
 PR=  5.84930E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 FUNCTION PRR(IS)
 PR=  5.84930E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 FUNCTION PRESU(T)
 REYU=   3.35920E 05     VIS=   2.16064E-05     DEN=   1.37883E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   2.08526E 02     2.12585E 02     2.10555E 02
 TEMPERTURE=  832.71PRESSURE D=   2.27193E-02
 FUNCTION PRR(IS)
 PR=  5.82657E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 PRESSURE IS   5.8265/E 00    VELOCITY   2.1258E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.4774E-07
  2    0.0000E-01    0.0000E-01    7.9707E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.4724E-03    1.2994E 02    0.0000E-01
  6    1.3459E-09    5.0364E-05    0.0000E-01
  7    1.2075E-09    4.5186E-05    0.0000E-01
  8    2.7677E-10    1.0357E-05    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    1.8722DE-03   7.00597E 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

 DL CHANGED TO    1.97467E 00     ZIC=   3.36334E 02
 I= 1  RA=   1.49804E-03  DXA(I)=   1.01384E-02  CF,CR=   1.06182E-03   6.41019E-08  REQC=   1.79470E 00

 RATE=   1.41097E 00
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.01496E 02FEET
TEMPERTURE 1109.70DEGREE-K MOLAR FLOW RATE 2.46192E 02POUND MOLES PER HOUR
PRESSURE IS 2.05023E 00 VELOCITY 1.0218E 03FEET/SEC.


SYSTEM 4 820 TO 1110 DEG K
REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 0. HOURS OF RUN

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.60160E 01FEET
TEMPERTURE 870.85DEGREE-K MOLAR FLOW RATE 2.00001E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.00%
PRESSURE IS 5.75581E 00 VELOCITY 2.2506E 02FEET/SEC.
ITERATION NUMBER= 1

NO	CONCENTRATION	TMPH	DXA
1	6.9505E-16	2.7526E-11	2.8885E-06
2	0.0000E-01	0.0000E-01	4.4513E-07
3	0.0000E-01	0.0000E-01	2.7594E-08
4	4.1865E-20	1.6581E-15	4.8535E-05
5	3.2809E-03	1.2994E 02	3.8228E-12
6	1.9288E-08	7.6391E-04	4.0692E-21
7	1.7771E-08	7.0383E-04	0.0000E-01
8	3.0340E-09	1.2016E-04	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.76894E-03	7.00596E 01	
12	6.74616E-20	0.00000E-01	
13	7.19814E-24	2.85085E-19	

REACTOR POSITION 3.20320E 01FEET
TEMPERTURE 921.70DEGREE-K MOLAR FLOW RATE 2.00011E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.01%
PRESSURE IS 5.65542E 00 VELOCITY 2.4244E 02FEET/SEC.
ITERATION NUMBER= 2

NO	CONCENTRATION	TMPH	DXA
1	1.0385E-13	4.4287E-09	3.6626E-05
2	0.0000E-01	0.0000E-01	3.4986E-06
3	0.0000E-01	0.0000E-01	2.8896E-07
4	5.4656E-17	2.3310E-12	3.2526E-04
5	3.0466E-03	1.2993E 02	3.5542E-10
6	2.5157E-07	1.0729E-02	1.0894E-17
7	2.3845E-07	1.0169E-02	0.0000E-01
8	2.6228E-08	1.1185E-03	0.0000E-01
9	0.0000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.64277E-03	7.00597E 01	
12	6.75359E-17	0.00000E-01	
13	2.11735E-20	9.02993E-16	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.80480E 01FEET
TEMPERTURE 953.04DEGREE-K MOLAR FLOW RATE 2.00074E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.06%
PRESSURE IS 5.54979E 00 VELOCITY 2.5553E 02FEET/SEC.
ITERATION NUMBER- 3

NO	CONCENTRATION	TMPH	DXA
1	3.8291E-12	1.7208E-07	1.4992E-04
2	0.0000E-01	0.0000E-01	1.0940E-05
3	0.0000E-01	0.0000E-01	1.0620E-06
4	1.1292E-14	5.0744E-10	9.2973E-04
5	2.8898E-03	1.2986E 02	8.4262E-09
6	1.6333E-06	7.3399E-02	4.3511E-15
7	1.5697E-06	7.0539E-02	0.0000E-01
8	1.2728E-07	5.7198E-03	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.55899E-03	7.00601E 01	
12	7.11319E-15	0.00000E-01	
13	1.03315E-17	4.64290E-13	

REACTOR POSITION 6.40640E 01FEET
TEMPERTURE 965.05DEGREE-K MOLAR FLOW RATE 2.00187E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.14%
PRESSURE IS 5.44347E 00 VELOCITY 2.6395E 02FEET/SEC.
ITERATION NUMBER- 4

NO	CONCENTRATION	TMPH	DXA
1	2.1366E-11	9.9156E-07	2.4891E-04
2	0.0000E-01	0.0000E-01	1.6459E-05
3	0.0000E-01	0.0000E-01	1.6951E-06
4	1.5249E-13	7.0771E-09	1.3535E-03
5	2.7958E-03	1.2975E 02	3.2649E-08
6	3.9892E-06	1.8513E-01	5.0938E-14
7	3.8481E-06	1.7858E-01	0.0000E-01
8	2.8240E-07	1.3106E-02	0.0000E-01
9	0.0000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.50964E-03	7.00605E 01	
12	5.77617E-14	0.00000E-01	
13	1.71251E-16	7.94756E-12	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 8.00800E 01FEET
TEMPERTURE 977.06DEGREE-K MOLAR FLOW RATE 2.00371E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.28%
PRESSURE IS 5.33464E 00 VELOCITY 2.7294E 02FEET/SEC.
ITERATION NUMBER- 5

NO	CONCENTRATION	TMPH	DXA
1	7.7026E-11	3.6952E-06	4.0739E-04
2	0.0000E-01	0.0000E-01	2.4468E-05
3	0.0000E-01	0.0000E-01	2.6696E-06
4	9.7775E-13	4.6907E-08	1.9487E-03
5	2.7007E-03	1.2956E-02	8.9911E-08
6	7.6732E-06	3.6811E-01	3.2662E-13
7	7.4220E-06	3.5606E-01	0.0000E-01
8	5.0272E-07	2.4118E-02	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.46040E-03	7.00612E 01	
12	2.99727E-13	0.00000E-01	
13	1.26982E-15	6.09181E-11	

REACTOR POSITION 9.60959E 01FEET
TEMPERTURE 988.27DEGREE-K MOLAR FLOW RATE 2.00663E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.51%
PRESSURE IS 5.22456E 00 VELOCITY 2.8230E 02FEET/SEC.
ITERATION NUMBER- 6

NO	CONCENTRATION	TMPH	DXA
1	2.2670E-10	1.1245E-05	6.3624E-04
2	0.0000E-01	0.0000E-01	3.5006E-05
3	0.0000E-01	0.0000E-01	4.0256E-06
4	4.4972E-12	2.2308E-07	2.7078E-03
5	2.6060E-03	1.2927E 02	2.0869E-07
6	1.3246E-05	6.5705E-01	1.5907E-12
7	1.2843E-05	6.3705E-01	0.0000E-01
8	8.3735E-07	4.0047E-02	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.41244E-03	7.00623E 01	
12	1.22543E-12	0.00000E-01	
13	6.76343E-15	3.35492E-10	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.12112E 02FEET
TEMPERTURE 999.48DEGREE-K MOLAR FLOW RATE 2.01113E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.85%
PRESSURE IS 5.11364E 00 VELOCITY 2.9235E 02FEET/SEC.
ITERATION NUMBER- 7

NO	CONCENTRATION	TMPH	DXA
1	5.9234E-10	3.0417E-05	9.8208E-04
2	0.0000E-01	0.0000E-01	4.9598E-05
3	0.0000E-01	0.0000E-01	6.0044E-06
4	1.6994E-11	8.7268E-07	3.7284E-03
5	2.5085E-03	1.2881E 02	4.4178E-07
6	2.1469E-05	1.1025E 00	6.6362E-12
7	2.0861E-05	1.0712E 00	0.0000E-01
8	1.2196E-06	6.2627E-02	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.36441E-03	7.0064E 01	
12	4.40788E-12	0.00000E-01	
13	2.96226E-14	1.52116E-09	

REACTOR POSITION 1.26128E 02FEET
TEMPERTURE 1008.05DEGREE-K MOLAR FLOW RATE 2.01767E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 1.35%
PRESSURE IS 2.00336E 00 VELOCITY 3.0234E 02FEET/SEC.
ITERATION NUMBER- 8

NO	CONCENTRATION	TMPH	DXA
1	1.3948E-09	7.4047E-05	1.3481E-03
2	0.0000E-01	0.0000E-01	6.3847E-05
3	0.0000E-01	0.0000E-01	8.0331E-06
4	5.4702E-11	2.9040E-06	4.6979E-03
5	2.4139E-03	1.2815E 02	8.0399E-07
6	3.2983E-05	1.7510E 00	2.3252E-11
7	3.2108E-05	1.7046E 00	0.0000E-01
8	1.7550E-06	9.3168E-02	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.31981E-03	7.00665E 01	
12	1.30744E-11	0.00000E-01	
13	1.12486E-13	5.97167E-09	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 1.44144E 02FEET

TEMPERTURE 1014.05DEGREE-K MOLAR FLOW RATE 2.02580E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 1.97%

PRESSURE IS 4.89207E 00 VELOCITY 3.1231E 02FEET/SEC.

ITERATION NUMBER= 9

NO	CONCENTRATION	TMPH	DXA
1	2.7980E-09	1.5338E-04	1.6644E-03
2	0.0000E-01	0.0000E-01	7.5408E-05
3	0.0000E-01	0.0000E-01	9.7435E-06
4	1.4095E-10	7.7268E-06	5.4671E-03
5	2.3228E-03	1.2733E 02	1.2299E-06
6	4.6626E-05	2.5560E 00	5.9885E-11
7	4.5452E-05	2.4916E 00	0.0000E-01
8	2.3604E-06	1.2939E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.27822E-03	7.00695E 01	
12	3.05174E-11	0.00000E-01	
13	3.33553E-13	1.82848E-08	

REACTOR POSITION 1.60160E 02FEET

TEMPERTURE 1020.02DEGREE-K MOLAR FLOW RATE 2.03573E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 2.72%

PRESSURE IS 4.77983E 00 VELOCITY 3.2310E 02FEET/SEC.

ITERATION NUMBER= 10

NO	CONCENTRATION	TMPH	DXA
1	5.0619E-09	2.8696E-04	2.0427E-03
2	0.0000E-01	0.0000E-01	8.8604E-05
3	0.0000E-01	0.0000E-01	1.1752E-05
4	3.0978E-10	1.7561E-05	6.3214E-03
5	2.2286E-03	1.2634E 02	1.7451E-06
6	6.2418E-05	3.5384E 00	1.3668E-10
7	6.0915E-05	3.4532E 00	0.0000E-01
8	3.0297E-06	1.7175E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.23611E-03	7.00735E 01	
12	6.39290E-11	0.00000E-01	
13	8.35251E-13	4.73495E-08	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.76176E 02FEET
TEMPERTURE 1022.02DEGREE-K MOLAR FLOW RATE 2.04664E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 3.55%
PRESSURE IS 4.66467E 00 VELOCITY 3.3350E 02FEET/SEC.
ITERATION NUMBER- 11

NO	CONCENTRATION	THPH	DXA
1	8.2029E-09	4.7979E-04	2.1419E-03
2	0.0000E-01	0.0000E-01	9.1572E-05
3	0.0000E-01	0.0000E-01	1.2752E-05
4	5.8333E-10	3.4119E-05	6.5119E-03
5	2.1412E-03	1.2524E 02	2.0794E-06
6	7.8965E-05	4.6187E 00	2.4660E-10
7	7.7127E-05	4.5111E 00	0.0000E-01
8	3.7137E-06	2.1721E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.1981IE-03	7.0077BE 01	
12	1.0653BE-10	0.0000E-01	
13	1.78764E-12	1.0455?E-07	

REACTOR POSITION 1.92192E 02FEET
TEMPERTURE 1024.02DEGREE-K MOLAR FLOW RATE 2.05798E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 4.42%
PRESSURE IS 4.5447?E 00 VELOCITY 3.4487E 02FEET/SEC.
ITERATION NUMBER- 12

NO	CONCENTRATION	THPH	DXA
1	1.2082E-08	7.3045E-04	2.2435E-03
2	0.0000E-01	0.0000E-01	9.4542E-05
3	0.0000E-01	0.0000E-01	1.2759E-05
4	9.6002E-10	5.8038E-05	6.6908E-03
5	2.0528E-03	1.2410E 02	2.3351E-06
6	9.4956E-05	5.7406E 00	3.0893E-10
7	9.2802E-05	5.6104E 00	0.0000E-01
8	4.3631E-06	2.6377E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.15925E-03	7.0682BE 01	
12	1.61232E-10	0.0000E-01	
13	3.27204E-12	1.97812E-07	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 2.08208E 02FEET
TEMPERTURE 1027.05DEGREE-K MOLAR FLOW RATE 2.06992E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 5.33%
PRESSURE IS 4.41954E 00 VELOCITY 3.5776E 02FEET/SEC.
ITERATION NUMBER= 13

NO	CONCENTRATION	TAPH	DXA
1	1.6729E-08	1.0466E-03	2.4396E-03
2	0.0000E-01	0.0000E-01	1.0059E-04
3	0.0000E-01	0.0000E-01	1.3753E-05
4	1.4400E-09	9.0255E-05	7.0676E-03
5	1.9609E-03	1.2290E 02	2.5966E-06
6	1.1042E-04	6.9210E 00	6.6554E-10
7	1.0797E-04	6.7675E 00	0.0000E-01
8	4.9768E-06	3.1193E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.1823E-03	7.0088E 01	
12	2.3581?E-10	0.0000E-01	
13	5.4098E-12	3.3902E-07	

REACTOR POSITION 2.24224E 02FEET
TEMPERTURE 1031.06DEGREE-K MOLAR FLOW RATE 2.08318E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 6.33%
PRESSURE IS 4.28964E 00 VELOCITY 3.7240E 02FEET/SEC.
ITERATION NUMBER= 14

NO	CONCENTRATION	TAPH	DXA
1	2.2467E-08	1.4649E-03	2.7429E-03
2	0.0000E-01	0.0000E-01	1.0992E-04
3	0.0000E-01	0.0000E-01	1.5268E-05
4	2.0468E-09	1.3345E-04	7.6496E-03
5	1.8645E-03	1.2158E 02	2.9051E-06
6	1.2623E-04	8.2300E 00	8.9284E-10
7	1.2349E-04	8.0516E 00	0.0000E-01
8	5.5814E-06	3.6391E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.0750?E-03	7.0094?E 01	
12	3.42769E-10	0.0000E-01	
13	8.5?815E-12	5.5473?E-07	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.40240E 02FEET

TEMPERTURE 1035.06DEGREE-K MOLAR FLOW RATE 2.09788E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 7.45%

PRESSURE IS 4.15415E 00 VELOCITY 3.8876E 02FEET/SEC.

ITERATION NUMBER- 15

NO	CONCENTRATION	TMPH	DXA
1	2.9449E-08	2.0030E-03	3.0720E-03
2	0.0000E-01	0.0000E-01	1.1967E-04
3	0.0000E-01	0.0000E-01	1.6930E-05
4	2.7927E-09	1.8994E-04	8.2500E-03
5	1.7659E-03	1.2011E 02	3.1987E-06
6	1.4233E-04	9.6806E 00	1.3227E-09
7	1.3932E-04	9.4755E 00	0.0000E-01
8	6.1742E-06	4.1993E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.03071E-03	7.01025E 01	
12	4.84554E-10	0.00000E-01	
13	1.29012E-11	8.77461E-07	

REACTOR POSITION 2.56256E 02FEET

TEMPERTURE 1039.06DEGREE-K MOLAR FLOW RATE 2.11411E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 8.68%

PRESSURE IS 4.01223E 00 VELOCITY 4.0720E 02FEET/SEC.

ITERATION NUMBER- 16

NO	CONCENTRATION	TMPH	DXA
1	3.7770E-08	2.6883E-03	3.4259E-03
2	0.0000E-01	0.0000E-01	1.2976E-04
3	0.0000E-01	0.0000E-01	1.8669E-05
4	3.6790E-09	2.6165E-04	8.8621E-03
5	1.6648E-03	1.1849E 02	3.4618E-06
6	1.5847E-04	1.1279E 01	1.9081E-09
7	1.5519E-04	1.1046E 01	0.0000E-01
8	6.7438E-06	4.8000E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	9.85650E-04	7.01119E 01	
12	6.67556E-10	0.00000E-01	
13	1.89299E-11	1.34735E-06	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 2.72271E 02FEET
TEMPERTURE 1043.07DEGREE-K MOLAR FLOW RATE 2.13190E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 10.03%
PRESSURE IS 3.86216E 00 VELOCITY 4.2822E 02FEET/SEC.
ITERATION NUMBER- 17

NO	CONCENTRATION	THPH	DXA
1	4.7463E-08	3.5489E-03	3.8021E-03
2	0.0000E-01	0.0000E-01	1.4005E-04
3	0.0000E-01	0.0000E-01	2.0489E-05
4	4.6942E-09	3.5099E-04	9.4764E-03
5	1.5610E-03	1.1672E 02	3.6773E-06
6	1.7427E-04	1.3030E 01	2.6839E-09
7	1.7075E-04	1.2767E 01	0.0000E-01
8	7.2758E-06	5.4402E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	9.37839E-04	7.01233E 01	
12	8.97036E-10	6.00000E-01	
13	2.69390E-11	2.01427E-06	

REACTOR POSITION 2.88267E 02FEET
TEMPERTURE 1050.18DEGREE-K MOLAR FLOW RATE 2.15224E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 11.56%
PRESSURE IS 3.79326E 00 VELOCITY 4.5393E 02FEET/SEC.
ITERATION NUMBER- 18

NO	CONCENTRATION	THPH	DXA
1	5.8966E-08	4.6672E-03	4.7082E-03
2	0.0000E-01	0.0000E-01	1.6513E-04
3	0.0000E-01	0.0000E-01	2.4880E-05
4	5.8464E-09	4.6274E-04	1.0992E-02
5	1.4492E-03	1.1471E 02	4.1811E-06
6	1.8985E-04	1.5027E 01	3.9818E-09
7	1.8612E-04	1.4732E 01	0.0000E-01
8	7.7628E-06	6.1443E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	8.96143E-04	7.01383E 01	
12	1.29284E-09	0.00000E-01	
13	3.74385E-11	2.96326E-06	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.04303E 02FEET
TEMPERTURE 1060.19DEGREE-K MOLAR FLOW RATE 2.17920E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 13.59%
PRESSURE IS 3.53821E 00 VELOCITY 4.8567E 02FEET/SEC.
ITERATION NUMBER- 19

NO	CONCENTRATION	TMPH	DXA
1	7.5259E-08	9.3623E-03	9.3987E-03
2	0.0000E-01	0.0000E-01	2.0969E-04
3	0.0000E-01	0.0000E-01	3.2908E-05
4	7.3617E-09	6.2235E-04	1.3647E-02
5	1.3255E-03	1.1205E 02	5.1815E-06
6	2.0895E-04	1.7665E 01	6.9125E-09
7	2.0500E-04	1.7331E 01	0.0000E-01
8	8.2995E-06	7.0163E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	8.2994IE-04	7.0162E 01	
12	2.0483E-09	0.0000E-01	
13	5.3922E-11	4.5585E-06	

REACTOR POSITION 3.20318E 02FEET
TEMPERTURE 1070.120EGREE-K MOLAR FLOW RATE 2.21457E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 16.25%
PRESSURE IS 3.36544E 00 VELOCITY 5.2372E 02FEET/SEC.
ITERATION NUMBER- 20

NO	CONCENTRATION	TMPH	DXA
1	9.8457E-08	8.9565E-03	8.5501E-03
2	0.0000E-01	0.0000E-01	2.6229E-04
3	0.0000E-01	0.0000E-01	4.2827E-05
4	9.4308E-09	8.5791E-04	1.6698E-02
5	1.1937E-03	1.0859E 02	6.3979E-06
6	2.3211E-04	2.1115E 01	1.2150E-08
7	2.2793E-04	2.0734E 01	0.0000E-01
8	8.8872E-06	8.0846E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	7.7169SE-04	7.0199E 01	
12	3.2786E-09	0.0000E-01	
13	8.0863E-11	7.3560IE-06	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.36334E 02FEET
TEMPERTURE 1076.13DEGREE-K MOLAR FLOW RATE 2.25599E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 19.35%
PRESSURE IS 3.17641E 00 VELOCITY 5.6844E 02FEET/SEC.
ITERATION NUMBER= 21

NO	CONCENTRATION	THPH	DXA
1	1.2736E-07	1.2540E-02	9.8133E-03
2	0.0000E-01	0.0000E-01	2.8942E-04
3	0.0000E-01	0.0000E-01	4.8387E-05
4	1.1923E-08	1.1739E-03	1.8185E-02
5	1.0618E-03	1.0455E 02	6.7806E-06
6	2.5538E-04	2.5145E 01	1.6729E-08
7	2.5101E-04	2.4715E 01	0.0000E-01
8	9.4201E-06	9.2752E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	7.13465E-04	7.02491E 01	
12	4.61874E-09	0.00000E-01	
13	1.21059E-10	1.19197E-05	

REACTOR POSITION 3.54105E 02FEET
TEMPERTURE 1082.79DEGREE-K MOLAR FLOW RATE 2.30460E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 23.02%
PRESSURE IS 2.93334E 00 VELOCITY 6.3270E 02FEET/SEC.
ITERATION NUMBER= 22

NO	CONCENTRATION	THPH	DXA
1	1.5879E-07	1.7538E-02	5.4186E-03
2	0.0000E-01	0.0000E-01	1.5306E-04
3	0.0000E-01	0.0000E-01	2.6261E-05
4	1.4140E-08	1.5617E-03	9.4799E-03
5	9.6307E-04	9.9740E 01	3.0322E-06
6	2.7088E-04	2.9918E 01	6.7225E-09
7	2.6651E-04	2.9435E 01	0.0000E-01
8	9.6270E-06	1.0633E 00	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	6.36366E-04	7.02845E 01	
12	3.00634E-09	0.00000E-01	
13	1.44312E-10	1.59387E-05	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.71877E 02FEET
TEMPERTURE 1092.42DEGREE-K MOLAR FLOW RATE 2.35887E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 27.11%
PRESSURE IS 2.64047E 00 VELOCITY 7.2583E 02FEET/SEC.
ITERATION NUMBER- 23

NO	CONCENTRATION	TAPH	DXA
1	1.9116E-07	2.4127E-02	6.6626E-03
2	0.0000E-01	0.0000E-01	1.7699E-04
3	0.0000E-01	0.0000E-01	3.1507E-05
4	1.5775E-08	1.9911E-03	1.6739E-02
5	7.4786E-04	9.4393E 01	2.8124E-06
6	2.7915E-04	3.5233E 01	9.9530E-09
7	2.7490E-04	3.4698E 01	0.0000E-01
8	9.5640E-06	1.2072E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	5.5721DE-04	7.0329?E 01	
12	4.1J025E-09	0.0000E-01	
13	1.68051E-10	2.1211DE-05	

REACTOR POSITION 3.89648E 02FEET
TEMPERTURE 1103.53DEGREE-K MOLAR FLOW RATE 2.42310E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 31.93%
PRESSURE IS 2.26581E 00 VELOCITY 8.7771E 02FEET/SEC.
ITERATION NUMBER- 24

NO	CONCENTRATION	TAPH	DXA
1	2.1995E-07	3.3311E-02	8.1791E-03
2	0.0000E-01	0.0000E-01	2.0268E-04
3	0.0000E-01	0.0000E-01	3.7619E-05
4	1.6058E-08	2.4320E-03	1.2017E-02
5	5.8188E-04	8.8124E 01	2.1944E-06
6	2.7394E-04	4.1487E 01	1.4342E-08
7	2.7007E-04	4.0901E 01	0.0000E-01
8	9.0162E-06	1.3655E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	4.6486?0E-04	7.0?9?69E 01	
12	5.2794DE-09	0.0000E-01	
13	1.92005E-10	2.9076?5E-05	

SYSTEM 4 820 T= 1110 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.15413E 01(1103.53, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42392E-01(1103.53, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.32921E 02(1103.53, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12510E-08(1103.53, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42397E 01(1103.53, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13014E 01(1103.53, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24930E 00(1103.53, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.22039E-02(1103.53, 8)

FUNCTION PRR(IS)
PR= 5.84930E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.85506E 05 VIS= 2.68175E-05 DEN= 1.00495E-01
FRICTION FACTOR= 1.27344E-02 V1,V2,VA= 8.77715E 02 3.72228E 02 6.24980E 02
TEMPERTURE= 1103.53PRESSURE D= 4.20913E-01

1-A	ACETYLENE	2.19949E-07	3.33106E-02
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	1.60562E-08	2.43197E-03
5-E	ETHANE	5.81879E-04	8.81237E 01
6-F	ETHYLENE	2.73941E-04	4.14874E 01
7-G	HYDROGEN	2.70070E-04	4.09013E 01
8-H	METHANE	9.01623E-06	1.36548E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	4.64830E-04	7.03969E 01
12-L	CARBON	5.27940E-09	0.00000E-01
13-M	CARBON MONOXIDE	1.92005E-10	2.90785E-05

CONVERSION OF ETHANE TO ETHYLENE IS 31.93%

REACTOR RADIUS PROFILE AFTER 100.00 HOURS

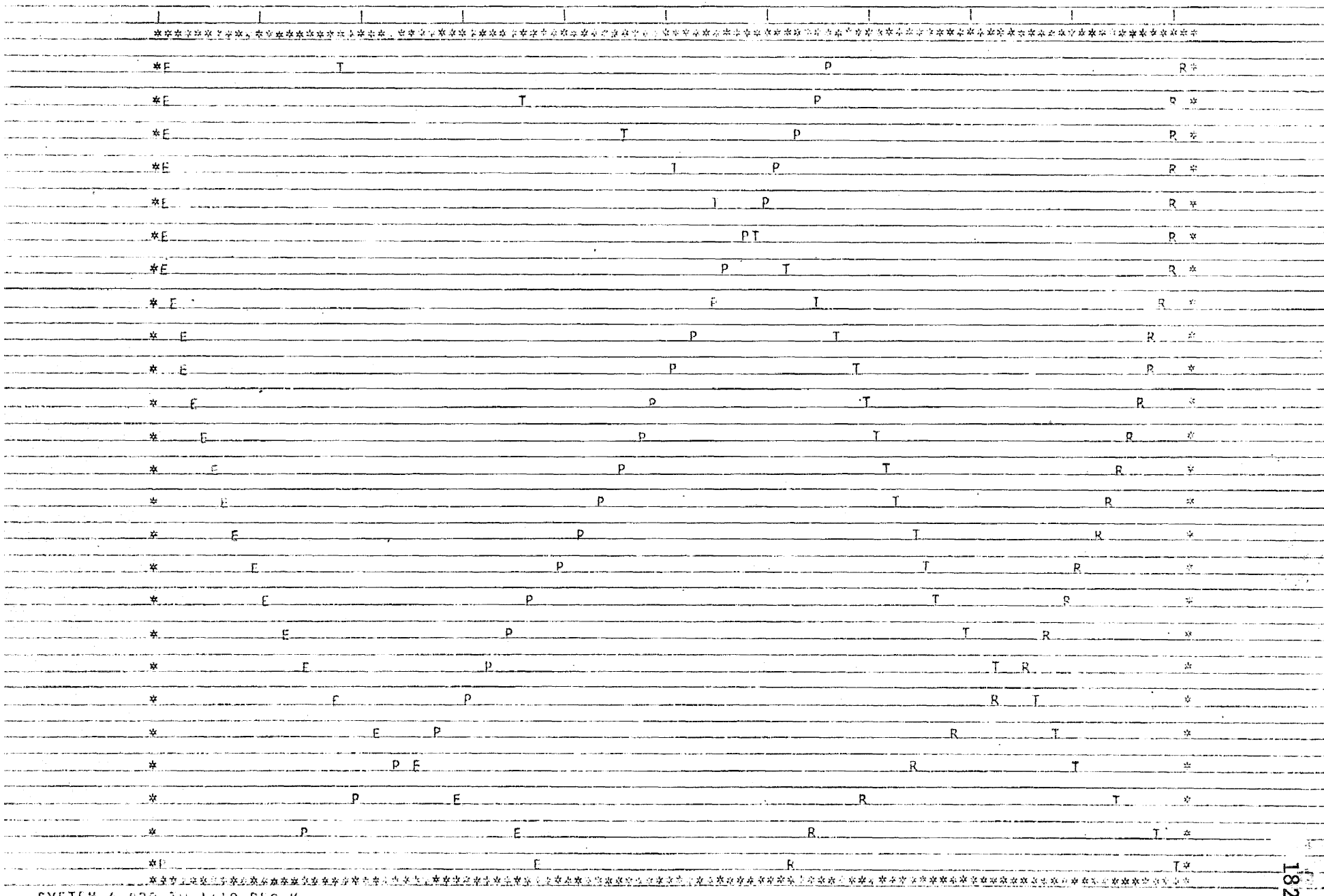
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.124999	0.124999	0.124999
0.124998	0.124998	0.124997	0.124997	0.124996	0.124995	0.124994	0.124993	0.124991	0.124990
0.124988	0.124986	0.124984	0.124982	0.124980	0.124978	0.124975	0.124972	0.124969	0.124966
0.124962	0.124958	0.124953	0.124948	0.124943	0.124937	0.124930	0.124923	0.124915	0.124907
0.124897	0.124886	0.124877	0.124865	0.124853	0.124840	0.124825	0.124810	0.124794	0.124775
0.124745	0.124710	0.124670	0.124624	0.124571	0.124509	0.124438	0.124356	0.124261	0.124153
0.124056	0.123949	0.123833	0.123039	0.123589	0.123451	0.123304	0.123147	0.122981	0.122790
0.122537	0.122260	0.121957	0.119771	0.121084	0.120694	0.120287	0.119873	0.119466	0.119466

```
 REACTOR IS    430.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0000 MOLES  AT PRESSURE   5.8494  VELOCITY OF  2.08526E 02 AT TEMPERATURE   820.0DEG R
 INITIAL REACTOR INCREMENT(DL 1.92467E 00FEET
 FUNCTION REQC(T,I)
 REQC(T,1)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,1)=   0.6e841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,1)=   0.14012E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,1)=   0.14637E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,1)=   0.52409E-01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,1)=   0.27599E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,1)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,1)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   5.84930E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRR(IS)
 PR=   5.84930E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(I)
 RENU=   3.35920E 05     VIS=   2.16064E-05     DEN=   1.37883E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   2.08526E 02        2.12585E 02        2.10555E 02
 TEMPERTURE=  832.71PRESSURE D=   2.27193E-02
  FUNCTION PRR(IS)
 PR=   5.82657E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   5.82657E 00    VELOCITY   2.12585E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.4774E-07
  2    0.0000E-01    0.0000E-01    7.9707E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.4724E-03    1.2994E 02    0.0000E-01
  6    1.3459E-09    5.0364E-05    0.0000E-01
  7    1.2075E-09    4.5186E-05    0.0000E-01
  8    2.7677E-10    1.0357E-05    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    1.8722DE-03   7.0059E 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

  DL CHANGED TO    1.92606E 00     ZIC=   3.40338E 02
 I= 1  RA=   1.51399E-03  DXA(I)=   1.00803E-02  CF,CR=   1.01745E-03   6.39166E-08  REQC=   1.77659E 00

 RATE=   1.48819E 00

 VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.93955E 02FEET
TEMPERTURE 1106.22DEGREE-K MOLAR FLOW RATE 2.42293E 02POUND MOLES PER HOUR
PRESSURE IS 2.000000E 00 VELOCITY 1.2709E 03FEET/SEC.

```
 REACTOR IS     400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES  AT PRESSURE   6.042A  VELOCITY OF  2.01632E 02 AT TEMPERATURE    820.0DEG K
 INITIAL REACTOR INCREMENT(DL 1.98606E 00FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.66841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14612E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52402E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27595E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.73939E-03( 832.71, 8)
 FUNCTION PRR(IS)
 PR=   6.04930E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRR(IS)
 PR=   6.04929E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   3.35919E 05     VIS=   2.16064E-05     DEN=   1.42616E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   2.01632E 02      2.05503E 02      2.03568E 02
 TEMPERTURE=  832.71PRESSURE D=   2.19422E-02
 FUNCTION PRR(IS)
 PR=   6.02735E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   6.02735E 00    VELOCITY   2.0550E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    2.6658E-07
  2    0.0000E-01    0.0000E-01    6.1104E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.5911E-03    1.2994E 02    0.0000E-01
  6    1.0670E-09    3.8610E-05    0.0000E-01
  7    9.5733E-10    3.4640E-05    0.0000E-01
  8    2.1943E-10    7.9398E-06    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    1.93621E-02   7.00596E 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

 DL CHANGED TO    1.97621E 00     ZIC=   3.24322E 02
 I= 1  RA=   1.54377E-03  DXA(I)=   1.01305E-02  CF,CR=   1.28505E-03   8.02306E-08  REQC=   1.84423E 00

 RATE=   1.20147E 00

 DL CHANGED TO    9.83156E-01     ZIC=   3.93484E 02
 I= 1  RA=   2.58433E-03  DXA(I)=   1.00504E-02  CF,CR=   6.59586E-04   1.33966E-07  REQC=   1.50958E 00

 RATE=   3.91931E 00
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.00366E 02FEET
TEMPERTURE 1109.61DEGREE-K MOLAR FLOW RATE 2.49734E 02POUND MOLES PER HOUR
PRESSURE IS 2.000000E 00 VELOCITY 8.5195E 02FEET/SEC.


SYSTEM 4 920 TO 1110 DEG K
REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 100 HOURS OF RUN

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.60160E 01FEET
TEMPERTURE 870.450EGREE-K MOLAR FLOW RATE 2.00001E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.00%
PRESSURE IS 5.95904E 00 VELOCITY 2.1738E 02FEET/SEC.
ITERATION NUMBER- 1

NO	CONCENTRATION	TNPH	DXA
1	7.5181E-16	2.8769E-11	2.9869E-06
2	0.0000E-01	0.0000E-01	4.6059E-07
3	0.0000E-01	0.0000E-01	2.8552E-08
4	4.6543E-26	1.7810E-15	5.0221E-05
5	3.3957E-03	1.2994E 02	4.0802E-12
6	2.0301E-08	7.7683E-04	4.4500E-21
7	1.8713E-08	7.1606E-04	0.0000E-01
8	3.1762E-09	1.2154E-04	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.8306E-03	7.0059E 01	
12	7.5505E-20	0.0000E-01	
13	8.1474E-24	3.1176E-19	

REACTOR POSITION 2.2032E 01FEET
TEMPERTURE 921.70EGREE-K MOLAR FLOW RATE 2.00011E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.01%
PRESSURE IS 5.9622E 00 VELOCITY 2.3388E 02FEET/SEC.
ITERATION NUMBER- 2

NO	CONCENTRATION	TNPH	DXA
1	1.1519E-13	4.7409E-09	3.7942E-05
2	0.0000E-01	0.0000E-01	3.6243E-06
3	0.0000E-01	0.0000E-01	2.9934E-07
4	6.4863E-17	2.6695E-12	3.3695E-04
5	3.1570E-03	1.2993E 02	3.9395E-10
6	2.6963E-07	1.1097E-02	1.2484E-17
7	2.5560E-07	1.0519E-02	0.0000E-01
8	2.8076E-08	1.1555E-03	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.7023IE-03	7.0059E 01	
12	7.7607OE-17	0.0000E-01	
13	2.5122OE-20	1.0339IE-15	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.80480E 01FEET
TEMPERTURE 953.04DEGREE-K MOLAR FLOW RATE 2.00077E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.06%
PRESSURE IS 5.76079E 00 VELOCITY 2.4618E 02FEET/SEC.
ITERATION NUMBER- 3

NO	CONCENTRATION	TMPH	OXA
1	4.2666E-12	1.8487E-07	1.5551E-04
2	0.0000E-01	0.0000E-01	1.1348E-05
3	0.0000E-01	0.0000E-01	1.1016E-06
4	1.3523E-14	5.8565E-10	9.6439E-04
5	2.9985E-03	1.2986E 02	9.3893E-09
6	1.7566E-06	7.6076E-02	5.0251E-15
7	1.6882E-06	7.3113E-02	0.0000E-01
8	1.3684E-07	5.9262E-03	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.61768E-03	7.00602E 01	
12	8.22509E-15	0.00000E-01	
13	1.23738E-17	5.35898E-13	

REACTOR POSITION 5.4064CE 01FEET
TEMPERTURE 965.05DEGREE-K MOLAR FLOW RATE 2.00194E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.15%
PRESSURE IS 5.65806E 00 VELOCITY 2.5391E 02FEET/SEC.
ITERATION NUMBER- 4

NO	CONCENTRATION	TMPH	OXA
1	2.3899E-11	1.0673E-06	2.5856E-04
2	0.0000E-01	0.0000E-01	1.7097E-05
3	0.0000E-01	0.0000E-01	1.7608E-06
4	1.8354E-13	8.1970E-09	1.4060E-03
5	2.9051E-03	1.2974E 02	3.6491E-08
6	4.3009E-06	1.9208E-01	5.9111E-14
7	4.1488E-06	1.8529E-01	0.0000E-01
8	3.0439E-07	1.3594E-02	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.56875E-03	7.00607E 01	
12	6.71111E-14	0.00000E-01	
13	2.06246E-16	9.21100E-12	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 5.70800E 01FEET
TEMPERTURE 977.36DEGREE-K MOLAR FLOW RATE 2.00386E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.29%
PRESSURE IS 5.55513E 00 VELOCITY 2.6213E 02FEET/SEC.
ITERATION NUMBER= 5

NO	CONCENTRATION	TMPH	DXA
1	8.6474E-11	3.9858E-06	4.2384E-04
2	0.0000E-01	0.0000E-01	2.5456E-05
3	0.0000E-01	0.0000E-01	2.7774E-06
4	1.1829E-12	5.4522E-08	2.0274E-03
5	2.8106E-03	1.2955E 02	1.0079E-07
6	8.2948E-06	3.8233E-01	3.8095E-13
7	8.0233E-06	3.6982E-01	0.0000E-01
8	5.4333E-07	2.5043E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.5200IE-03	7.0061BE-01	
12	3.5059E-13	0.0000E-01	
13	1.5385AE-15	7.0915TE-11	

REACTOR POSITION 9.60959E 01FEET
TEMPERTURE 988.27DEGREE-K MOLAR FLOW RATE 2.00689E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.53%
PRESSURE IS 5.45056E 00 VELOCITY 2.7063E 02FEET/SEC.
ITERATION NUMBER= 6

NO	CONCENTRATION	TMPH	DXA
1	2.5553E-10	1.2157E-05	6.6307E-04
2	0.0000E-01	0.0000E-01	3.6482E-05
3	0.0000E-01	0.0000E-01	4.1953E-06
4	5.4703E-12	2.6025E-07	2.9220E-03
5	2.7166E-03	1.2924E 02	2.3486E-07
6	1.4361E-05	6.8322E-01	1.6658E-12
7	1.3924E-05	6.6243E-01	0.0000E-01
8	9.7509E-07	4.1632E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.47269E-03	7.0062AE 01	
12	1.43944E-12	0.0000E-01	
13	8.24990E-15	3.92486E-10	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.12112E 02FEET
TEMPERTURE 999.45DEGREE-K MOLAR FLOW RATE 2.01158E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.88%
PRESSURE IS 5.34620E 00 VELOCITY 2.7970E 02FEET/SEC.
ITERATION NUMBER- 7

NO	CONCENTRATION	THPH	DXA
1	6.7066E-10	3.2966E-05	1.0254E-03
2	0.0000E-01	0.0000E-01	5.1768E-05
3	0.0000E-01	0.0000E-01	6.2695E-06
4	2.0792E-11	1.0220E-06	3.6930E-03
5	2.6196E-03	1.2877E 02	4.9817E-07
6	2.3352E-05	1.1479E 00	7.8318E-12
7	2.2691E-05	1.1153E 00	0.0000E-01
8	1.3261E-06	5.5186E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.42539E-03	7.00641E 01	
12	5.21063E-12	0.0000E-01	
13	3.64036E-14	1.78932E-09	

REACTOR POSITION 1.28128E 02FEET
TEMPERTURE 1008.050EGREE-K MOLAR FLOW RATE 2.01842E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 1.40%
PRESSURE IS 5.24331E 00 VELOCITY 2.8861E 02FEET/SEC.
ITERATION NUMBER- 8

NO	CONCENTRATION	THPH	DXA
1	1.5866E-09	8.0463E-05	1.4106E-03
2	0.0000E-01	0.0000E-01	6.6806E-05
3	0.0000E-01	0.0000E-01	8.4054E-06
4	6.7328E-11	3.4140E-06	4.9156E-03
5	2.5258E-03	1.2808E 02	9.0919E-07
6	3.6003E-05	1.8256E 00	2.7628E-11
7	3.5049E-05	1.7772E 00	0.0000E-01
8	1.9150E-06	9.7101E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.38180E-03	7.00666E 01	
12	1.55624E-11	0.0000E-01	
13	1.39372E-13	7.06712E-09	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 1.44144E 02FEET

TEMPERTURE 1014.05DEGREE-K MOLAR FLOW RATE 2.02692E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 2.05%

PRESSURE IS 5.14034E 00 VELOCITY 2.9741E 02FEET/SEC.

ITERATION NUMBER- 9

NO	CONCENTRATION	TLPH	DXA
1	3.1991E-09	1.6710E-04	1.7455E-03
2	0.0000E-01	0.0000E-01	7.9085E-05
3	0.0000E-01	0.0000E-01	1.0219E-05
4	1.7453E-10	9.1162E-06	5.7338E-03
5	2.4356E-03	1.2722E 02	1.3946E-06
6	5.1087E-05	2.6684E 00	7.1663E-11
7	4.9801E-05	2.6013E 00	0.0000E-01
8	2.5852E-06	1.3503E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.3414BE-03	7.0669E 01	
12	3.6589BE-11	0.0000E-01	
13	4.1677BE-13	2.1769BE-08	

REACTOR POSITION 1.60160E 02FEET

TEMPERTURE 1020.02DEGREE-K MOLAR FLOW RATE 2.03733E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 2.85%

PRESSURE IS 5.03746E 00 VELOCITY 3.0686E 02FEET/SEC.

ITERATION NUMBER- 10

NO	CONCENTRATION	TLPH	DXA
1	5.8187E-09	3.1346E-04	2.1477E-03
2	0.0000E-01	0.0000E-01	9.3166E-05
3	0.0000E-01	0.0000E-01	1.2356E-05
4	3.8599E-10	2.0794E-05	6.6569E-03
5	2.3421E-03	1.2617E 02	1.9850E-06
6	6.8669E-05	3.6993E 00	1.6481E-10
7	6.7016E-05	3.6102E 00	0.0000E-01
8	3.3316E-06	1.7947E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.3607BE-03	7.0674IE 01	
12	7.7254BE-11	0.0000E-01	
13	1.0531IE-12	5.6731BE-08	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 1.76176E 02FEET

TEMPERTURE 1022.02DEGREE-K MOLAR FLOW RATE 2.04880E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 3.72%

PRESSURE IS 4.93200E 00 VELOCITY 3.1580E 02FEET/SEC.

ITERATION NUMBER- 11

NO	CONCENTRATION	TMPH	DXA
1	9.4821E-09	5.2546E-04	2.2584E-03
2	0.0000E-01	0.0000E-01	9.6551E-05
3	0.0000E-01	0.0000E-01	1.2918E-05
4	7.3169E-10	4.0547E-05	6.8660E-03
5	2.2560E-03	1.2502E 02	2.3738E-06
6	8.7253E-05	4.8352E 00	2.9978E-10
7	8.5224E-05	4.7227E 00	0.0000E-01
8	4.1014E-06	2.2728E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.26460E-03	7.00785E 01	
12	1.29830E-10	0.00000E-01	
13	2.27536E-12	1.26091E-07	

REACTOR POSITION 1.92192E 02FEET

TEMPERTURE 1024.02DEGREE-K MOLAR FLOW RATE 2.06075E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 4.63%

PRESSURE IS 4.82397E 00 VELOCITY 3.2548E 02FEET/SEC.

ITERATION NUMBER- 12

NO	CONCENTRATION	TMPH	DXA
1	1.4050E-08	8.0204E-04	2.3729E-03
2	0.0000E-01	0.0000E-01	9.9994E-05
3	0.0000E-01	0.0000E-01	1.3495E-05
4	1.2129E-09	6.9238E-05	7.0767E-03
5	2.1690E-03	1.2381E 02	2.6776E-06
6	1.0542E-04	6.0179E 00	4.7695E-10
7	1.0303E-04	5.8816E 00	0.0000E-01
8	4.8413E-06	2.7636E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.22771E-03	7.00833E 01	
12	1.96269E-10	0.00000E-01	
13	4.20611E-12	2.40104E-07	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 2.08208E 02FEET
TEMPERTURE 1027.050EGREE-K MOLAR FLOW RATE 2.07336E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 5.59%
PRESSURE IS 4.71106E 00 VELOCITY 3.3639E 02FEET/SEC.
ITERATION NUMBER- 13

NO	CONCENTRATION	TAPH	DXA
1	1.9581E-08	1.1545E-03	2.5892E-03
2	0.0000E-01	0.0000E-01	1.0676E-04
3	0.0000E-01	0.0000E-01	1.4597E-05
4	1.8343E-09	1.0814E-04	7.5012E-03
5	2.0786E-03	1.2255E 02	2.9949E-06
6	1.2324E-04	7.2657E 00	7.2493E-10
7	1.2051E-04	7.1046E 00	0.0000E-01
8	5.5510E-06	3.2727E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.18879E-03	7.00887E 01	
12	2.92906E-10	0.0000E-01	
13	7.02803E-12	4.14358E-07	

REACTOR POSITION 2.24224E 02FEET
TEMPERTURE 1031.060EGREE-K MOLAR FLOW RATE 2.08740E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 6.66%
PRESSURE IS 4.59490E 00 VELOCITY 3.4870E 02FEET/SEC.
ITERATION NUMBER- 14

NO	CONCENTRATION	TAPH	DXA
1	2.6492E-08	1.6178E-03	2.9225E-03
2	0.0000E-01	0.0000E-01	1.1711E-04
3	0.0000E-01	0.0000E-01	1.6289E-05
4	2.6325E-09	1.6075E-04	8.1505E-03
5	1.9838E-03	1.2114E 02	3.3760E-06
6	1.4171E-04	8.6538E 00	1.1172E-09
7	1.3865E-04	8.4665E 00	0.0000E-01
8	6.2620E-06	3.8239E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.14782E-03	7.00954E 01	
12	4.36572E-10	0.0000E-01	
13	1.11891E-11	6.83263E-07	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.40240E 02FEET

TEMPERTURE 1035.06DEGREE-K MOLAR FLOW RATE 2.10303E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 7.85%

PRESSURE IS 4.47482E 00 VELOCITY 3.6231E 02FEET/SEC.

ITERATION NUMBER- 15

NO	CONCENTRATION	THPH	UXA
1	3.5019E-08	2.2196E-03	3.2874E-03
2	0.0000E-01	0.0000E-01	1.2806E-04
3	0.0000E-01	0.0000E-01	1.8117E-05
4	3.6329E-09	2.3026E-04	6.6287E-03
5	1.8866E-03	1.1958E 02	3.7520E-06
6	1.6288E-04	1.0197E 01	1.6748E-09
7	1.5748E-04	9.9816E 00	0.0000E-01
8	6.9736E-06	4.4200E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.1+605E-03	7.01034E 01	
12	6.16496E-10	0.0000E-01	
13	1.72004E-11	1.09019E-06	

REACTOR POSITION 2.56256E 02FEET

TEMPERTURE 1039.06DEGREE-K MOLAR FLOW RATE 2.12034E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 9.16%

PRESSURE IS 4.35024E 00 VELOCITY 3.7745E 02FEET/SEC.

ITERATION NUMBER- 16

NO	CONCENTRATION	THPH	UXA
1	4.5346E-08	2.9903E-03	3.6843E-03
2	0.0000E-01	0.0000E-01	1.3955E-04
3	0.0000E-01	0.0000E-01	2.0077E-05
4	4.8505E-09	3.1986E-04	9.5307E-03
5	1.7871E-03	1.1786E 02	4.1070E-06
6	1.8052E-04	1.1904E 01	2.4488E-09
7	1.7680E-04	1.1659E 01	0.0000E-01
8	7.6753E-06	5.0615E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.06321E-03	7.01130E 01	
12	8.61755E-10	0.0000E-01	
13	2.56329E-11	1.69036E-06	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.72271E 02FEET

TEMPERTURE 1043.07DEGREE-K MOLAR FLOW RATE 2.13940E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 10.61%

PRESSURE IS 4.21976E 00 VELOCITY 3.9447E 02FEET/SEC.

ITERATION NUMBER= 17

NO	CONCENTRATION	TIPH	DXA
1	5.7616E-08	3.9643E-03	4.1121E-03
2	0.0000E-01	0.0000E-01	1.5147E-04
3	0.0000E-01	0.0000E-01	2.2160E-05
4	6.2873E-09	4.3260E-04	1.0249E-02
5	1.6852E-03	1.1595E 02	4.4240E-06
6	2.0031E-04	1.5783E 01	3.4971E-09
7	1.9628E-04	1.5505E 01	0.0000E-01
8	8.3542E-06	5.7452E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.01917E-03	7.01245E 01	
12	1.17746E-09	0.0000E-01	
13	3.71282E-11	2.55463E-06	

REACTOR POSITION 2.82287E 02FEET

TEMPERTURE 1050.18DEGREE-K MOLAR FLOW RATE 2.16129E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 12.26%

PRESSURE IS 4.08341E 00 VELOCITY 4.1523E 02FEET/SEC.

ITERATION NUMBER= 18

NO	CONCENTRATION	TIPH	DXA
1	7.2517E-08	5.2392E-03	5.1241E-03
2	0.0000E-01	0.0000E-01	1.7972E-04
3	0.0000E-01	0.0000E-01	2.7078E-05
4	7.9810E-09	5.7661E-04	1.1964E-02
5	1.5742E-03	1.1378E 02	5.1175E-06
6	2.2055E-04	1.5934E 01	5.2779E-09
7	2.1623E-04	1.5622E 01	0.0000E-01
8	9.0065E-06	6.5070E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	9.70824E-04	7.01396E 01	
12	1.73000E-09	0.0000E-01	
13	5.26677E-11	3.80511E-06	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.04303E 02FEET
TEMPERTURE 1060.19DEGREE-K MOLAR FLOW RATE 2.19042E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 14.46%
PRESSURE IS 3.94491E 00 VELOCITY 4.4112E 02FEET/SEC.
ITERATION NUMBER- 19

NO	CONCENTRATION	TAPH	DXA
1	9.4040E-08	7.1864E-03	7.6073E-03
2	0.0000E-01	0.0000E-01	2.2964E-04
3	0.0000E-01	0.0000E-01	3.6038E-05
4	1.0296E-08	7.8650E-04	1.4945E-02
5	1.4512E-03	1.1090E 02	6.4662E-06
6	2.4587E-04	1.8789E 01	9.3315E-09
7	2.4125E-04	1.8436E 01	0.0000E-01
8	9.7501E-06	7.4508E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	9.1816ZE-04	7.0164E 01	
12	2.8023E-09	0.0000E-01	
13	7.7802DE-11	5.9454DE-06	

REACTOR POSITION 3.20318E 02FEET
TEMPERTURE 1070.12DEGREE-K MOLAR FLOW RATE 2.22874E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 17.34%
PRESSURE IS 3.80355E 00 VELOCITY 4.7254E 02FEET/SEC.
ITERATION NUMBER- 20

NO	CONCENTRATION	TAPH	DXA
1	1.2535E-07	1.0187E-02	9.4153E-03
2	0.0000E-01	0.0000E-01	2.8884E-04
3	0.0000E-01	0.0000E-01	4.7161E-05
4	1.3586E-08	1.1041E-03	1.8388E-02
5	1.3182E-03	1.0713E 02	8.1375E-06
6	2.7728E-04	2.2535E 01	1.6705E-08
7	2.7232E-04	2.2132E 01	0.0000E-01
8	1.0595E-05	8.6107E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	8.6381DE-04	7.0203IE 01	
12	4.5954TE-09	0.0000E-01	
13	1.2020JE-10	9.7690TE-06	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.38155E 02FEET
TEMPERTURE 1076.81DEGREE-K MOLAR FLOW RATE 2.27774E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 21.05%
PRESSURE IS 3.62464E 00 VELOCITY 5.2267E 02FEET/SEC.
ITERATION NUMBER- 21

NO	CONCENTRATION	TMPH	DXA
1	1.6767E-07	1.4783E-02	5.2802E-03
2	0.2000E-01	0.1000E-01	1.5504E-04
3	0.0000E-01	0.0000E-01	2.5990E-05
4	1.7649E-08	1.5737E-03	9.7274E-03
5	1.1600E-03	1.0227E 02	4.1505E-06
6	3.1022E-04	2.7352E 01	6.6070E-09
7	3.0500E-04	2.6891E 01	0.0000E-01
8	1.1300E-05	1.0033E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	7.9663SE-04	7.0238IE 01	
12	3.2566E-09	0.0000E-01	
13	1.6324TE-10	1.4393ZE-05	

REACTOR POSITION 3.55939E 02FEET
TEMPERTURE 1083.48DEGREE-K MOLAR FLOW RATE 2.33140E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 25.11%
PRESSURE IS 3.42514E 00 VELOCITY 5.6649E 02FEET/SEC.
ITERATION NUMBER- 22

NO	CONCENTRATION	TMPH	DXA
1	2.1698E-07	2.0823E-02	6.1739E-03
2	0.0000E-01	0.0000E-01	1.7364E-04
3	0.0000E-01	0.0000E-01	2.9870E-05
4	2.2401E-08	2.1498E-03	1.0738E-02
5	1.2101E-03	9.6943E 01	4.1897E-06
6	3.4003E-04	2.2633E 01	1.0131E-08
7	3.3465E-04	3.2116E 01	0.0000E-01
8	1.2013E-05	1.1529E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	7.3224IE-04	7.0272GE 01	
12	4.6525OE-09	0.0000E-01	
13	2.0653BE-10	1.9821BE-05	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.73724E 02FEET
TEMPERTURE 1093.58DEGREE-K MOLAR FLOW RATE 2.39234E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 29.71%
PRESSURE IS 3.18283E 00 VELOCITY 6.3094E 02FEET/SEC.
ITERATION NUMBER- 23

NO	CONCENTRATION	THPH	DXA
1	2.7092E-07	2.8968E-02	7.5134E-03
2	0.0000E-01	0.0000E-01	2.0870E-04
3	0.0000E-01	0.0000E-01	3.7316E-05
4	2.6426E-08	2.6256E-03	1.2633E-02
5	8.5029E-04	9.0920E 01	4.2447E-06
6	3.6108E-04	3.6610E 01	1.5843E-08
7	3.5573E-04	3.8038E 01	0.0000E-01
8	1.2285E-05	1.3137E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	6.5764TE-04	7.0320E 01	
12	6.8345E-09	0.0000E-01	
13	2.6177E-10	2.7990E-05	

REACTOR POSITION 3.91509E 02FEET
TEMPERTURE 1104.690EGREE-K MOLAR FLOW RATE 2.46384E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 35.08%
PRESSURE IS 2.84375E 00 VELOCITY 7.6399E 02FEET/SEC.
ITERATION NUMBER- 24

NO	CONCENTRATION	THPH	DXA
1	3.2611E-07	4.0326E-02	9.6728E-03
2	0.0000E-01	0.0000E-01	2.3799E-04
3	0.0000E-01	0.0000E-01	4.4364E-05
4	2.8882E-08	3.5714E-03	1.4076E-02
5	6.7854E-04	8.3906E 01	3.6693E-06
6	3.6866E-04	4.5568E 01	2.3119E-08
7	3.6363E-04	4.4965E 01	0.0000E-01
8	1.2043E-05	1.4891E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	5.6925E-04	7.0392E 01	
12	9.1677E-09	0.0000E-01	
13	3.2664E-10	4.0390E-05	

SYSTEM 4 820 TO 1110 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.15310E 01(1104.69, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.45675E-01(1104.69, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.34972E 02(1104.69, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12602E-08(1104.69, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42361E 01(1104.69, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13177E 01(1104.69, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24886E 00(1104.69, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.22116E-02(1104.69, 8)

FUNCTION PRR(IS)
PR= 6.04930E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.39640E 05 VIS= 2.68387E-05 DEN= 1.04906E-01
FRICTION FACTOR= 1.29231E-02 V1,V2,VA= 7.63988E 02 3.91634E 02 5.77815E 02
TEMPERTURE= 1104.69PRESSURE D= 3.13544E-01

1-A	ACETYLENE	3.26108E-07	4.03256E-02
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	2.88816E-08	3.57141E-03
5-E	ETHANE	6.78536E-04	8.39059E 01
6-F	ETHYLENE	3.68664E-04	4.55880E 01
7-G	HYDROGEN	3.63629E-04	4.49653E 01
8-H	METHANE	1.20425E-05	1.48915E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	5.69253E-04	7.03922E 01
12-L	CARBON	9.16776E-09	0.00000E-01
13-M	CARBON MONOXIDE	3.20634E-10	4.03907E-05

CONVERSION OF ETHANE TO ETHYLENE IS 35.08%

REACTOR RADIUS PROFILE AFTER 200.00 HOURS

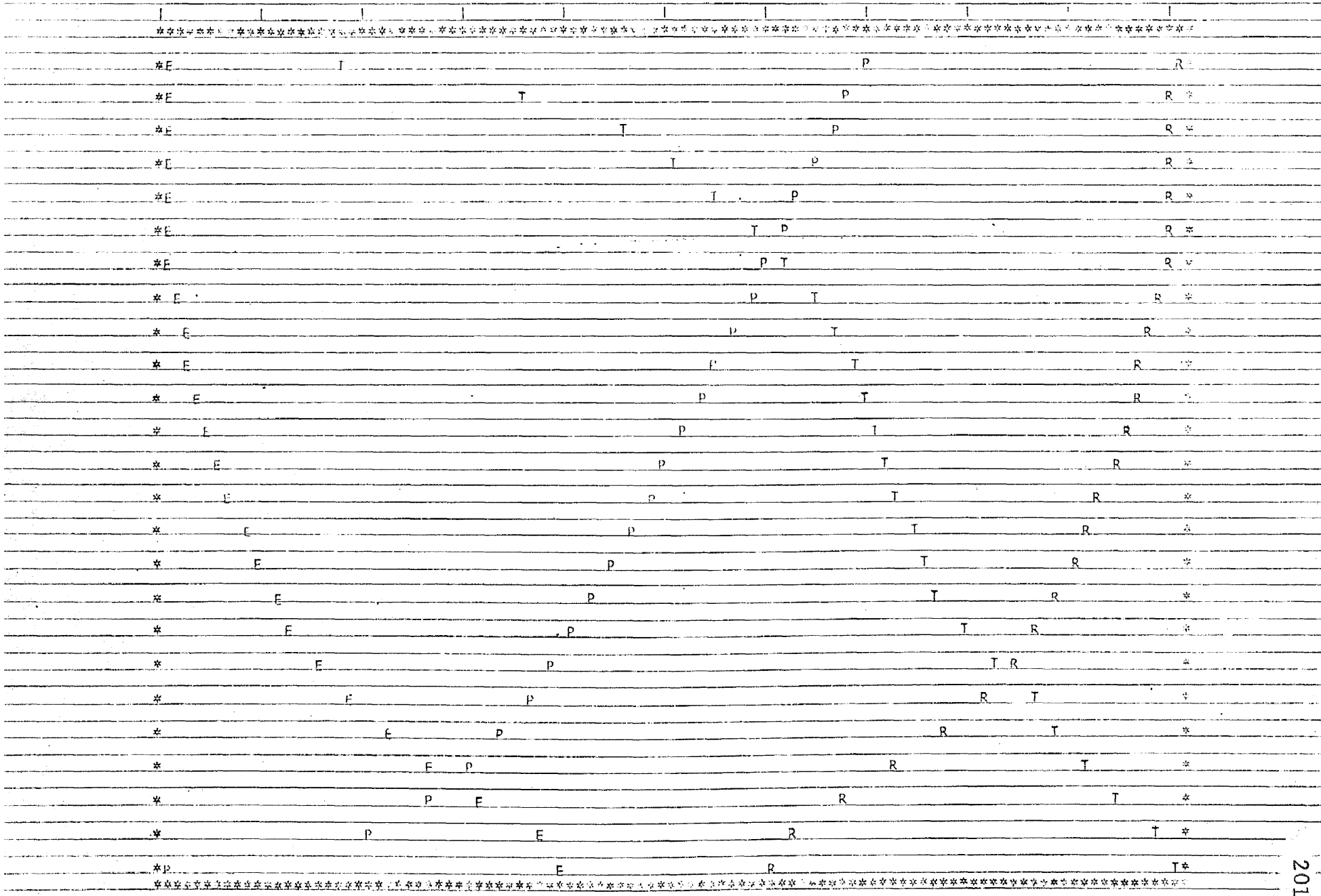
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.125000	0.125000	0.124999	0.124999	0.124999	0.124999	0.124998	0.124997
0.124997	0.124996	0.124995	0.124993	0.124992	0.124990	0.124987	0.124985	0.124982	0.124978
0.124974	0.124971	0.124967	0.124962	0.124957	0.124952	0.124946	0.124940	0.124934	0.124927
0.124919	0.124909	0.124899	0.124888	0.124875	0.124862	0.124848	0.124832	0.124815	0.124796
0.124776	0.124754	0.124730	0.124704	0.124677	0.124647	0.124615	0.124580	0.124543	0.124502
0.124433	0.124355	0.124265	0.124160	0.124039	0.123899	0.123737	0.123549	0.123331	0.123084
0.122237	0.122616	0.122344	0.121415	0.121776	0.121449	0.121098	0.120722	0.120321	0.119859
0.119251	0.118577	0.115413	0.115040	0.115683	0.114668	0.113613	0.112641	0.111747	0.111747

```
 REACTOR IS      400.00 FEET LONG AND   0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MILES  AT PRESSURE   6.049A  VELOCITY OF  2.01632E 02 AT TEMPERATURE   820.00EG K
 INITIAL REACTOR INCREMENT(DL 9.83156E-01FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.68841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14612E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14637E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52402E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   6.04930E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=   6.04929E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 KENU=   3.35919E 05      VIS=   2.16064E-05      DEN=   1.42616E-01
 FRICTION FACTOR=   1.41227E-02      V1,V2,VA=   2.01632E 02      2.05504E 02      2.03568E 02
 TEMPERTURE=  832.71PRESSURE D=   2.19422E-02
  FUNCTION PRR(IS)
 PR=   6.02734E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   6.02734E 00    VELOCITY    2.0550E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.5963E-07
  2    0.0000E-01    0.0000E-01    8.2432E-08
  3    0.00005-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.5911E-03    1.2994E 02    0.0000E-01
  6    1.4395E-09    5.2066E-05    0.0000E-01
  7    1.2915E-09    4.6731E-05    0.0000E-01
  8    2.9602E-10    1.0711E-05    0.0000E-01
  9    0.00000E-01   0.0000CE-01
 10    0.00000E-01   0.00000E-01
 11    1.93621E-03   7.00597E 01
 12    0.00000E-01   0.00000E-01
 13    0.00000E-01   0.00000E-01

  DL CHANGED TO    1.96211E 00      ZIC=   3.28326E 02
 I= 1  KA=   1.57703E-03  DXA(I)=   1.02033E-02  CF,CR=   1.24408E-03   8.25100E-08  REQC=   1.82748E 00

 RATE=   1.26778E 00

 VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.90955E 02FEET
TEMPERTURE 1109.35DEGREE-K MOLAR FLOW RATE 2.47060E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.2705E 03FEET/SEC.

```
 REACTOR IS      400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES  AT PRESSURE    6.249A  VELOCITY OF   1.95179E 02 AT TEMPERATURE    820.0DEG R
 INITIAL REACTOR INCREMENT(DL 1.96211E 00FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=    0.11963E 02( 832.71,  1)
 FUNCTION REQC(T,I)
 REQC(T,I)=    0.68841E-02( 832.71,  2)
 FUNCTION REQC(T,I)
 REQC(T,I)=    0.14012E 06( 832.71,  3)
 FUNCTION REQC(T,I)
 REQC(T,I)=    0.14837E-08( 832.71,  4)
 FUNCTION REQC(T,I)
 REQC(T,I)=    0.52409E 01( 832.71,  5)
 FUNCTION REQC(T,I)
 REQC(T,I)=    0.27599E-01( 832.71,  6)
 FUNCTION REQC(T,I)
 REQC(T,I)=    0.5538IE 00( 832.71,  7)
 FUNCTION REQC(T,I)
 REQC(T,I)=    0.79139E-03( 832.71,  8)
 FUNCTION PRR(IS)
 PR=   6.24929E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRR(IS)
 PR=   6.24929E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   3.35919E 05      VIS=   2.16064E-05      DEN=   1.47348E-01
 FRICTION FACTOR=    1.41227E-02      V1,V2,VA=   1.95179E 02          1.98880E 02          1.97030E 02
 TEMPERTURE=   832.71PRESSURE D=   2.12174E-02
 FUNCTION PRR(IS)
 PR=   6.22807E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   6.22807E 00    VELOCITY    1.9888E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    2.7462E-07
  2    0.0000E-01    0.0000E-01    6.2946E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.7095E-03    1.2994E-02    0.0000E-01
  6    1.1356E-09    3.9774E-05    0.0000E-01
  7    1.0188E-09    3.5664E-05    0.0000E-01
  8    2.3352E-10    8.1792E-06    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    2.0002JE-03   7.0059GE 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

  DL CHANGED TO     1.96839E 00      ZIC=   3.16314E 02
 I= 1  RA=    1.57878E-03  DXA(I)=    1.01708E-02  CF,CR=    1.46206E-03   9.52185E-08  REQC=    1.87819E 00

 RATE=    1.07857E 00

  DL CHANGED TO     9.77499E-01      ZIC=   3.93076E 02
 I= 1  RA=    2.85336E-03  DXA(I)=    1.00665E-02  CF,CR=    7.34717E-04   1.89908E-07  REQC=    1.51182E 00

 RATE=    3.88513E 00
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.00895E 02FEET
TEMPERTURE 1109.95DEGREE-K MOLAR FLOW RATE 2.51995E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 8.6908E 02FEET/SEC.



SYSTEM 4 820 TO 1110 DEG K

REACTOR PRODUCT (E) REACTANT(P) TEMPERATURE(T) PRESSURE(P) AFTER 200 HOURS OF RUN

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.60160E 01FEET
TEMPERTURE 870.65DEGREE-K MOLAR FLOW RATE 2.00001E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.00%
PRESSURE IS 6.16205E 00 VELOCITY 2.1022E 02FEET/SEC.
ITERATION NUMBER- 1

NO	CONCENTRATION	TMPH	OXA
1	8.2987E-16	3.0717E-11	3.0891E-06
2	0.0000E-01	0.0000E-01	4.7605E-07
3	0.0000E-01	0.0000E-01	2.9510E-08
4	5.4845E-20	2.0300E-15	5.1906E-05
5	3.5105E-03	1.2994E 02	4.5019E-12
6	2.1685E-08	8.0265E-04	5.0715E-21
7	1.9989E-08	7.3987E-04	0.0000E-01
8	3.3925E-09	1.2557E-04	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.8927BE-03	7.0059TE 01	
12	8.61403E-20	0.0000E-01	
13	9.59924E-24	3.5530BE-19	

REACTOR POSITION 3.20320E 01FEET
TEMPERTURE 921.70DEGREE-K MOLAR FLOW RATE 2.00012E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.01%
PRESSURE IS 6.06850E 00 VELOCITY 2.2593E 02FEET/SEC.
ITERATION NUMBER- 2

NO	CONCENTRATION	TMPH	OXA
1	1.2755E-13	5.0722E-09	3.9255E-05
2	0.0000E-01	0.0000E-01	3.7498E-06
3	0.0000E-01	0.0000E-01	3.0970E-07
4	7.6629E-17	3.0553E-12	3.4861E-04
5	3.2672E-03	1.2993E 02	4.3602E-10
6	2.8862E-07	1.1478E-02	1.4286E-17
7	2.7360E-07	1.0880E-02	0.0000E-01
8	3.0051E-08	1.1951E-03	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.76173E-03	7.0059BE 01	
12	8.89025E-17	0.0000E-01	
13	2.97463E-20	1.1829AE-15	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.80480E 01FEET
TEMPERTURE 953.04DEGREE-K MOLAR FLOW RATE 2.00080E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.06%
PRESSURE IS 5.97103E 00 VELOCITY 2.3751E 02FEET/SEC.
ITERATION NUMBER- 3

NO	CONCENTRATION	TAPH	DXA
1	4.7405E-12	1.9814E-07	1.6108E-04
2	0.0000E-01	0.0000E-01	1.1755E-05
3	0.0000E-01	0.0000E-01	1.1411E-06
4	1.6094E-14	6.7268E-10	9.9896E-04
5	3.1058E-03	1.2986E 02	1.0422E-08
6	1.8843E-06	7.8760E-02	5.7748E-15
7	1.8109E-06	7.5693E-02	0.0000E-01
8	1.4677E-07	6.1348E-03	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.67616E-03	7.00601E 01	
12	9.46151E-15	0.00000E-01	
13	1.47276E-17	6.15583E-13	

REACTOR POSITION 5.40640E 01FEET
TEMPERTURE 965.05DEGREE-K MOLAR FLOW RATE 2.00201E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.15%
PRESSURE IS 5.87335E 00 VELOCITY 2.4465E 02FEET/SEC.
ITERATION NUMBER- 4

NO	CONCENTRATION	TAPH	DXA
1	2.6617E-11	1.1458E-06	2.6817E-04
2	0.0000E-01	0.0000E-01	1.7732E-05
3	0.0000E-01	0.0000E-01	1.8262E-06
4	2.1933E-13	9.4415E-09	1.4582E-03
5	3.0139E-03	1.2973E 02	4.0604E-08
6	4.6233E-06	1.9902E-01	6.8203E-14
7	4.4598E-06	1.9198E-01	0.0000E-01
8	3.2718E-07	1.4084E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.62757E-03	7.00606E 01	
12	7.75169E-14	0.00000E-01	
13	2.46628E-16	1.06164E-11	

SYSTEM 4 920 TO 1110 DEG K

REACTOR POSITION 8.00800E 01FEET
TEMPERTURE 977.06DEGREE-K MOLAR FLOW RATE 2.00400E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.31%
PRESSURE IS 5.77415E 00 VELOCITY 2.5220E 02FEET/SEC.
ITERATION NUMBER- 5

NO	CONCENTRATION	TAPH	DXA
1	9.6615E-11	4.2862E-06	4.4019E-04
2	0.0000E-01	0.0000E-01	2.6438E-05
3	0.0000E-01	0.0000E-01	2.6845E-06
4	1.4197E-12	6.2984E-08	2.1056E-03
5	2.9198E-03	1.2953E 02	1.1243E-07
6	8.9373E-06	3.9649E-01	4.4150E-13
7	8.6448E-06	3.8352E-01	0.0000E-01
8	5.8534E-07	2.5968E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.5792JE-03	7.0061ZE 01	
12	4.06178E-13	0.0000E-01	
13	1.84947E-15	8.20501E-11	

REACTOR POSITION 9.60959E 01FEET
TEMPERTURE 988.27DEGREE-K MOLAR FLOW RATE 2.00715E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.55%
PRESSURE IS 5.67490E 00 VELOCITY 2.5997E 02FEET/SEC.
ITERATION NUMBER- 6

NO	CONCENTRATION	TAPH	DXA
1	2.6650E-10	1.3099E-05	6.8970E-04
2	0.0000E-01	0.0000E-01	3.7947E-05
3	0.0000E-01	0.0000E-01	4.3638E-06
4	6.5959E-12	3.0156E-07	2.9353E-03
5	2.8262E-03	1.2921E 02	2.6261E-07
6	1.5513E-05	7.0925E-01	2.1729E-12
7	1.5041E-05	6.8767E-01	0.0000E-01
8	9.4512E-07	4.3211E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.53244E-03	7.0062JE 01	
12	1.67859E-12	0.0000E-01	
13	9.97549E-15	4.56075E-10	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.12112E 02FEET
TEMPERTURE 999.48DEGREE-K MOLAR FLOW RATE 2.01203E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.92%
PRESSURE IS 5.5763bE 00 VELOCITY 2.6822E 02FEET/SEC.
ITERATION NUMBER- 7

NO	CONCENTRATION	TMPH	DXA
1	7.5485E-10	3.5597E-05	1.0684E-03
2	0.0000E-01	0.0000E-01	5.3956E-05
3	0.0000E-01	0.0000E-01	6.5721E-06
4	2.5192E-11	1.1882E-06	4.0561E-03
5	2.7296E-03	1.2872E 02	5.5833E-07
6	2.5297E-05	1.1929E 00	9.1702E-12
7	2.4580E-05	1.1591E 00	0.0000E-01
8	1.4362E-06	6.7729E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.48576E-03	7.0064E 01	
12	6.1098E-12	0.0000E-01	
13	4.4305lE-14	2.0893E-09	

REACTOR POSITION 1.20128E 02FEET
TEMPERTURE 1008.05DEGREE-K MOLAR FLOW RATE 2.01916E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 1.46%
PRESSURE IS 5.4803bE 00 VELOCITY 2.7624E 02FEET/SEC.
ITERATION NUMBER- 8

NO	CONCENTRATION	TMPH	DXA
1	1.7934E-09	8.7061E-05	1.4723E-03
2	0.0000E-01	0.0000E-01	6.9730E-05
3	0.0000E-01	0.0000E-01	8.7733E-06
4	8.1981E-11	3.9806E-06	5.1308E-03
5	2.6362E-03	1.2800E 02	1.0212E-06
6	3.9120E-05	1.8995E 00	3.2538E-11
7	3.8084E-05	1.8492E 00	0.0000E-01
8	2.2801E-06	1.1070E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.44302E-03	7.0066E 01	
12	1.83566E-11	0.0000E-01	
13	1.7830E-13	8.29472E-09	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.44144E 02FEET
TEMPERTURE 1014.05DEGREE-K MOLAR FLOW RATE 2.02803E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 2.14%
PRESSURE IS 5.38508E 00 VELOCITY 2.8407E 02FLET/SEC.
ITERATION NUMBER- 9

NO	CONCENTRATION	TEPH	DXA
1	3.6310E-09	1.8124E-04	1.8755E-03
2	0.0000E-01	0.0000E-01	8.2710E-05
3	0.0000E-01	0.0000E-01	1.0687E-05
4	2.1354E-10	1.0659E-05	5.9965E-03
5	2.5465E-03	1.2710E 02	1.5695E-06
6	5.5685E-05	2.7796E 00	5.4914E-11
7	5.4258E-05	2.7097E 00	0.0000E-01
8	2.8171E-06	1.4061E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.40381E-03	7.00697E 01	
12	4.34272E-11	2.0000E-01	
13	5.14555E-13	2.56834E-08	

REACTOR POSITION 1.60160E 02FEET
TEMPERTURE 1020.02DEGREE-K MOLAR FLOW RATE 2.03892E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 2.97%
PRESSURE IS 5.29087E 00 VELOCITY 2.9244E 02FEET/SEC.
ITERATION NUMBER- 10

NO	CONCENTRATION	TEPH	DXA
1	6.6339E-09	3.4073E-04	2.2509E-03
2	0.0000E-01	0.0000E-01	9.7637E-05
3	0.0000E-01	0.0000E-01	1.2950E-05
4	4.7464E-10	2.4378E-05	6.9768E-03
5	2.4333E-03	1.2601E 02	2.2386E-06
6	7.5113E-05	3.8579E 00	1.9654E-10
7	7.3306E-05	3.7651E 00	0.0000E-01
8	3.6428E-06	1.8715E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.36432E-03	7.00743E 01	
12	9.22979E-11	0.0000E-01	
13	1.31016E-12	6.72923E-08	

SYSTEM 4 920 TO 1110 DEG K

REACTOR POSITION 1.76176E 02FEET

TEMPERTURE 1022.02DEGREE-K MOLAR FLOW RATE 2.05093E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 3.89%

PRESSURE IS 5.19547E 00 VELOCITY 3.0023E 02FEET/SEC.

ITERATION NUMBER- 11

NO	CONCENTRATION	T&PH	DXA
1	1.0861E-08	5.7239E-04	2.3724E-03
2	0.0000E-01	0.0000E-01	1.0143E-04
3	0.0000E-01	0.0000E-01	1.3570E-05
4	9.0445E-10	4.7666E-05	7.2127E-03
5	2.3660E-03	1.2480E 02	2.6838E-06
6	9.5789E-05	5.0483E 00	3.5991E-10
7	9.3564E-05	4.9310E 00	0.0000E-01
8	4.5007E-06	2.3720E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.32971E-03	7.0078E6 01	
12	1.56193E-10	0.0000E-01	
13	2.85330E-12	1.5037E-07	

REACTOR POSITION 1.92192E 02FEET

TEMPERTURE 1024.02DEGREE-K MOLAR FLOW RATE 2.06346E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 4.84%

PRESSURE IS 5.09696E 00 VELOCITY 3.0861E 02FEET/SEC.

ITERATION NUMBER- 12

NO	CONCENTRATION	T&PH	DXA
1	1.6171E-08	8.7549E-04	2.4990E-03
2	0.0000E-01	0.0000E-01	1.0531E-04
3	0.0000E-01	0.0000E-01	1.4212E-05
4	1.5077E-09	8.1627E-05	7.4527E-03
5	2.2818E-03	1.2354E 02	3.0370E-06
6	1.1618E-04	6.2901E 00	5.7667E-10
7	1.1356E-04	6.147RE 00	0.0000E-01
8	5.3332E-06	2.6873E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.29452E-03	7.0083E6 01	
12	2.4[illegible]294E-10	0.0000E-01	
13	5.31767E-12	2.8789ZE-07	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.0620E 02FEET

TEMPERTURE 1027.05DEGREE-K MOLAR FLOW RATE 2.07673E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 5.95%

PRESSURE IS 4.29509E 00 VELOCITY 3.1801E 02FEET/SEC.

ITERATION NUMBER= 13

NO	CONCENTRATION	TMPH	DXA
1	2.2656E-08	1.2629E-03	2.7344E-03
2	0.0000E-01	0.0000E-01	1.1275E-04
3	0.0000E-01	0.0000E-01	1.5415E-05
4	2.2946E-09	1.2791E-04	7.9217E-03
5	2.1923E-03	1.2223E 02	3.4112E-06
6	1.3640E-04	7.6036E 00	8.0317E-10
7	1.3338E-04	7.4349E 00	0.0000E-01
8	5.1406E-06	5.4230E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.25738E-03	7.00891E 01	
12	3.57845E-10	0.00000E-01	
13	8.96314E-12	4.99624E-07	

REACTOR POSITION 2.24224E 02FEET

TEMPERTURE 1031.06DEGREE-K MOLAR FLOW RATE 2.09153E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 6.98%

PRESSURE IS 4.89112E 00 VELOCITY 3.2860E 02FEET/SEC.

ITERATION NUMBER= 14

NO	CONCENTRATION	TMPH	DXA
1	3.3832E-08	1.7739E-03	3.0955E-03
2	0.0000E-01	0.0000E-01	1.2405E-04
3	0.0000E-01	0.0000E-01	1.7254E-05
4	3.3176E-09	1.9088E-04	8.6332E-03
5	2.0982E-03	1.2072E 02	3.8663E-06
6	1.5759E-04	9.0669E 00	1.3722E-09
7	1.5419E-04	8.8710E 00	0.0000E-01
8	6.9599E-06	4.0043E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.21834E-03	7.00958E 01	
12	5.30691E-10	0.00000E-01	
13	1.44086E-11	8.28984E-07	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 2.40240E 02FEET
TEMPERTURE 1035.060EGREE-K MOLAR FLOW RATE 2.10804E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 6.23%
PRESSURE IS 4.78421E 00 VELOCITY 3.4024E 02FEET/SEC.
ITERATION NUMBER- 15

NO	CONCENTRATION	TMPH	DXA
1	4.1021E-08	2.6401E-03	3.4934E-03
2	0.0000E-01	0.0000E-01	1.3609E-04
3	0.0000E-01	0.0000E-01	1.9252E-05
4	4.6180E-09	2.7470E-04	9.3818E-03
5	2.3016E-03	1.1906E 02	4.3252E-06
6	1.7985E-04	1.0698E 01	2.0756E-09
7	1.7606E-04	1.0473E 01	0.0000E-01
8	7.7912E-06	4.6344E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.1785E-03	7.0103E 01	
12	7.6726E-10	0.0000E-01	
13	2.2388E-11	1.3317E-06	

REACTOR POSITION 2.50256E 02FEET
TEMPERTURE 1039.060EGREE-K MOLAR FLOW RATE 2.12637E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 9.63%
PRESSURE IS 4.67483E 00 VELOCITY 3.5311E 02FEET/SEC.
ITERATION NUMBER- 16

NO	CONCENTRATION	TMPH	DXA
1	5.3503E-08	3.2965E-03	3.9289E-03
2	0.0000E-01	0.0000E-01	1.4881E-04
3	0.0000E-01	0.0000E-01	2.1410E-05
4	6.2275E-09	3.8370E-04	1.0163E-02
5	1.9026E-03	1.1723E 02	4.7718E-06
6	2.0300E-04	1.2508E 01	3.0643E-09
7	1.9882E-04	1.2250E 01	0.0000E-01
8	8.6251E-06	5.3143E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.1379E-03	7.0113E 01	
12	1.0840E-09	0.0000E-01	
13	3.3761E-11	2.0802E-06	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.72271E 02FEET

TEMPERTURE 1043.07DEGREE-K MOLAR FLOW RATE 2.14660E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 11.16%

PRESSURE IS 4.56083E 00 VELOCITY 3.6751E 02FEET/SEC.

ITERATION NUMBER- 17

NO	CONCENTRATION	TMPH	DXA
1	6.8528E-08	4.3832E-03	4.4019E-03
2	0.0000E-01	0.0000E-01	1.6214E-04
3	0.0000E-01	0.0000E-01	2.3722E-05
4	8.1653E-09	5.2228E-04	1.0971E-02
5	1.8012E-03	1.1521E 02	5.1860E-06
6	2.2675E-04	1.4503E 01	4.4222E-09
7	2.2220E-04	1.4212E 01	0.0000E-01
8	9.4492E-06	6.0440E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.09635E-03	7.01254E 01	
12	1.49885E-09	0.0000E-01	
13	4.95459E-11	3.16908E-06	

REACTOR POSITION 2.88287E 02FEET

TEMPERTURE 1050.18DEGREE-K MOLAR FLOW RATE 2.16989E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 12.93%

PRESSURE IS 4.44289E 00 VELOCITY 3.8524E 02FEET/SEC.

ITERATION NUMBER- 18

NO	CONCENTRATION	TMPH	DXA
1	8.7041E-08	5.8119E-03	5.5058E-03
2	0.0000E-01	0.0000E-01	1.9311E-04
3	0.0000E-01	0.0000E-01	2.9095E-05
4	1.0504E-08	7.0141E-04	1.2855E-02
5	1.6907E-03	1.1289E 02	6.0638E-06
6	2.5153E-04	1.6795E 01	6.7468E-09
7	2.4663E-04	1.6468E 01	0.0000E-01
8	1.0262E-05	6.8524E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.05045E-03	7.01409E 01	
12	2.23070E-09	0.0000E-01	
13	7.13155E-11	4.76189E-06	

SYSTEM 4 920 TO 1110 DEG K

REACTOR POSITION 3.04303E 02FEET

TEMPERTURE 1060.19DEGREE-K MOLAR FLOW RATE 2.20093E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 15.27%

PRESSURE IS 4.32591E 00 VELOCITY 4.0804E 02FEET/SEC.

ITERATION NUMBER- 19

NO	CONCENTRATION	TMPH	DXA
1	1.1405E-07	8.0015E-03	7.5463E-03
2	0.0000E-01	0.0000E-01	2.4737E-04
3	0.0000E-01	0.0000E-01	3.6821E-05
4	1.3771E-08	9.6614E-04	1.6099E-02
5	1.5654E-03	1.0982E 02	7.7433E-06
6	2.8281E-04	1.9841E 01	1.2037E-08
7	2.7752E-04	1.9470E 01	0.0000E-01
8	1.1203E-05	7.8592E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.0015E-03	7.0264E 01	
12	3.6603E-09	0.0000E-01	
13	1.0712DE-10	7.5150DE-06	

REACTOR POSITION 3.22219E 02FEET

TEMPERTURE 1070.83DEGREE-K MOLAR FLOW RATE 2.24668E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 18.72%

PRESSURE IS 4.19514E 00 VELOCITY 4.3538E 02FEET/SEC.

ITERATION NUMBER- 21

NO	CONCENTRATION	TMPH	DXA
1	1.5784E-07	1.1832E-02	5.0636E-03
2	0.0000E-01	0.0000E-01	1.5462E-04
3	0.0000E-01	0.0000E-01	2.5317E-05
4	1.8953E-08	1.4207E-03	9.6278E-03
5	1.4047E-03	1.0529E 02	4.7752E-06
6	3.2458E-04	2.4330E 01	5.9065E-09
7	3.1885E-04	2.3901E 01	0.0000E-01
8	1.2335E-05	9.2465E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	9.3656DE-04	7.0204E 01	
12	3.0968BE-09	0.0000E-01	
13	1.6662GE-10	1.2490BE-05	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.39933E 02FEET
TEMPERTURE 1077.47DEGREE-K MOLAR FLOW RATE 2.29837E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 22.65%
PRESSURE IS 4.03925E 00 VELOCITY 4.8009E 02FEET/SEC.
ITERATION NUMBER= 21

NO	CONCENTRATION	TMPH	DXA
1	2.1320E-07	1.7070E-02	5.8360E-03
2	0.0000E-01	0.0000E-01	1.7063E-04
3	0.0000E-01	0.0000E-01	2.6677E-05
4	2.5355E-09	2.0300E-03	1.0690E-02
5	1.2508E-03	1.0014E 02	5.1184E-06
6	3.6758E-04	2.9430E 01	8.9776E-09
7	3.6147E-04	2.8941E 01	0.0000E-01
8	1.3422E-05	1.0746E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	8.7722BE-04	7.0233bE 01	
12	4.5502BE-09	0.0000E-01	
13	2.1537AE-10	1.7243bE-05	

REACTOR POSITION 3.57648E 02FEET
TEMPERTURE 1084.12DEGREE-K MOLAR FLOW RATE 2.35529E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 16.96%
PRESSURE IS 3.8556/E 00 VELOCITY 5.2948E 02FEET/SEC.
ITERATION NUMBER= 22

NO	CONCENTRATION	TMPH	DXA
1	2.7768E-07	2.3973E-02	6.7141E-03
2	0.0000E-01	0.0000E-01	1.8806E-04
3	0.0000E-01	0.0000E-01	3.2432E-05
4	3.2274E-08	2.7863E-03	1.1615E-02
5	1.0943E-03	9.4479E 01	5.1270E-06
6	4.0579E-04	3.5033E 01	1.3370E-08
7	3.9946E-04	3.4487E 01	0.0000E-01
8	1.4279E-05	1.2327E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	8.1393/E-04	7.0270E 01	
12	6.4394bE-09	0.0000E-01	
13	2.8351IE-10	2.4476bE-05	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.75362E 02FEET
TEMPERTURE 1094.600EGREE-K MOLAR FLOW RATE 2.41969E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 31.82%
PRESSURE IS 3.59973E 00 VELOCITY 6.3819E 02FEET/SEC.
ITERATION NUMBER- 23

NO	CONCENTRATION	THPH	DXA
1	3.4799E-07	3.3243E-02	8.1449E-03
2	0.0000E-01	0.0000E-01	2.1344E-04
3	0.0000E-01	0.0000E-01	3.8311E-05
4	3.8521E-08	3.6799E-03	1.2892E-02
5	9.2233E-04	8.8111E 01	5.0942E-06
6	4.3285E-04	4.1350E 01	1.6845E-08
7	4.2656E-04	4.0749E 01	0.0000E-01
8	1.4672E-05	1.4017E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	7.3610?E-04	7.0320?E 01	
12	8.95876E-09	0.0000E-01	
13	3.69494E-10	3.52980E-05	

REACTOR POSITION 3.93076E 02FEET
TEMPERTURE 1105.670EGREE-K MOLAR FLOW RATE 2.49184E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 37.24%
PRESSURE IS 3.21056E 00 VELOCITY 7.8242E 02FEET/SEC.
ITERATION NUMBER- 24

NO	CONCENTRATION	THPH	DXA
1	4.1291E-07	4.5540E-02	9.7528E-03
2	0.0000E-01	0.0000E-01	2.3853E-04
3	0.0000E-01	0.0000E-01	4.4626E-05
4	4.1453E-08	4.5720E-03	1.4080E-02
5	7.3472E-04	8.1034E 01	3.7958E-06
6	4.3873E-04	4.8388E 01	2.6662E-08
7	4.3286E-04	4.7741E 01	0.0000E-01
8	1.4304E-05	1.5777E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	6.38240E-04	7.03931E 01	
12	1.16103E-08	0.0000E-01	
13	4.5507?E-10	5.0190?E-05	

SYSTEM 4 820 TO 1110 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.15225E 01(1105.67, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.45916E-01(1105.67, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.34193E 02(1105.67, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12596E-08(1105.67, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42331E 01(1105.67, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13516E 01(1105.67, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24612E 00(1105.67, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.22180E-02(1105.67, 8)

FUNCTION PRR(IS)
PR= 6.24929E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.49806E 05 VIS= 2.66566E-05 DEN= 1.08389E-01
FRICTION FACTOR= 1.28795E-02 V1,V2,VA= 7.82417E 02 4.36677E 02 6.09553E 02
TEMPERTURE= 1105.67PRESSURE D= 3.11505E-01

1-A	ACETYLENE	4.12906E-07	4.55404E-02
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	4.14533E-08	4.57199E-03
5-E	ETHANE	7.34717E-04	8.10336E 01
6-F	ETHYLENE	4.38728E-04	4.83884E 01
7-G	HYDROGEN	4.32860E-04	4.77413E 01
8-H	METHANE	1.43044E-05	1.57767E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	6.36240E-04	7.03931E 01
12-L	CARBON	1.16103E-08	0.00000E-01
13-M	CARBON MONOXIDE	4.55070E-10	5.01905E-05

CONVERSION OF ETHANE TO ETHYLENE IS 37.24%

REACTOR RADIUS PROFILE AFTER 300.00 HOURS

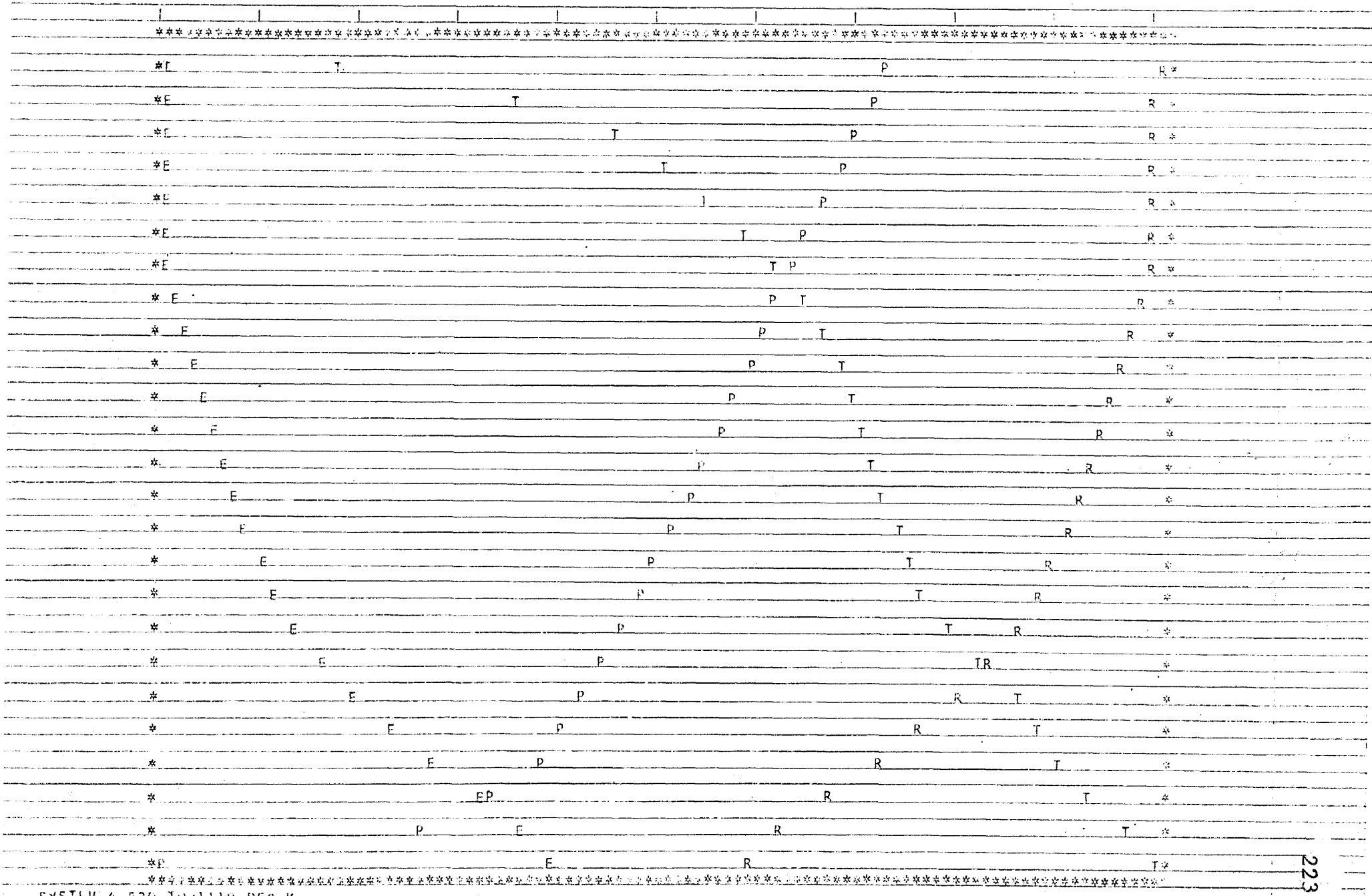
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.124999	0.124999	0.124999	0.124999	0.124998	0.124998	0.124997	0.124996
0.124995	0.124993	0.124991	0.124989	0.124987	0.124984	0.124980	0.124976	0.124970	0.124964
0.124959	0.124953	0.124946	0.124939	0.124931	0.124922	0.124913	0.124903	0.124893	0.124882
0.124868	0.124853	0.124836	0.124817	0.124797	0.124776	0.124752	0.124725	0.124697	0.124666
0.124633	0.124597	0.124557	0.124515	0.124469	0.124419	0.124365	0.124307	0.124245	0.124176
0.124062	0.123930	0.123779	0.123608	0.123420	0.123164	0.122890	0.122573	0.121609	0.121784
0.120807	0.121009	0.120547	0.119450	0.119582	0.119022	0.118422	0.117778	0.117091	0.114303
0.114996	0.113667	0.110208	0.109350	0.109199	0.107485	0.105734	0.104208	0.100441	0.100441

```
 REACTOR IS    400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES AT PRESSURE   6.249A VELOCITY OF  1.95179E 02 AT TEMPERATURE   820.0DEG K
 INITIAL REACTOR INCREMENT(DL 9.77499E-01FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.6o841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=  6.24929E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=  6.24929E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 REYN=  3.35919E 05     VIS=   2.16064E-05     DEN=   1.47348E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   1.95179E 02        1.98831E 02        1.97030E 02
 TEMPERTURE=  832.71PRESSURE D=   2.12174E-02
  FUNCTION PRR(IS)
 PR=  6.22807E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS  6.22807E 00    VELOCITY   1.9888E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.7152E-07
  2    0.0000E-01    0.0000E-01    6.5157E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.7098E-03    1.2994E 02    0.0000E-01
  6    1.5362E-09    5.3808E-05    0.0000E-01
  7    1.3783E-09    4.8276E-05    0.0000E-01
  8    3.1592E-10    1.1065E-05    0.0000E-01
  9  0.0000E-01    0.0000E-01
 10  0.0000E-01    0.0000E-01
 11  2.0023E-03    7.0097E 01
 12  0.0000E-01    0.0000E-01
 13  0.0000E-01    0.0000E-01

  DL CHANGED TO    1.98369E 00     ZIC=   3.20318E 02
 I= 1  RA=   1.6195DE-03  DXA(I)=   1.00923E-02  CF,CR=   1.42274E-03   9.93093E-08  REQC=   1.86110E 00

 RATE=   1.13845E 00

 VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 820 TO 1110 DEG K.
REACTOR POSITION 3.97660E 02FEET
TEMPERTURE 1108.55DEGREE-K MOLAR FLOW RATE 2.48173E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.4997E 03FEET/SEC.

```
 REACTOR IS      400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES  AT PRESSURE   6.449A  VELOCITY OF  1.89127E 02 AT TEMPERATURE    820.0DEG K
  INITIAL REACTOR INCREMENT(DL 1.98362E 00FEET
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.60841E-02( 832.71, 2)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.52469E 01( 832.71, 5)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   6.44929E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=   6.44929E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
  FUNCTION PRESD(T)
 RENO=   3.35919E 05     VIS=   2.16064E-05     DEN=   1.52080E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   1.89127E 02        1.92672E 02        1.90899E 02
 TEMPERTURE=  832.71PRESSURE D=   2.05395E-02
  FUNCTION PRR(IS)
 PR=   6.42874E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   6.42874E 00     VELOCITY    1.9267E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    2.8361E-07
  2    0.0000E-01    0.0000E-01    6.5007E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.8286E-03    1.2924E 02    0.0000E-01
  6    1.2103E-09    4.1076E-05    0.0000E-01
  7    1.3859E-09    3.6853E-05    0.0000E-01
  8    2.4838E-10    3.4470E-06    0.0000E-01
  9    0.00000E-01   0.00000E-01
 10    0.00000E-01   0.00000E-01
 11    2.06424E-03   7.00527E 01
 12    0.00000E-01   0.00000E-01
 13    0.00000E-01   0.00000E-01

  DL CHANGED  TO    1.85786E 00     ZIC=   3.16314E 02
 I= 1  RA=   1.68209E-03  DXA(I)=   1.07758E-02  CF,CR=   1.56629E-03   1.22712E-07  REQC=   1.87819E 00

 RATE=   1.07857E 00
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.01767E 02FEET
TEMPERTURE 1109.94DEGREE-K MOLAR FLOW RATE 2.52759E 02POUND MOLES PER HOUR
PRESSURE IS 2.000000E 00 VELOCITY 1.0854E 03FEET/SEC.


SYSTEM 4 820 TO 1110 DEG K
REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 300. HOURS OF RUN

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 1.60160E 01FEET
TEMPERTURE 870.65DEGREE-K MOLAR FLOW RATE 2.00001E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.00%
PRESSURE IS 6.36487E 00 VELOCITY 2.0352E 02FEET/SEC.
ITERATION NUMBER- 1

NO	CONCENTRATION	TMPH	DXA
1	9.1332E-16	3.2736E-11	3.1894E-06
2	0.0000E-01	0.0000E-01	4.9149E-07
3	0.0000E-01	0.0000E-01	3.0467E-08
4	6.4327E-20	2.3057E-15	5.3590E-05
5	3.6252E-03	1.2994E 02	4.9533E-12
6	2.3118E-08	8.2861E-04	5.7584E-21
7	2.1309E-08	7.6379E-04	0.0000E-01
8	3.6167E-09	1.2963E-04	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.9546BE-03	7.0059TE 01	
12	9.787o3E-20	0.0000E-01	
13	1.12555E-23	4.0343BE-19	

REACTOR POSITION 3.20320E 01FEET
TEMPERTURE 921.70DEGREE-K MOLAR FLOW RATE 2.00012E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.01%
PRESSURE IS 6.27463E 00 VELOCITY 2.1851E 02FEET/SEC.
ITERATION NUMBER- 2

NO	CONCENTRATION	TMPH	DXA
1	1.4073E-13	5.4143E-09	4.0567E-05
2	0.0000E-01	0.0000E-01	3.6751E-06
3	0.0000E-01	0.0000E-01	3.2005E-07
4	9.0431E-17	3.4810E-12	3.6026E-04
5	3.3772E-03	1.2993E 02	4.8093E-10
6	3.0823E-07	1.1858E-02	1.6275E-17
7	2.9213E-07	1.1241E-02	0.0000E-01
8	3.2C91E-08	1.2346E-03	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.82105E-03	7.0059BE 01	
12	1.01370E-16	0.0000E-01	
13	3.50217E-20	1.34736E-15	

SYSTEM 4 820 TO 1110 DEG.K
REACTOR POSITION 4.80480E 01FEET
TEMPERTURE 953.04DEGREE-K MOLAR FLOW RATE 2.00082E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.06%
PRESSURE IS 6.16057E 00 VELOCITY 2.2946E 02FEET/SEC.
ITERATION NUMBER- 3

NO	CONCENTRATION	TMPH	DXA
1	5.2447E-12	2.1185E-07	1.6664E-04
2	0.0000E-01	3.0000E-01	1.2160E-05
3	0.0000E-01	3.0000E-01	1.1804E-06
4	1.9034E-14	7.6883E-10	1.0334E-03
5	3.2148E-03	1.2986E 02	1.1525E-08
6	2.0161E-06	8.1436E-02	6.6033E-15
7	1.9376E-06	7.8267E-02	0.0000E-01
8	1.5703E-07	6.3431E-03	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.73447E-03	7.00601E 01	
12	1.08286E-14	0.0000E-01	
13	1.74198E-17	7.03633E-13	

REACTOR POSITION 6.40640E 01FEET
TEMPERTURE 965.05DEGREE-K MOLAR FLOW RATE 2.00208E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.16%
PRESSURE IS 6.08676E 00 VELOCITY 2.3608E 02FEET/SEC.
ITERATION NUMBER- 4

NO	CONCENTRATION	TMPH	DXA
1	2.9523E-11	1.2267E-06	2.7773E-04
2	0.0000E-01	0.0000E-01	1.8364E-05
3	0.0000E-01	0.0000E-01	1.8914E-06
4	2.6033E-13	1.0817E-08	1.5102E-03
5	3.1221E-03	1.2973E 02	4.4994E-08
6	4.9561E-06	2.0593E-01	7.8270E-14
7	4.7808E-06	1.9865E-01	0.0000E-01
8	3.5070E-07	1.4572E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.68613E-03	7.00605E 01	
12	8.99423E-14	0.0000E-01	
13	2.92933E-16	1.21717E-11	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 8.00800E 01FEET
TEMPERTURE 977.06DEGREE-K MOLAR FLOW RATE 2.00414E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.32%
PRESSURE IS 5.99186E 00 VELOCITY 2.4306E 02FEET/SEC.
ITERATION NUMBER= 5

NO	CONCENTRATION	THPH	OXA
1	1.0747E-10	4.5962E-06	4.5645E-04
2	0.0000E-01	0.0000E-01	2.7415E-05
3	0.0000E-01	0.0000E-01	2.9911E-06
4	1.6914E-12	7.2341E-08	2.1834E-03
5	3.0283E-03	1.2952E 02	1.2484E-07
6	9.6003E-06	4.1060E-01	5.0866E-13
7	9.2862E-06	3.9717E-01	0.0000E-01
8	6.2869E-07	2.6889E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.63812E-03	7.00612E 01	
12	4.68457E-13	0.0000E-01	
13	2.2070OE-15	9.43916E-11	

REACTOR POSITION 9.60959E 01FEET
TEMPERTURE 984.27DEGREE-K MOLAR FLOW RATE 2.00741E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.57%
PRESSURE IS 5.99744E 00 VELOCITY 2.5019E 02FEET/SEC.
ITERATION NUMBER= 6

NO	CONCENTRATION	THPH	OXA
1	3.1966E-10	1.4070E-05	7.1614E-04
2	0.0000E-01	0.0000E-01	3.9402E-05
3	0.0000E-01	0.0000E-01	4.5311E-06
4	7.9895E-12	3.4726E-07	3.0478E-03
5	2.9350E-03	1.2919E 02	2.9218E-07
6	1.6702E-05	7.3513E-01	2.5143E-12
7	1.6194E-05	7.1277E-01	0.0000E-01
8	1.0174E-06	4.4781E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.59175E-03	7.00622E 01	
12	1.94454E-12	0.0000E-01	
13	1.19656E-14	5.26696E-10	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 1.12112E 02FEET

TEMPERTURE 999.480EGREE-K MOLAR FLOW RATE 2.01248E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.95%

PRESSURE IS 5.80447E 00 VELOCITY 2.5774E 02FEET/SEC.

ITERATION NUMBER- 7

NO	CONCENTRATION	THPH	DXA
1	8.4507E-10	3.6309E-05	1.1110E-03
2	0.0000E-01	0.0000E-01	5.6106E-05
3	0.0000E-01	0.0000E-01	6.7924E-06
4	3.0256E-11	1.3716E-06	4.2177E-03
5	2.8385E-03	1.2867E 02	6.2232E-07
6	2.7303E-05	1.2377E 00	1.0691E-11
7	2.6529E-05	1.2026E 00	0.0000E-01
8	1.5498E-06	7.0255E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.54557E-03	7.00639E 01	
12	7.11201E-12	0.0000E-01	
13	5.34497E-14	2.42298E-09	

REACTOR POSITION 1.28128E 02FEET

TEMPERTURE 1008.05DEGREE-K MOLAR FLOW RATE 2.01989E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 1.52%

PRESSURE IS 5.71484E 00 VELOCITY 2.6501E 02FEET/SEC.

ITERATION NUMBER- 8

NO	CONCENTRATION	THPH	DXA
1	2.0150E-09	9.3899E-05	1.5334E-03
2	0.0000E-01	0.0000E-01	7.2623E-05
3	0.0000E-01	0.0000E-01	9.1373E-06
4	9.8853E-11	4.6070E-06	5.3437E-03
5	2.7452E-03	1.2792E 02	1.1400E-06
6	4.2334E-05	1.9728E 00	3.8020E-11
7	4.1213E-05	1.9205E 00	0.0000E-01
8	2.2505E-06	1.0487E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.50357E-03	7.00664E 01	
12	2.14778E-11	0.0000E-01	
13	2.07370E-13	9.6634[illegible]E-09	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 1.44144E 02FEET

TEMPERTURE 1014.05DEGREE-K MOLAR FLOW RATE 2.02913E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 2.224

PRESSURE IS 5.62676E 00 VELOCITY 2.7204E 02FEET/SEC.

ITERATION NUMBER- 9

NO	CONCENTRATION	THPH	OXA
1	4.0944E-09	1.9579E-04	1.9045E-03
2	0.0000E-01	0.0000E-01	8.6287E-05
3	0.0000E-01	0.0000E-01	1.1149E-05
4	2.5851E-10	1.2362E-05	6.2559E-03
5	2.6557E-03	1.2699E 02	1.7544E-06
6	6.0430E-05	2.8897E 00	9.9737E-11
7	5.8912E-05	2.8171E 00	0.0000E-01
8	3.0561E-06	1.4614E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.46533E-03	7.0069E 01	
12	5.10818E-11	0.0000E-01	
13	6.28531E-13	3.0054E-08	

REACTOR POSITION 1.60160E 02FEET

TEMPERTURE 1020.02DEGREE-K MOLAR FLOW RATE 2.04049E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 3.09%

PRESSURE IS 5.54062E 00 VELOCITY 2.7953E 02FEET/SEC.

ITERATION NUMBER- 10

NO	CONCENTRATION	THPH	OXA
1	7.5090E-09	3.6876E-04	2.3525E-03
2	0.0000E-01	0.0000E-01	1.0204E-04
3	0.0000E-01	0.0000E-01	1.3534E-05
4	5.7689E-10	2.8331E-05	7.2916E-03
5	2.5626E-03	1.2585E 02	2.5059E-06
6	8.1743E-05	4.0146E 00	2.3211E-10
7	7.9784E-05	3.9182E 00	0.0000E-01
8	3.9633E-06	1.9466E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.42689E-03	7.0074E 01	
12	1.09174E-10	0.0000E-01	
13	1.61088E-12	7.9109E-08	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.7e176E 02FEET
TEMPERTURE 1022.02DEGREE-K MOLAR FLOW RATE 2.05303E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 4.05%
PRESSURE IS 5.45327E 00 VELOCITY 2.8639E 02FEET/SEC.
ITERATION NUMBER- 11

NO	CONCENTRATION	TMPH	DXA
1	1.2341E-08	6.2057E-04	2.4843E-03
2	0.0000E-01	0.0000E-01	1.0621E-04
3	0.0000E-01	0.0000E-01	1.4210E-05
4	1.1038E-09	5.5505E-05	7.5528E-03
5	2.4776E-03	1.2458E 02	3.0093E-06
6	1.2457E-04	6.2583E 00	4.2741E-10
7	1.2214E-04	6.1362E 00	0.0000E-01
8	4.9116E-06	2.4698E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.39366E-03	7.00786E 01	
12	1.85826E-10	0.00000E-01	
13	3.53178E-12	1.77592E-07	

REACTOR POSITION 1.92192E 02FEET
TEMPERTURE 1024.02DEGREE-K MOLAR FLOW RATE 2.06614E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 5.05%
PRESSURE IS 5.36481E 00 VELOCITY 2.9374E 02FEET/SEC.
ITERATION NUMBER- 12

NO	CONCENTRATION	TMPH	DXA
1	1.3442E-08	9.5077E-04	2.6223E-03
2	0.0000E-01	0.0000E-01	1.1050E-04
3	0.0000E-01	0.0000E-01	1.4913E-05
4	1.8482E-09	9.5246E-05	7.8203E-03
5	2.3918E-03	1.2326E 02	3.4127E-06
6	1.2725E-04	6.5577E 00	6.8879E-10
7	1.2437E-04	6.4095E 00	0.0000E-01
8	5.8388E-06	3.0090E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.35995E-03	7.00837E 01	
12	2.87622E-10	0.00000E-01	
13	6.62715E-12	3.41525E-07	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 2.08208E 02FEET
TEMPERTURE 1027.35DEGREE-K MOLAR FLOW RATE 2.08003E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 6.11%
PRESSURE IS 5.27278E 00 VELOCITY 3.0199E 02FEET/SEC.
ITERATION NUMBER- 13

NO	CONCENTRATION	TMPH	OXA
1	2.5959E-08	1.3739E-03	2.8756E-03
2	0.0000E-01	0.0000E-01	1.1857E-04
3	0.0000E-01	0.0000E-01	1.6212E-05
4	2.8267E-09	1.4960E-04	8.3308E-03
5	2.3026E-03	1.2186E 02	3.8448E-06
6	1.4991E-04	7.9337E 00	1.0613E-09
7	1.4660E-04	7.7586E 00	0.0000E-01
8	6.7464E-06	3.5705E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.32433E-03	7.00895E 01	
12	4.31107E-10	0.00000E-01	
13	1.12506E-11	5.95437E-07	

REACTOR POSITION 2.24224E 02FEET
TEMPERTURE 1031.06DEGREE-K MOLAR FLOW RATE 2.09557E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 7.29%
PRESSURE IS 5.18002E 00 VELOCITY 3.1125E 02FEET/SEC.
ITERATION NUMBER- 14

NO	CONCENTRATION	TMPH	OXA
1	3.5491E-08	1.9332E-03	3.2629E-03
2	0.0000E-01	0.0000E-01	1.3076E-04
3	0.0000E-01	0.0000E-01	1.6187E-05
4	4.1102E-09	2.2389E-04	9.0999E-03
5	2.2086E-03	1.2030E 02	4.3747E-06
6	1.7366E-04	9.4705E 00	1.6595E-09
7	1.7011E-04	9.2662E 00	0.0000E-01
8	7.6752E-06	4.1807E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.28666E-03	7.00965E 01	
12	6.43799E-10	0.00000E-01	
13	1.92278E-11	9.92838E-07	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 2.40240E 02FEET
TEMPERTURE 1035.06DEGREE-K MOLAR FLOW RATE 2.11292E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 9.61%
PRESSURE IS 5.08547E 00 VELOCITY 3.2148E 02FEET/SEC.
ITERATION NUMBER- 15

NO	CONCENTRATION	TMPH	DXA
1	4.7460E-08	2.6644E-03	3.6911E-03
2	0.0000E-01	0.0000E-01	1.4379E-04
3	0.0000E-01	0.0000E-01	2.0342E-05
4	5.7592E-09	3.2332E-04	9.9128E-03
5	2.1119E-03	1.1856E 02	4.9172E-06
6	1.9925E-04	1.1186E 01	2.5269E-09
7	1.9506E-04	1.0951E 01	0.0000E-01
8	8.6273E-06	4.8433E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.24876E-03	7.01048E 01	
12	9.37767E-10	0.00000E-01	
13	2.85639E-11	1.60356E-06	

REACTOR POSITION 2.56256E 02FEET
TEMPERTURE 1039.06DEGREE-K MOLAR FLOW RATE 2.13221E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 10.07%
PRESSURE IS 4.98891E 00 VELOCITY 3.3276E 02FEET/SEC.
ITERATION NUMBER- 15

NO	CONCENTRATION	TMPH	DXA
1	6.2241E-08	3.6067E-03	4.1615E-03
2	0.0000E-01	0.0000E-01	1.5762E-04
3	0.0000E-01	0.0000E-01	2.2678E-05
4	7.8247E-09	4.5343E-04	1.0765E-02
5	2.0127E-03	1.1663E 02	5.4543E-06
6	2.2592E-04	1.3091E 01	3.7564E-09
7	2.2128E-04	1.2823E 01	0.0000E-01
8	9.5937E-06	5.5593E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.20996E-03	7.01148E 01	
12	1.33552E-09	0.00000E-01	
13	4.34688E-11	2.51893E-06	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.72271E 02FEET

TEMPERTURE 1043.07DEGREE-K MOLAR FLOW RATE 2.15354E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 11.69%

PRESSURE IS 4.88917E 00 VELOCITY 3.4539E 02FEET/SEC.

ITERATION NUMBER- 17

NO	CONCENTRATION	TMPH	DXA
1	8.0193E-08	4.8054E-03	4.6740E-03
2	0.0000E-01	0.0000E-01	1.7217E-04
3	0.0000E-01	0.0000E-01	2.5189E-05
4	1.0346E-08	6.1996E-04	1.1650E-02
5	1.9108E-03	1.1450E 02	5.9662E-06
6	2.5360E-04	1.5196E 01	5.4569E-09
7	2.4853E-04	1.4892E 01	0.0000E-01
8	1.0562E-05	6.3290E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.1703OE-03	7.0126BE 01	
12	1.86210E-09	0.0000E-01	
13	6.44141E-11	3.85984E-06	

REACTOR POSITION 2.88267E 02FEET

TEMPERTURE 1050.18DEGREE-K MOLAR FLOW RATE 2.17811E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 13.56%

PRESSURE IS 4.78681E 00 VELOCITY 3.6125E 02FEET/SEC.

ITERATION NUMBER- 18

NO	CONCENTRATION	TMPH	DXA
1	1.0251E-07	6.3848E-03	5.8578E-03
2	0.0000E-01	0.0000E-01	2.0545E-04
3	0.0000E-01	0.0000E-01	3.6956E-05
4	1.3437E-08	8.3689E-04	1.3677E-02
5	1.7991E-03	1.1205E 02	7.0210E-06
6	2.8285E-04	1.7617E 01	8.3814E-09
7	2.7736E-04	1.7275E 01	0.0000E-01
8	1.1532E-05	7.1827E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.12621E-03	7.01427E 01	
12	2.79472E-09	0.0000E-01	
13	9.36839E-11	5.83484E-06	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.04303E 02FEET
TEMPERTURE 1060.19DEGREE-K MOLAR FLOW RATE 2.21083E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 16.03%
PRESSURE IS 4.60664E 00 VELOCITY 3.8260E 02FEET/SEC.
ITERATION NUMBER- 19

NO	CONCENTRATION	TAPH	DXA
1	1.3523E-07	3.2065E-03	8.0298E-03
2	0.0000E-01	0.0000E-01	2.6316E-04
3	0.0000E-01	0.0000E-01	4.1298E-05
4	1.7805E-08	1.1595E-03	1.7127E-02
5	1.6708E-03	1.0881E 02	9.0023E-06
6	3.1965E-04	2.0830E 01	1.4987E-08
7	3.1389E-04	2.0442E 01	0.0000E-01
8	1.2660E-05	8.2449E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.07748E-03	7.01691E 01	
12	4.61584E-09	0.0000E-01	
13	1.42218E-10	9.26175E-06	

REACTOR POSITION 3.21857E 02FEET
TEMPERTURE 1070.71DEGREE-K MOLAR FLOW RATE 2.25766E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 19.57%
PRESSURE IS 4.57552E 00 VELOCITY 4.0956E 02FEET/SEC.
ITERATION NUMBER- 20

NO	CONCENTRATION	TAPH	DXA
1	1.8683E-07	1.2914E-02	5.0456E-03
2	0.0000E-01	0.0000E-01	1.5420E-04
3	0.0000E-01	0.0000E-01	2.5236E-05
4	2.4579E-08	1.6990E-03	9.6039E-03
5	1.5070E-03	1.0417E 02	5.1976E-06
6	3.5787E-04	2.5428E 01	6.4445E-09
7	3.6141E-04	2.4981E 01	0.0000E-01
8	1.3986E-05	9.6672E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.01570E-03	7.02074E 01	
12	3.65684E-09	0.0000E-01	
13	2.2[illegible]328E-10	1.52296E-05	

SYSTEM 4.820 TO 1110 DEG K
REACTOR POSITION 3.38606E 02FEET
TEMPERTURE 1076.98DEGREE-K MOLAR FLOW RATE 2.30835E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 23.42%
PRESSURE IS 4.44401E 00 VELOCITY 4.5644E 02FEET/SEC.
ITERATION NUMBER= 21

NO	CONCENTRATION	TMPH	DXA
1	2.4984E-07	1.8258E-02	5.6910E-03
2	0.0000E-01	0.0000E-01	1.6694E-04
3	0.0000E-01	0.0000E-01	2.8002E-05
4	3.2721E-08	2.3913E-03	1.0470E-02
5	1.3561E-03	9.9104E 01	5.5810E-06
6	4.1643E-04	3.0433E 01	9.4038E-09
7	4.0953E-04	2.9929E 01	0.0000E-01
8	1.5247E-05	1.1143E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	9.6103AE-04	7.0234E 01	
12	5.2223GE-09	0.0000E-01	
13	2.7856OE-10	2.0357TE-05	

REACTOR POSITION 3.55325E 02FEET
TEMPERTURE 1083.25DEGREE-K MOLAR FLOW RATE 2.36328E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 27.59%
PRESSURE IS 4.23682E 00 VELOCITY 4.9482E 02FEET/SEC.
ITERATION NUMBER= 22

NO	CONCENTRATION	TMPH	DXA
1	3.2220E-07	2.5122E-02	6.5513E-03
2	0.0000E-01	0.0000E-01	1.8454E-04
3	0.0000E-01	0.0000E-01	3.1718E-05
4	4.1508E-08	3.2363E-03	1.1418E-02
5	1.2609E-03	9.3632E 01	5.5842E-06
6	4.5975E-04	3.5846E 01	1.3770E-08
7	4.5253E-04	3.5257E 01	0.0000E-01
8	1.6259E-05	1.2677E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	9.0122GE-04	7.0266BE 01	
12	7.3457GE-09	0.0000E-01	
13	3.5686GE-10	2.7824GE-05	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.72044E 02FEET
TEMPERTURE 1092.53DEGREE-K MOLAR FLOW RATE 2.42223E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 32.04%
PRESSURE IS 4.01745E 00 VELOCITY 6.2947E 02FEET/SEC.
ITERATION NUMBER- 23

NO	CONCENTRATION	THPH	DXA
1	3.9744E-07	3.3754E-02	7.2130E-03
2	0.0000E-01	0.0000E-01	1.9152E-04
3	0.0000E-01	0.0000E-01	3.4107E-05
4	4.9127E-08	4.1724E-03	1.1618E-02
5	1.0336E-03	8.7784E 01	4.8762E-06
6	4.9027E-04	4.1639E 01	1.8002E-08
7	4.6310E-04	4.1030E 01	0.0000E-01
8	1.6771E-05	1.4243E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	8.2783AE-04	7.0308E 01	
12	9.2207E-09	0.0000E-01	
13	4.4757E-10	3.8012AE-05	

REACTOR POSITION 3.88763E 02FEET
TEMPERTURE 1102.98DEGREE-K MOLAR FLOW RATE 2.48571E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 36.81%
PRESSURE IS 3.57742E 00 VELOCITY 7.9163E 02FEET/SEC.
ITERATION NUMBER- 24

NO	CONCENTRATION	THPH	DXA
1	4.5376E-07	4.4539E-02	8.3198E-03
2	0.0000E-01	0.0000E-01	2.0692E-04
3	0.0000E-01	0.0000E-01	3.8326E-05
4	5.1302E-08	5.0355E-03	1.2282E-02
5	8.3038E-04	8.1554E 01	3.4764E-06
6	4.8734E-04	4.7834E 01	2.1455E-08
7	4.8071E-04	4.7184E 01	0.0000E-01
8	1.6114E-05	1.5816E 00	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	7.1691AE-04	7.0367E 01	
12	1.1130BE-08	0.0000E-01	
13	5.1453AE-10	5.0508ZE-05	

SYSTEM 4 820 TO 1110 DEG K

```
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.15462E 01(1102.98, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   2.45258E-01(1102.98, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.36384E 02(1102.98, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.12614E-08(1102.98, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.42414E 01(1102.98, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.12937E 01(1102.98, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.24960E 00(1102.98, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.22003E-02(1102.98, 8)

  FUNCTION PRR(IS)
 PR=   6.44929E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENO=   5.53597E 05     VIS=   2.66074E-05     DEN=   1.13022E-01
 FRICTION FACTOR=   1.28635E-02     V1,V2,VA=   7.91628E 02     5.15670E 02     6.53648E 02
 TEMPERATURE= 1102.9 PRESSURE D=   2.21701E-01
  1-A  ACETYLENE              4.53763E-07     4.45387E-02
  2-B  ISO-BUTANE             0.00000E-01     0.00000E-01
  3-C  N-BUTANE               0.00000E-01     0.00000E-01
  4-D  ISO-BUTENE             5.13023E-08     5.03553E-03
  5-E  ETHANE                 8.30876E-04     8.15538E 01
  6-F  ETHYLENE               4.87339E-04     4.78343E 01
  7-G  HYDROGEN               4.80709E-04     4.71835E 01
  8-H  METHANE                1.61135E-05     1.58161E 00
  9-I  PROPANE                0.00000E-01     0.00000E-01
 10-J  PROPENE                0.00000E-01     0.00000E-01
 11-K  WATER                  7.16910E-04     7.03677E 01
 12-L  CARBON                 1.11303E-08     0.00000E-01
 13-M  CARBON MONOXIDE        5.14560E-10     5.05082E-05

 CONVERSION OF ETHANE          TO  ETHYLENE          IS 36.81%
```

REACTOR RADIUS PROFILE AFTER 400.00 HOURS

0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.124999	0.124999	0.124999	0.124998	0.124998	0.124997	0.124996	0.124994
0.124992	0.124990	0.124988	0.124985	0.124981	0.124977	0.124971	0.124965	0.124958	0.124949
0.124941	0.124932	0.124922	0.124912	0.124901	0.124888	0.124875	0.124861	0.124846	0.124830
0.124810	0.124788	0.124764	0.124737	0.124708	0.124676	0.124641	0.124603	0.124562	0.124517
0.124468	0.124415	0.124357	0.124294	0.124227	0.124153	0.124075	0.123989	0.123898	0.123795
0.123626	0.123433	0.123209	0.122948	0.122647	0.122297	0.121891	0.121417	0.119637	0.120350
0.119238	0.118697	0.118428	0.117224	0.117109	0.116308	0.115454	0.112760	0.113297	0.110358
0.110509	0.108040	0.104896	0.100356	0.102426	0.100159	0.097921	0.095781	0.087396	0.087396

```
 REACTOR IS     400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES AT PRESSURE   6.449A  VELOCITY OF  1.89127E 02 AT TEMPERATURE    820.0DEG R
 INITIAL REACTOR INCREMENT(DL 1.857b6E 00FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.68841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14937E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   6.44929E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=   6.44928E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENO=   3.35919E 05      VIS=   2.16064E-05      DEN=   1.52080E-01
 FRICTION FACTOR=   1.41227E-02      V1,V2,VA=   1.89127E 02          1.92672E 02          1.90899E 02
 TEMPERTURE=  832.71PRESSURE D=   2.05395E-02
  FUNCTION PRR(IS)
 PR=   6.42874E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   6.42874E 00    VELOCITY    1.9267E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.8341E-07
  2    0.0000E-01    0.0000E-01    8.7882E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.8286E-03    1.2994E 02    0.0000E-01
  6    1.6361E-09    5.5530E-05    0.0000E-01
  7    1.4679E-09    4.9821E-05    0.0000E-01
  8    3.3646E-10    1.1419E-05    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    2.0642AE-03   7.0659AE 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

 DL CHANGED TO    1.9088OE 00      ZIC=   3.16314E 02
I= 1  KA=   1.68480E-03  DXA(I)=   1.04803E-02  CF,CR=   1.56230E-03   1.20146E-07  REQC=   1.87819E 00

RATE=   1.07857E 00

VELOCITY OF GAS GREATER THAN SOUND
```

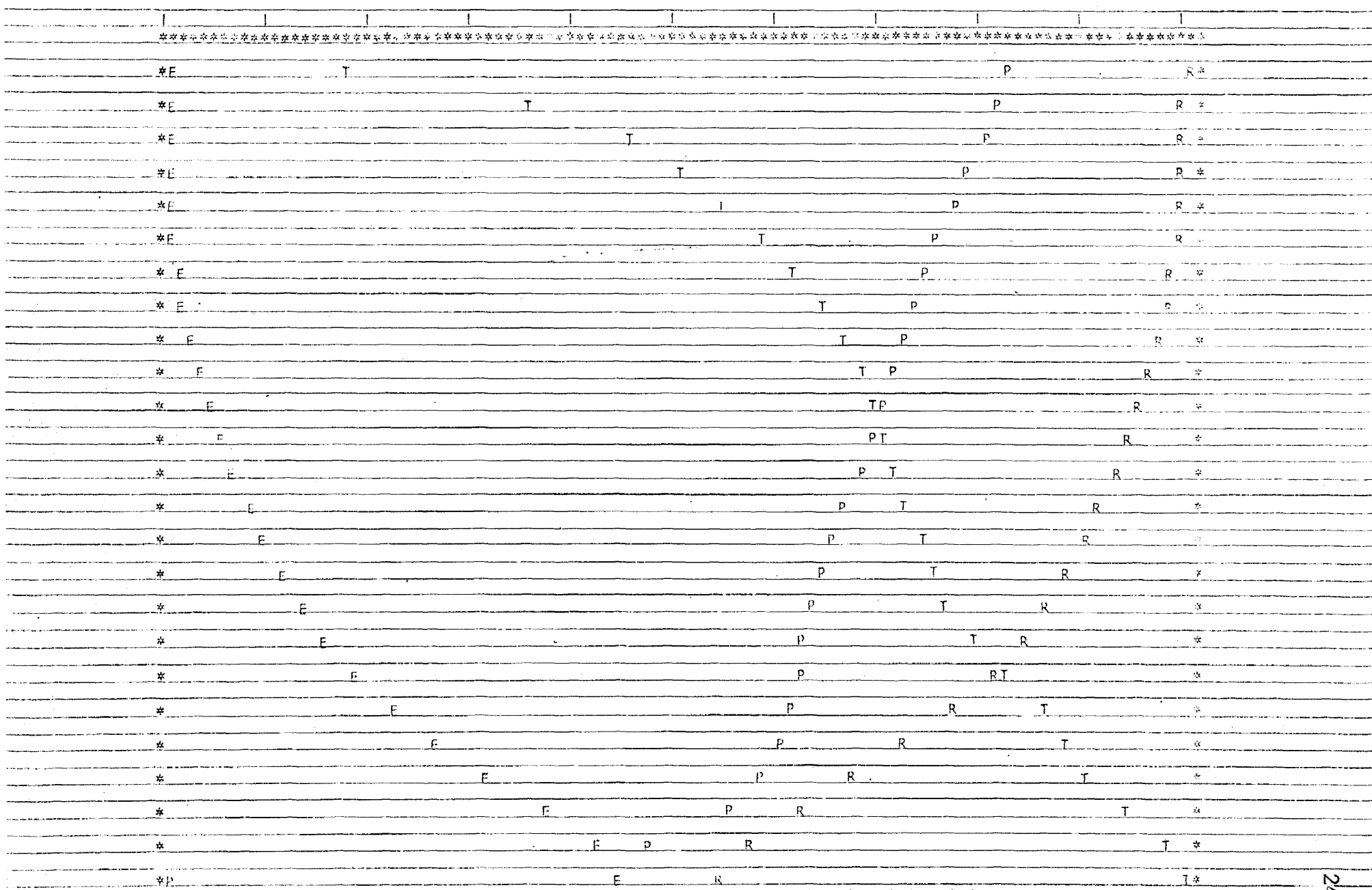
SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.92662E 02FEET
TEMPERTURE 1105.41DEGREE-K MOLAR FLOW RATE 2.47460E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.3165E 03FEET/SEC.

```
 REACTOR IS     400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES  AT PRESSURE   6.649A  VELOCITY OF  1.83438E 02 AT TEMPERATURE   820.0DEG R
 INITIAL REACTOR INCREMENT(DL 1.20880E 00FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.68841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.140125 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52459E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   6.64929E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=   6.64928E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   3.35910E 05     VIS=   2.16064E-05     DEN=   1.56811E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   1.83438E 02        1.86841E 02        1.85140E 02
 TEMPERTURE= 832.71PRESSURE D=   1.99041E-02
  FUNCTION PRR(IS)
 PR=   6.62937E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   6.62937E 00    VELOCITY    1.8684E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    2.9324E-07
  2    0.0000E-01    0.0000E-01    6.7213E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    3.9473E-03    1.2994E 02    0.0000E-01
  6    1.2901E-09    4.2479E-05    0.0000E-01
  7    1.1575E-09    3.8103E-05    0.0000E-01
  8    2.6531E-10    8.7337E-06    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    2.12826E-03   7.00596E 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

 DL CHANGED TO    1.95486E 00      ZIC=   3.12310E 02
 I= 1  RA=   1.67718E-03  DXA(I)=   1.02411E-02  CF,CR=   1.69749E-03   1.43398E-07  REQC=   1.99643E 00

 RATE=   9.88194E-01

 VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 B20 TO 1110 DEG K
REACTOR POSITION 3.97912E 02FEET
TEMPERTURE 1108.69DEGREE-K MOLAR FLOW RATE 2.55264E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.2425E 03FEET/SEC.

```
 REACTOR IS     400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES  AT PRESSURE   6.849A  VELOCITY OF  1.78082E 02 AT TEMPERATURE   820.0DEG R
 INITIAL REACTOR INCREMENT(DL 1.95486E 00FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.66841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27593E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
 FUNCTION PRR(IS)
 PR=   6.84928E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 FUNCTION PRR(IS)
 PR=   6.84928E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   3.35918E 05     VIS=   2.16064E-05     DEN=   1.61542E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   1.78082E 02     1.81354E 02     1.79718E 02
 TEMPERTURE=  832.71PRESSURE D=   1.93074E-02
 FUNCTION PRR(IS)
 PR=   6.82997E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 PRESSURE IS   6.82997E 00    VELOCITY    1.8135E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.0143E-07
  2    0.0000E-01    0.0000E-01    6.9090E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    4.0660E-03    1.2994E 02    0.0000E-01
  6    1.3661E-09    4.3656E-05    0.0000E-01
  7    1.2256E-09    3.9167E-05    0.0000E-01
  8    2.8092E-10    8.9776E-06    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    2.19227E-03    7.00596E 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

 DL CHANGED TO    1.90666E 00     ZIC=   3.08306E 02
 I= 1  RA=   1.64962E-03  DXA(I)=   1.05000E-02  CF,CR=   1.82833E-03   1.65892E-07  REQC=   1.93574E 00

 RATE=   9.02414E-01

 VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.00781E 02FEET
TEMPERTURE 1109.88DEGREE-K MOLAR FLOW RATE 2.58703E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.0528E 03FEET/SEC.


SYSTEM 4 820 TO 1110 DEG K
REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 400. HOURS OF RUN

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.60160E 01FEET
TEMPERTURE 870.85DEGREE-K MOLAR FLOW RATE 2.00001E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.00%
PRESSURE IS 6.97230E 00 VELOCITY 1.8579E 02FEET/SEC.
ITERATION NUMBER- 1

NO	CONCENTRATION	TMPH	DXA
1	1.1964E-15	3.9170E-11	3.4898E-06
2	0.0000E-01	0.0000E-01	5.3779E-07
3	0.0000E-01	0.0000E-01	3.3337E-08
4	1.0082E-19	3.3006E-15	5.8638E-05
5	3.9689E-03	1.2994E 02	6.4839E-12
6	2.7684E-08	9.0634E-04	8.2379E-21
7	2.5518E-08	8.3545E-04	0.0000E-01
8	4.3308E-09	1.4179E-04	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	2.13994E-03	7.00595E 01	
12	1.40296E-19	0.00000E-01	
13	1.76287E-23	5.77147E-19	

REACTOR POSITION 3.20320E 01FEET
TEMPERTURE 921.70DEGREE-K MOLAR FLOW RATE 2.00013E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.01%
PRESSURE IS 6.89031E 00 VELOCITY 1.9899E 02FEET/SEC.
ITERATION NUMBER- 2

NO	CONCENTRATION	TMPH	DXA
1	1.8555E-13	6.5050E-09	4.4491E-05
2	0.0000E-01	0.0000E-01	4.2499E-06
3	0.0000E-01	0.0000E-01	3.5101E-07
4	1.4329E-16	5.0235E-12	3.9511E-04
5	3.7062E-03	1.2993E 02	6.3352E-10
6	3.7074E-07	1.2997E-02	2.3479E-17
7	3.5145E-07	1.2321E-02	0.0000E-01
8	3.8594E-08	1.3530E-03	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.99844E-03	7.00594E 01	
12	1.46581E-16	0.00000E-01	
13	5.54244E-20	1.94302E-15	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 4.80480E 01FEET
TEMPERTURE 953.04DEGREE-K MOLAR FLOW RATE 2.00090E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.07%
PRESSURE IS 6.83564E 00 VELOCITY 2.0840E 02FEET/SEC.
ITERATION NUMBER- 3

NO	CONCENTRATION	THPH	UXA
1	6.9608E-12	2.5553E-07	1.6324E-04
2	0.0000E-01	0.0000E-01	1.3371E-05
3	0.0000E-01	0.0000E-01	1.2980E-06
4	3.0453E-14	1.1179E-09	1.1303E-03
5	3.5372E-03	1.2985E 02	1.5273E-08
6	2.4365E-06	8.9441E-02	9.6152E-15
7	2.3416E-06	8.5959E-02	0.0000E-01
8	1.8974E-07	6.9651E-03	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.90849E-03	7.00595E 01	
12	1.58015E-14	0.0000E-01	
13	2.78837E-17	1.02360E-12	

REACTOR POSITION 6.40640E 01FEET
TEMPERTURE 965.05DEGREE-K MOLAR FLOW RATE 2.00228E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.17%
PRESSURE IS 6.72199E 00 VELOCITY 2.1380E 02FEET/SEC.
ITERATION NUMBER- 4

NO	CONCENTRATION	THPH	UXA
1	3.9427E-11	1.4847E-06	3.0624E-04
2	0.0000E-01	0.0000E-01	2.0249E-05
3	0.0000E-01	0.0000E-01	2.0855E-06
4	4.2002E-13	1.5816E-08	1.6652E-03
5	3.4445E-03	1.2971E 02	5.9907E-08
6	6.0167E-06	2.2657E-01	1.1497E-13
7	5.8040E-06	2.1856E-01	0.0000E-01
8	4.2566E-07	1.6029E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.86052E-03	7.00598E 01	
12	1.31097E-13	0.0000E-01	
13	4.73696E-16	1.78375E-11	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 8.06800E 01FEET
TEMPERTURE 977.06DEGREE-K MOLAR FLOW RATE 2.00456E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.35%
PRESSURE IS 6.63843E 00 VELOCITY 2.1943E 02FEET/SEC.
ITERATION NUMBER= 5

NO	CONCENTRATION	TMPH	DXA
1	1.4449E-10	5.5835E-06	5.0481E-04
2	0.0000E-01	0.0000E-01	3.0319E-05
3	0.0000E-01	0.0000E-01	3.3080E-06
4	2.7526E-12	1.0637E-07	2.4147E-03
5	3.3506E-03	1.2948E 02	1.6694E-07
6	1.1713E-05	4.5262E-01	7.5433E-13
7	1.1330E-05	4.3782E-01	0.0000E-01
8	7.6684E-07	2.9633E-02	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.81304E-03	7.00604E 01	
12	6.96450E-13	0.00000E-01	
13	3.60951E-15	1.39481E-10	

REACTOR POSITION 9.60959E 01FEET
TEMPERTURE 988.27DEGREE-K MOLAR FLOW RATE 2.00818E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 0.62%
PRESSURE IS 6.55682E 00 VELOCITY 2.2512E 02FEET/SEC.
ITERATION NUMBER= 6

NO	CONCENTRATION	TMPH	DXA
1	4.3298E-10	1.7163E-05	7.9455E-04
2	0.0000E-01	0.0000E-01	4.3716E-05
3	0.0000E-01	0.0000E-01	5.0272E-06
4	1.2953E-11	5.1343E-07	3.3815E-03
5	3.2571E-03	1.2911E 02	3.9223E-07
6	2.0488E-05	8.1211E-01	3.7674E-12
7	1.9865E-05	7.8742E-01	0.0000E-01
8	1.2476E-06	4.9451E-02	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.76752E-03	7.00614E 01	
12	2.92157E-12	0.00000E-01	
13	1.98156E-14	7.85465E-10	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.12112E 02FEET
TEMPERTURE 999.48DEGREE-K MOLAR FLOW RATE 2.01381E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 1.05%
PRESSURE IS 6.47863E 00 VELOCITY 2.3107E 02FEET/SEC.
ITERATION NUMBER- 7

NO	CONCENTRATION	TMPH	DXA
1	1.1538E-09	4.6934E-05	1.2369E-03
2	0.0000E-01	0.0000E-01	6.2466E-05
3	0.0000E-01	0.0000E-01	7.5622E-06
4	5.0110E-11	2.0385E-06	4.6957E-03
5	3.1598E-03	1.2854E 02	8.3804E-07
6	3.3689E-05	1.3704E 00	1.6153E-11
7	3.2736E-05	1.3317E 00	0.0000E-01
8	1.9114E-06	7.7753E-02	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.72232E-03	7.00631E 01	
12	1.08076E-11	0.0000E-01	
13	8.97258E-14	3.6500E-09	

REACTOR POSITION 1.28128E 02FEET
TEMPERTURE 1008.050EGREE-K MOLAR FLOW RATE 2.02206E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 1.69%
PRESSURE IS 6.40617E 00 VELOCITY 2.3667E 02FEET/SEC.
ITERATION NUMBER- 8

NO	CONCENTRATION	TMPH	DXA
1	2.7740E-09	1.1556E-04	1.7136E-03
2	0.0000E-01	0.0000E-01	8.1157E-05
3	0.0000E-01	0.0000E-01	1.0211E-05
4	1.6513E-10	6.8787E-06	5.9716E-03
5	3.0655E-03	1.2770E 02	1.5385E-06
6	5.2562E-05	2.1896E 00	5.8796E-11
7	5.1172E-05	2.1317E 00	0.0000E-01
8	2.7925E-06	1.1633E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.68195E-03	7.00657E 01	
12	3.3031?E-11	0.0000E-01	
13	3.53220E-13	1.47142E-08	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.44144E 02FEET
TEMPERTURE 1014.05DEGREE-K MOLAR FLOW RATE 2.03239E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 2.47%
PRESSURE IS 6.33739E 00 VELOCITY 2.4194E 02FEET/SEC.
ITERATION NUMBER- 9

NO	CONCENTRATION	TMPH	OXA
1	5.6835E-09	2.4195E-04	2.1368E-03
2	0.0000E-01	0.0000E-01	9.6812E-05
3	0.0000E-01	0.0000E-01	1.2509E-05
4	4.3512E-10	1.8523E-05	7.0189E-03
5	2.9753E-03	1.2666E 02	2.3708E-06
6	7.5510E-05	3.2145E 00	1.5479E-10
7	7.3615E-05	3.1338E 00	0.0000E-01
8	3.8161E-06	1.6245E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.6459E-03	7.0069E-01	
12	7.9529E-11	0.0000E-01	
13	1.0863E-12	4.6245E-08	

REACTOR POSITION 1.60160E 02FEET
TEMPERTURE 1020.02DEGREE-K MOLAR FLOW RATE 2.04510E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 3.44%
PRESSURE IS 6.27299E 00 VELOCITY 2.4751E 02FEET/SEC.
ITERATION NUMBER- 10

NO	CONCENTRATION	TMPH	OXA
1	1.0513E-08	4.5759E-04	2.6507E-03
2	0.0000E-01	0.0000E-01	1.1498E-04
3	0.0000E-01	0.0000E-01	1.5250E-05
4	9.7850E-10	4.2589E-05	8.2159E-03
5	2.8805E-03	1.2537E 02	3.3916E-06
6	1.0283E-04	4.4759E 00	3.6476E-10
7	1.0037E-04	4.3685E 00	0.0000E-01
8	4.9818E-06	2.1683E-01	0.0000E-01
9	0.0000E-01	0.0000E-01	
10	0.0000E-01	0.0000E-01	
11	1.6099E-03	7.0073E-01	
12	1.7216E-10	0.0000E-01	
13	2.8266E-12	1.2303E-07	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 1.76176E 02FEET
TEMPERTURE 1022.02DEGREE-K MOLAR FLOW RATE 2.05920E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 4.52%
PRESSURE IS 6.20942E 00 VELOCITY 2.5238E 02FEET/SEC.
ITERATION NUMBER- 11

NO	CONCENTRATION	TMPH	DXA
1	1.7429E-08	7.7299E-04	2.8120E-03
2	0.0000E-01	0.0000E-01	1.2022E-04
3	0.0000E-01	0.0000E-01	1.6084E-05
4	1.8872E-09	8.3702E-05	8.5491E-03
5	2.7947E-03	1.2395E 02	4.0811E-06
6	1.3246E-04	5.5747E 00	6.8041E-10
7	1.2939E-04	5.7387E 00	0.0000E-01
8	6.2164E-06	2.7571E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.58007E-03	7.00786E 01	
12	2.96924E-10	0.00000E-01	
13	6.29374E-12	2.79138E-07	

REACTOR POSITION 1.92192E 02FEET
TEMPERTURE 1024.02DEGREE-K MOLAR FLOW RATE 2.07398E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 5.65%
PRESSURE IS 6.14582E 00 VELOCITY 2.5755E 02FEET/SEC.
ITERATION NUMBER- 12

NO	CONCENTRATION	TMPH	DXA
1	2.6286E-08	1.1886E-03	2.9927E-03
2	0.0000E-01	0.0000E-01	1.2569E-04
3	0.0000E-01	0.0000E-01	1.6962E-05
4	3.1871E-09	1.4412E-04	8.8951E-03
5	2.7082E-03	1.2246E 02	4.6434E-06
6	1.6235E-04	7.3411E 00	1.1112E-09
7	1.5869E-04	7.1757E 00	0.0000E-01
8	7.4432E-06	3.3657E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.54991E-03	7.00840E 01	
12	4.65914E-10	0.00000E-01	
13	1.19953E-11	5.42403E-07	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.08208E 02FEET

TEMPERTURE 1027.05DEGREE-K MOLAR FLOW RATE 2.08970E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 6.85%

PRESSURE IS 6.08086E 00 VELOCITY 2.6334E 02FEET/SEC.

ITERATION NUMBER- 13

NO	CONCENTRATION	TMPH	DXA
1	3.7332E-08	1.7238E-03	3.2878E-03
2	0.0000E-01	0.0000E-01	1.3557E-04
3	0.0000E-01	0.0000E-01	1.8536E-05
4	4.9223E-09	2.2729E-04	9.5252E-03
5	2.6177E-03	1.2087E 02	5.2595E-06
6	1.9273E-04	8.8996E 00	1.7361E-09
7	1.8849E-04	8.7038E 00	0.0000E-01
8	8.6660E-06	4.0016E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.51790E-03	7.00902E 01	
12	7.08551E-10	0.00000E-01	
13	2.06988E-11	9.55783E-07	

REACTOR POSITION 2.24224E 02FEET

TEMPERTURE 1031.06DEGREE-K MOLAR FLOW RATE 2.10734E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 8.19%

PRESSURE IS 6.01734E 00 VELOCITY 2.6988E 02FEET/SEC.

ITERATION NUMBER- 14

NO	CONCENTRATION	TMPH	DXA
1	5.1560E-08	2.4353E-03	3.7512E-03
2	0.0000E-01	0.0000E-01	1.5033E-04
3	0.0000E-01	0.0000E-01	2.0909E-05
4	7.2408E-09	3.4200E-04	1.0462E-02
5	2.5216E-03	1.1910E 02	6.0303E-06
6	2.2540E-04	1.0646E 01	2.7551E-09
7	2.2057E-04	1.0418E 01	0.0000E-01
8	9.9409E-06	4.6953E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.48412E-03	7.00978E 01	
12	1.07476E-09	0.00000E-01	
13	3.41358E-11	1.61230E-06	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 2.40240E 02FEET
TEMPERTURE 1035.06DEGREE-K MOLAR FLOW RATE 2.12711E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 9.70%
PRESSURE IS 5.95508E 00 VELOCITY 2.7701E 02FEET/SEC.
ITERATION NUMBER- 15

NO	CONCENTRATION	TMPH	DXA
1	6.9706E-08	3.3703E-03	4.2684E-03
2	0.0000E-01	0.0000E-01	1.6628E-04
3	0.0000E-01	0.0000E-01	2.3523E-05
4	1.0284E-08	4.9722E-04	1.1463E-02
5	2.4222E-03	1.1711E 02	6.8421E-06
6	2.6066E-04	1.2603E 01	4.2615E-09
7	2.5521E-04	1.2339E 01	0.0000E-01
8	1.1274E-05	5.4512E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.44998E-03	7.01070E 01	
12	1.59196E-09	0.00000E-01	
13	5.45316E-11	2.63663E-06	

REACTOR POSITION 2.56256E 02FEET
TEMPERTURE 1039.06DEGREE-K MOLAR FLOW RATE 2.14917E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 11.38%
PRESSURE IS 5.89394E 00 VELOCITY 2.8487E 02FEET/SEC.
ITERATION NUMBER- 16

NO	CONCENTRATION	TMPH	DXA
1	9.2501E-08	4.5823E-03	4.8420E-03
2	0.0000E-01	0.0000E-01	1.8340E-04
3	0.0000E-01	0.0000E-01	2.6387E-05
4	1.4190E-08	7.0294E-04	1.2526E-02
5	2.3194E-03	1.1490E 02	7.6729E-06
6	2.9845E-04	1.4785E 01	6.4403E-09
7	2.9237E-04	1.4483E 01	0.0000E-01
8	1.2659E-05	6.2710E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.41544E-03	7.01182E 01	
12	2.30819E-09	0.00000E-01	
13	8.47251E-11	4.19713E-06	

SYSTEM 4 820 TO 1110 DEG K

REACTOR POSITION 2.72271E 02FEET
TEMPERTURE 1043.07DEGREE-K MOLAR FLOW RATE 2.17364E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 13.24%
PRESSURE IS 5.83301E 00 VELOCITY 2.9365E 02FEET/SEC.
ITERATION NUMBER- 17

NO	CONCENTRATION	TMPH	DXA
1	1.2070E-07	6.1326E-03	5.4736E-03
2	0.0000E-01	0.0000E-01	2.0163E-04
3	0.0000E-01	0.0000E-01	2.9499E-05
4	1.9093E-08	9.7004E-04	1.3643E-02
5	2.2132E-03	1.1245E 02	8.4988E-06
6	3.3858E-04	1.7202E 01	9.5222E-09
7	3.3187E-04	1.6861E 01	0.0000E-01
8	1.4083E-05	7.1552E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.38036E-03	7.01316E 01	
12	3.28047E-09	0.00000E-01	
13	1.28376E-10	6.52233E-06	

REACTOR POSITION 2.88287E 02FEET
TEMPERTURE 1050.18DEGREE-K MOLAR FLOW RATE 2.20192E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 15.38%
PRESSURE IS 5.77399E 00 VELOCITY 3.0508E 02FEET/SEC.
ITERATION NUMBER- 18

NO	CONCENTRATION	TMPH	DXA
1	1.5646E-07	8.1869E-03	6.9023E-03
2	0.0000E-01	0.0000E-01	2.4210E-04
3	0.0000E-01	0.0000E-01	3.6477E-05
4	2.5295E-08	1.3236E-03	1.6117E-02
5	2.0949E-03	1.0962E 02	1.0142E-05
6	3.8204E-04	1.9991E 01	1.4874E-08
7	3.7470E-04	1.9607E 01	0.0000E-01
8	1.5554E-05	8.1390E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.34060E-03	7.01496E 01	
12	5.02311E-09	0.00000E-01	
13	1.91260E-10	1.00081E-05	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.04303E 02FEET
TEMPERTURE 1060.19DEGREE-K MOLAR FLOW RATE 2.23958E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 18.23%
PRESSURE IS 5.72573E 00 VELOCITY 3.2156E 02FEET/SEC.
ITERATION NUMBER- 19

NO	CONCENTRATION	TMPH	DXA
1	2.0956E-07	1.1348E-02	9.5013E-03
2	0.0000E-01	0.0000E-01	3.1140E-04
3	0.0000E-01	0.0000E-01	4.8869E-05
4	3.4310E-08	1.8580E-03	2.0267E-07
5	1.9551E-03	1.0588E 02	1.3171E-05
6	4.3752E-04	2.3693E 01	2.6969E-08
7	4.2947E-04	2.3258E 01	0.0000E-01
8	1.7290E-05	9.3634E-01	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.29593E-03	7.01800E 01	
12	8.45911E-09	0.00000E-01	
13	2.98219E-10	1.61498E-05	

REACTOR POSITION 3.21870E 02FEET
TEMPERTURE 1070.70DEGREE-K MOLAR FLOW RATE 2.29218E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 22.23%
PRESSURE IS 5.67926E 00 VELOCITY 3.4250E 02FEET/SEC.
ITERATION NUMBER- 20

NO	CONCENTRATION	TMPH	DXA
1	2.9326E-07	1.6602E-02	6.3187E-03
2	0.0000E-01	0.0000E-01	1.9313E-04
3	0.0000E-01	0.0000E-01	3.1607E-05
4	4.8423E-08	2.7413E-03	1.2279E-02
5	1.7772E-03	1.0061E 02	8.2298E-06
6	5.1035E-04	2.8892E 01	1.2903E-08
7	5.0152E-04	2.8393E 01	0.0000E-01
8	1.9388E-05	1.0976E 00	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.24011E-03	7.02062E 01	
12	7.18618E-09	0.00000E-01	
13	4.04671E-10	2.29096E-05	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.39437E 02FEET
TEMPERTURE 1077.29DEGREE-K MOLAR FLOW RATE 2.35281E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 26.84%
PRESSURE IS 5.60907E 00 VELOCITY 3.8285E 02FEET/SEC.
ITERATION NUMBER- 21

NO	CONCENTRATION	TMPH	OXA
1	4.0450E-07	2.3918E-02	7.1725E-03
2	0.0000E-01	0.0000E-01	2.1000E-04
3	0.0000E-01	0.0000E-01	3.5268E-05
4	6.7312E-08	3.9801E-03	1.3162E-02
5	1.5990E-03	9.4548E 01	8.7405E-06
6	5.8984E-04	3.4877E 01	1.9335E-08
7	5.8031E-04	3.4313E 01	0.0000E-01
8	2.1545E-05	1.2740E 00	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.18792E-03	7.02404E 01	
12	1.06248E-08	0.00000E-01	
13	5.61066E-10	3.31753E-05	

REACTOR POSITION 3.57004E 02FEET
TEMPERTURE 1083.88DEGREE-K MOLAR FLOW RATE 2.41850E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 31.82%
PRESSURE IS 5.51037E 00 VELOCITY 4.2278E 02FEET/SEC.
ITERATION NUMBER- 22

NO	CONCENTRATION	TMPH	OXA
1	5.3640E-07	3.3408E-02	8.2057E-03
2	0.0000E-01	0.0000E-01	2.3026E-04
3	0.0000E-01	0.0000E-01	3.9672E-05
4	8.8754E-08	5.5278E-03	1.4228E-02
5	1.4129E-03	8.7999E 01	8.7097E-06
6	6.6386E-04	4.1347E 01	2.7225E-08
7	6.5388E-04	4.0725E 01	0.0000E-01
8	2.3393E-05	1.4570E 00	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.12845E-03	7.02827E 01	
12	1.52332E-08	0.00000E-01	
13	7.81082E-10	4.86477E-05	

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.74571E 02FEET
TEMPERTURE 1094.11DEGREE-K MOLAR FLOW RATE 2.48852E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 37.11%
PRESSURE IS 5.30644E 00 VELOCITY 5.1023E 02FEET/SEC.
ITERATION NUMBER- 23

NO	CONCENTRATION	TMPH	DXA
1	6.7675E-07	4.5381E-02	9.8033E-03
2	0.0000E-01	0.0000E-01	2.5778E-04
3	0.0000E-01	0.0000E-01	4.6184E-05
4	1.0837E-07	7.2670E-03	1.5587E-02
5	1.2087E-03	8.1055E 01	8.6063E-06
6	7.1906E-04	4.8218E 01	3.6467E-08
7	7.0906E-04	4.7548E 01	0.0000E-01
8	2.4479E-05	1.6415E 00	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	1.04891E-03	7.03372E 01	
12	2.10587E-08	0.00000E-01	
13	1.03821E-09	6.96199E-05	

REACTOR POSITION 3.91088E 02FEET
TEMPERTURE 1104.43DEGREE-K MOLAR FLOW RATE 2.55397E 02POUND MOLES PER HOUR

CONVERSION OF ETHANE TO ETHYLENE IS 42.05%
PRESSURE IS 4.82639E 00 VELOCITY 6.8434E 02FEET/SEC.
ITERATION NUMBER- 24

NO	CONCENTRATION	TMPH	DXA
1	7.6637E-07	5.8481E-02	5.1289E-03
2	0.0000E-01	0.0000E-01	1.2646E-04
3	0.0000E-01	0.0000E-01	2.3550E-05
4	1.1280E-07	8.6080E-03	7.4838E-03
5	9.7730E-04	7.4577E 01	2.4433E-06
6	7.1596E-04	5.4635E 01	9.7332E-09
7	7.0676E-04	5.3932E 01	0.0000E-01
8	2.3631E-05	1.8032E 00	0.0000E-01
9	0.00000E-01	0.00000E-01	
10	0.00000E-01	0.00000E-01	
11	9.22339E-04	7.03829E 01	
12	1.14618E-08	0.00000E-01	
13	1.10873E-09	8.46060E-05	

SYSTEM 4 820 TO 1110 DEG K

```
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.15334E 01(1104.43, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.45611E-01(1104.43, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.35184E 02(1104.43, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.12604E-08(1104.43, 4)
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.42369E 01(1104.43, 5)
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.13140E 01(1104.43, 6)
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.24880E 00(1104.43, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.22098E-02(1104.43, 8)

 FUNCTION PRR(IS)
 PR=  7.04928E 00    RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   5.31869E 05     VIS=   2.68339E-05     DEN=   1.25325E-01
 FRICTION FACTOR=   1.29572E-02     V1,V2,VA=   6.84337E 02     6.18705E 02     6.51521E 02
 TEMPERTURE= 1104.43PRESSURE D=   2.32607E-02
  1-A  ACETYLENE              7.66377E-07        5.84813E-02
  2-B  ISO BUTANE             0.00000E-01        0.00000E-01
  3-C  N-BUTANE               0.00000E-01        0.00000E-01
  4-D  ISO-BUTENE             1.12804E-07        8.60799E-03
  5-E  ETHANE                 9.77296E-04        7.45766E 01
  6-F  ETHYLENE               7.15964E-04        5.46346E 01
  7-G  HYDROGEN               7.06757E-04        5.39320E 01
  8-H  METHANE                2.36308E-05        1.80374E 00
  9-I  PROPANE                0.00000E-01        0.00000E-01
 10-J  PROPENE                0.00000E-01        0.00000E-01
 11-K  WATER                  9.22339E-04        7.03829E 01
 12-L  CARBON                 1.14618E-08        0.00000E-01
 13-M  CARBON MONOXIDE        1.10873E-09        8.46060E-05

 CONVERSION OF ETHANE          TO  ETHYLENE          IS 42.05%
```

REACTOR RADIUS PROFILE AFTER 500.00 HOURS

0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000	0.125000
0.124999	0.124999	0.124999	0.124999	0.124998	0.124998	0.124997	0.124996	0.124994	0.124992
0.124989	0.124986	0.124983	0.124978	0.124973	0.124967	0.124960	0.124951	0.124940	0.124928
0.124916	0.124904	0.124890	0.124875	0.124858	0.124841	0.124822	0.124801	0.124780	0.124756
0.124727	0.124695	0.124660	0.124621	0.124578	0.124532	0.124481	0.124425	0.124364	0.124298
0.124226	0.124147	0.124061	0.123968	0.123868	0.123758	0.123641	0.123513	0.123375	0.123220
0.122968	0.122677	0.122340	0.121948	0.121494	0.120963	0.120350	0.119624	0.117639	0.118015
0.116638	0.115428	0.115245	0.113659	0.110891	0.111625	0.110172	0.107261	0.106971	0.103696
0.102843	0.099964	0.095399	0.090840	0.086352	0.088091	0.084987	0.076404	0.073938	0.073938

```
 REACTOR IS     400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES  / HOUR ARE 200.0POUND MOLES  AT PRESSURE   7.049A  VELOCITY OF  1.73029E 02 AT TEMPERATURE    820.0DEG K
  INITIAL REACTOR INCREMENT(DL 9.69399E-01FEET
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.68841E-02( 832.71, 2)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   7.04928E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=   7.04928E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
  FUNCTION PRESD(T)
 RENU=   3.35918E 05     VIS=   2.16064E-05     DEN=   1.66272E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   1.73029E 02          1.76180E 02          1.74605E 02
 TEMPERIURE=  832.71PRESSURE D=   1.87458E-02
  FUNCTION PRR(IS)
 PR=   7.03053E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 PRESSURE IS   7.03053E 00    VELOCITY    1.7618E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    4.1908E-07
  2    0.0000E-01    0.0000E-01    9.6058E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    4.1847E-03    1.2994E 02    0.0000E-01
  6    1.9547E-09    0.0696E-05    0.0000E-01
  7    1.7538E-09    5.4456E-05    0.0000E-01
  8    4.0195E-10    1.2482E-05    0.0000E-01
  9    0.00000E-01   0.00000E-01
 10    0.00000E-01   0.00000E-01
 11    2.25628E-03   7.00596E 01
 12    0.00000E-01   0.00000E-01
 13    0.00000E-01   0.00000E-01

 DL CHANGED  TO    1.85975E 00     ZIC=   3.08306E 02
 I= 1  RA=   1.72639E-03  DXA(I)=   1.07649E-02  CF,CR=   1.91346E-03   1.97715E-07  REQC=   1.93574E 00

 RATE=   9.02414E-01
 I PT P(1)-P(12), GC AMWT   1104.99     3.62     0.00     0.00     0.00     0.00     1.13     0.73     0.72     0.02
     0.00     0.00     1.01     0.00     0.00     1.31    20.61  -500.64
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.91989E 02FEET
TEMPERTURE 1104.99DEGREE-K MOLAR FLOW RATE 2.51592E 02POUND MOLES PER HOUR
PRESSURE IS 5.00000E-01 VELOCITY 1.1055E 03FEET/SEC.

```
 REACTOR IS      400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES  AT PRESSURE   7.249A  VELOCITY OF  1.68256E 02 AT TEMPERATURE   820.0DEG R
  INITIAL REACTOR INCREMENT(DL 1.85975E 00FEET
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.68841E-02( 832.71, 2)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
  FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
   FUNCTION PRR(IS)
 PR=   7.24928E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
   FUNCTION PRR(IS)
 PR=   7.24928E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   3.35915E 05     VIS=   2.16064E-05     DEN=   1.71002E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   1.68256E 02          1.71295E 02          1.69775E 02
 TEMPERTURE=  832.71PRESSURE D=   1.82164E-02
   FUNCTION PRR(IS)
 PR=   7.23105E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   7.23105E 00    VELOCITY    1.7129E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.1982E-07
  2    0.0000E-01    0.0000E-01    7.3306E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    4.3035E-03    1.2994E 02    0.0000E-01
  6    1.5341E-09    4.6320E-05    0.0000E-01
  7    1.3763E-09    4.1557E-05    0.0000E-01
  8    3.1547E-10    9.5254E-06    0.0000E-01
  9    0.00000E-01   0.00000E-01
 10    0.00000E-01   0.00000E-01
 11    2.32030E-03   7.00596E 01
 12    0.00000E-01   0.00000E-01
 13    0.00000E-01   0.00000E-01

 DL CHANGED TO    1.90289E 02     ZIC=   3.04302E 02
 I= 1  RA=   1.67941E-03  DXA(I)=   1.05208E-02  CF,CR=   2.03923E-03   2.21298E-07  REQC=   1.96590E 00

 RATE=   8.23729E-01

 VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.93736E 02FEET
TEMPERTURE 1106.08DEGREE-K MOLAR FLOW RATE 2.54508E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.6800E 03FEET/SEC.

```
 REACTOR IS     400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.00POUND MOLES AT PRESSURE   7.449A  VELOCITY OF  1.63738E 02 AT TEMPERATURE    820.0DEG K
 INITIAL REACTOR INCREMENT(DL 1.90289E 00FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.68841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   7.44928E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=   7.44927E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   3.35917E 05     VIS=   2.16064E-05     DEN=   1.75731E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   1.63738E 02     1.66673E 02     1.65206E 02
 TEMPERTURE=  832.71PRESSURE D=   1.77163E-02
  FUNCTION PRR(IS)
 PR=   7.43155E 00     RADI(1)=   1.25000E-01     VOL=   0.00000E-01
 PRESSURE IS   7.43155E 00     VELOCITY    1.6667E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.2832E-07
  2    0.0000E-01    0.0000E-01    7.5254E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    4.4222E-03    1.2994E 02    0.0000E-01
  6    1.6163E-09    4.7551E-05    0.0000E-01
  7    1.4519E-09    4.2662E-05    0.0000E-01
  8    3.3279E-10    9.7785E-06    0.0000E-01
  9    0.00000E-01   0.00000E-01
 10    0.00000E-01   0.00000E-01
 11    2.38431E-03   7.00596E 01
 12    0.00000E-01   0.00000E-01
 13    0.00000E-01   0.00000E-01

 DL CHANGED TO    1.98252E 00     ZIC=   3.00299E 02
 I= 1  RA=   1.62353E-03  DXA(I)=   1.00983E-02  CF,CR=   2.16064E-03   2.44135E-07  REQC=   1.99667E 00

 RATE=   7.51563E-01

 VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.93472E 02FEET
TEMPERTURE 1105.92DEGREE-K MOLAR FLOW RATE 2.56811E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.2836E 03FEET/SEC.

```
 REACTOR IS    400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES AT PRESSURE   7.649A  VELOCITY OF  1.59457E 02 AT TEMPERATURE   820.0DEG K
 INITIAL REACTOR INCREMENT(DL 1.98252E 00FEET
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.68841E-02( 832.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.27599E-01( 832.71, 6)
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,1)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   7.64927E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=   7.64927E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   3.35917E 05     VIS=   2.16064E-05     DEN=   1.80461E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=   1.59457E 02        1.62295E 02        1.60876E 02
 TEMPERTURE=  832.71PRESSURE D=   1.72432E-02
  FUNCTION PRR(IS)
 PR=   7.63202E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   7.63202E 00    VELOCITY    1.6230E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.3718E-07
  2    0.0000E-01    0.0000E-01    7.7286E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    4.5409E-03    1.2994E 02    0.0000E-01
  6    1.7966E-09    4.6835E-05    0.0000E-01
  7    1.5311E-09    4.3813E-05    0.0000E-01
  8    3.5095E-10    1.0043E-05    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    2.4483E-03    7.0059E 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

 DL CHANGED TO   1.89579E 00    ZIC=   3.00299E 02
 I= 1  RA=   1.6639AE-03  DXA(I)=   1.05602E-02  CF,CR=   2.24114E-03   2.85769E-07  REQC=   1.99667E 00

RATE=   7.51583E-01

VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.96982E 02FEET
TEMPERTURE 1108.11DEGREE-K MOLAR FLOW RATE 2.59804E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.5530E 03FEET/SEC.

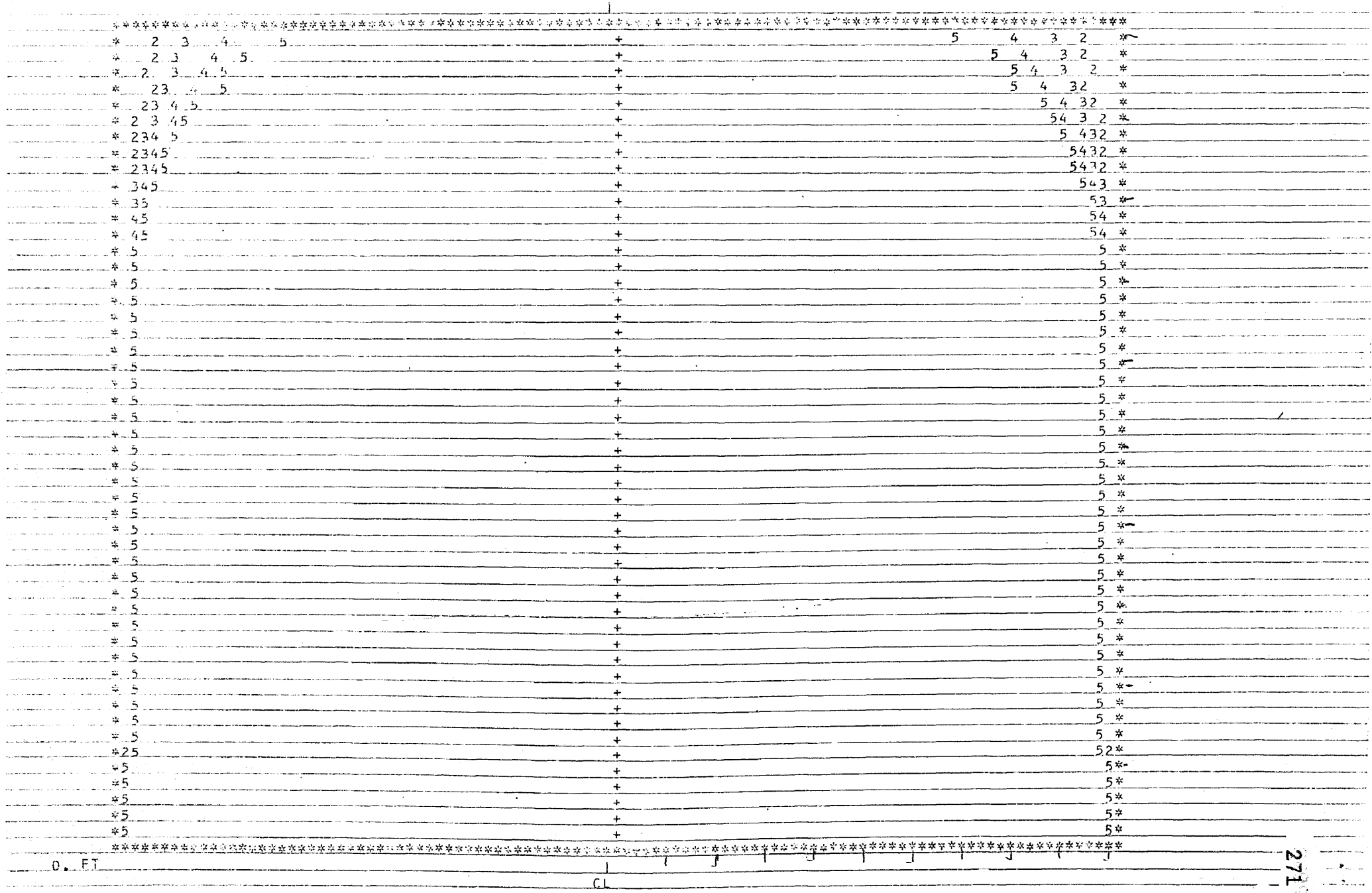
```
 REACTOR IS     400.00 FEET LONG AND  0.125 FEET IN RADIUS
 TOTAL MOLES / HOUR ARE 200.0POUND MOLES  AT PRESSURE   7.849A  VELOCITY OF  1.55394E 02 AT TEMPERATURE    820.0DEG K
 INITIAL REACTOR INCREMENT(DL 1.89579E 00FEET
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.11963E 02( 832.71, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.6e841E-02( 932.71, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14012E 06( 832.71, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.14837E-08( 832.71, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.52409E 01( 832.71, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.27599L-01( 832.71, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.55381E 00( 832.71, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.79039E-03( 832.71, 8)
  FUNCTION PRR(IS)
 PR=   7.84927E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
  FUNCTION PRR(IS)
 PR=   7.84927E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   3.35917E 05     VIS=   2.16064E-05     DEN=   1.65190E-01
 FRICTION FACTOR=   1.41227E-02     V1,V2,VA=  1.55394E 02        1.58142E 02        1.56768E 02
 TEMPERTURE=  832.71PRESSURE D=   1.67949E-02
  FUNCTION PRR(IS)
 PR=   7.83247E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 PRESSURE IS   7.83247E 00    VELOCITY    1.5814E 02FEET/SEC.
  1    0.0000E-01    0.0000E-01    3.4531E-07
  2    0.0000E-01    0.0000E-01    7.9150E-08
  3    0.0000E-01    0.0000E-01    0.0000E-01
  4    0.0000E-01    0.0000E-01    0.0000E-01
  5    4.6596E-03    1.2994E 02    0.0000E-01
  6    1.7934E-09    5.0012E-05    0.0000E-01
  7    1.6090E-09    4.4870E-05    0.0000E-01
  8    3.6881E-10    1.0285E-05    0.0000E-01
  9    0.0000E-01    0.0000E-01
 10    0.0000E-01    0.0000E-01
 11    2.51234E-03   7.0059eE 01
 12    0.0000E-01    0.0000E-01
 13    0.0000E-01    0.0000E-01

 DL CHANGED TO    1.92601E 00     ZIC=   2.96295E 02
 I= 1  RA=   1.01700E-03  DXA(I)=   1.03945E-02  CF,CR=   2.35965E-03   3.08253E-07  REQC=   2.02796E 00

RATE=   6.35453E-01

 DL CHANGED TO    9.53695E-01     ZIC=   3.6562eE 02
 I= 1  RA=   3.30363E-03  DXA(I)=   1.00976E-02  CF,CR=   1.53235E-03   9.03224E-07  REQC=   1.67012E 00

RATE=   2.15805E 00

VELOCITY OF GAS GREATER THAN SOUND
```

SYSTEM 4 820 TO 1110 DEG K
REACTOR POSITION 3.96138E 02FEET
TEMPERTURE 1107.59DEGREE-K MOLAR FLOW RATE 2.61283E 02POUND MOLES PER HOUR
PRESSURE IS 2.[illegible]E 00 VELOCITY 1.2499E 03FEET/SEC.

```
REACTOR IS      400.00 FEET LONG AND  0.125 FEET IN RADIUS
TOTAL MOLES / HOUR ARE 200.00000 MOLES AT PRESSURE   8.049A VELOCITY OF  1.51533E 02 AT TEMPERATURE   820.00EG R
INITIAL REACTOR INCREMENT(DL 9.53695E-01FEET
FUNCTION REQC(T,I)
REQC(T,I)=   0.11963E 02( 832.71, 1)
FUNCTION REQC(T,I)
REQC(T,I)=   0.66841E-02( 832.71, 2)
FUNCTION REQC(T,I)
REQC(T,I)=   0.14017E 06( 832.71, 3)
FUNCTION REQC(T,I)
REQC(T,I)=   0.14637E-08( 832.71, 4)
FUNCTION REQC(T,I)
REQC(T,I)=   0.52409E 01( 832.71, 5)
FUNCTION REQC(T,I)
REQC(T,I)=   0.27599E-01( 832.71, 6)
FUNCTION REQC(T,I)
REQC(T,I)=   0.55381E 00( 832.71, 7)
FUNCTION REQC(T,I)
REQC(T,I)=   0.79039E-03( 832.71, 8)
 FUNCTION PRR(IS)
PR=  8.04927E 00     RADI(1)=  1.25000E-01     VOL=  0.00000E-01
 FUNCTION PRR(IS)
PR=  8.04926E 00     RADI(1)=  1.25000E-01     VOL=  0.00000E-01
FUNCTION PRESD(T)
RENU=  3.35917E 05     VIS=  2.16064E-05     DEN=  1.89918E-01
FRICTION FACTOR=  1.41227E-02     V1,V2,VA=  1.51533E 02     1.54196E 02     1.52865E 02
TEMPERTURE=  832.71PRESSURE D=  1.63696E-02
 FUNCTION PRR(IS)
PR=  8.03289E 00     RADI(1)=  1.25000E-01     VOL=  0.00000E-01
PRESSURE IS   8.03289E 00     VELOCITY   1.5420E 02FEET/SEC.
 1   0.0000E-01   0.0000E-01   3.5428E-07
 2   0.0000E-01   0.0000E-01   8.1205E-08
 3   0.0000E-01   0.0000E-01   0.0000E-01
 4   0.0000E-01   0.0000E-01   0.0000E-01
 5   4.7784E-03   1.2994E 02   0.0000E-01
 6   1.8869E-09   5.1311E-05   0.0000E-01
 7   1.6929E-09   4.6035E-05   0.0000E-01
 8   3.8803E-10   1.0552E-05   0.0000E-01
 9   0.0000E-01   0.0000E-01
10   0.0000E-01   0.0000E-01
11   2.57635E-03   7.00596E 01
12   0.00000E-01   0.00000E-01
13   0.00000E-01   0.00000E-01

 DL CHANGED TO   1.85175E 00     ZIC=  2.96295E 02
I= 1  RA=  1.66921E-03  DXA(I)=  1.03114E-02  CF,CR=  2.43591E-03  3.54529E-07  REQC=  2.02796E 00

RATE=  6.35453E-01

 DL CHANGED TO   9.03262E-01     ZIC=  3.68505E 02
I= 1  RA=  3.53758E-03  DXA(I)=  1.02503E-02  CF,CR=  1.54420E-03  1.10122E-06  REQC=  1.65298E 00

RATE=  2.29359E 00

VELOCITY OF GAS GREATER THAN SOLID
```

SYSTEM 4.820 TO 1110 DEG K
REACTOR POSITION 3.92210E 02FEET
TEMPERTURE 1109.510DEGREE-K MOLAR FLOW RATE 2.64115E 02POUND MOLES PER HOUR
PRESSURE IS 2.00000E 00 VELOCITY 1.2390E 03FEET/SEC.

REACTOR RADIUS PROFILE FROM START TO CLOSE DOWN



0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 0 Hours of Run
Pressure (P) 8-2 At.
Temperature (T) 820-1050°K
272
SYSTEM 1 820 TO 1050 DEG K

SYSTEM 1 820 TO 1050 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 0.HOURS OF RUN

SYSTEM 1 820 TO 1050 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.21468E 01(1048.65, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.33349E-01(1048.65, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13617E 03(1048.65, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13002E-08(1048.65, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.44133E 01(1048.65, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.70039E 00(1048.65, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.28340E 00(1048.65, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.18575E-02(1048.65, 8)

FUNCTION PRR(IS)
PR= 5.84930E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.94496E 05 VIS= 2.58054E-05 DEN= 1.05844E-01
FRICTION FACTOR= 1.26997E-02 V1,V2,VA= 8.60155E 02 2.99372E 02 5.79768E 02
TEMPERTURE= 1048.65PRESSURE D= 4.11471E-01

1-A	ACETYLENE	1.06958E-08	1.53804E-03
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	5.11583E-10	7.35651E-05
5-E	ETHANE	8.43818E-04	1.21340E 02
6-F	ETHYLENE	5.93251E-05	8.53086E 00
7-G	HYDROGEN	5.80189E-05	8.34305E 00
8-H	METHANE	2.66216E-06	3.82815E-01
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	4.87716E-04	7.01330E 01
12-L	CARBON	1.28123E-10	0.00000E-01
13-M	CARBON MONOXIDE	2.46968E-12	3.55137E-07

CONVERSION OF ETHANE TO ETHYLENE IS 6.57%

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 4800. Hours of Run
Temperature (T) 820-1050°K
Pressure (P) 8-2 AT.
SYSTEM 1 820 TO 1050 DEG K

SYSTEM 1 820 TO 1050 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 4800.HOURS OF RUN

SYSTEM 1 820 TO 1050 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.21468E 01(1048.65, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.33349E-01(1048.65, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13617E 03(1048.65, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13002E-08(1048.65, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.44133E 01(1048.65, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.70039E 00(1048.65, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.28340E 00(1048.65, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.18575E-02(1048.65, 8)

FUNCTION PRR(IS)
PR= 5.89929E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.97020E 05 VIS= 2.58054E-05 DEN= 1.06733E-01
FRICTION FACTOR= 1.26901E-02 V1,V2,VA= 8.69077E 02 3.09439E 02 5.89263E 02
TEMPERTURE= 1048.65PRESSURE D= 4.16534E-01

1-A	ACETYLENE	1.13499E-08	1.57896E-03
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	5.66668E-10	7.88331E-05
5-E	ETHANE	8.71383E-04	1.21224E 02
6-F	ETHYLENE	6.21353E-05	8.64406E 00
7-G	HYDROGEN	6.07669E-05	8.45369E 00
8-H	METHANE	2.78951E-06	3.88068E-01
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	5.04126E-04	7.01324E 01
12-L	CARBON	1.35138E-10	0.00000E-01
13-M	CARBON MONOXIDE	2.69394E-12	3.74773E-07

CONVERSION OF ETHANE TO ETHYLENE IS 6.65%

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 7200. Hours of Run
Temperature (T) 820-1050°K
Pressure (P) 8-2 AT.
SYSTEM 1 820 TO 1050 DEG K

SYSTEM 1 820 TO 1050 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 7200.HOURS OF RUN

SYSTEM 1 820 TO 1050 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.21468E 01(1048.65, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.33349E-01(1048.65, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13617E 03(1048.65, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13002E-08(1048.65, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.44133E 01(1048.65, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.70039E 00(1048.65, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.29340E 00(1048.65, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.18575E-02(1048.65, 8)

FUNCTION PRR(IS)
PR= 5.89929E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 6.21273E 05 VIS= 2.58054E-05 DEN= 1.06154E-01
FRICTION FACTOR= 1.26003E-02 V1,V2,VA= 9.26640E 02 3.19467E 02 6.23063E 02
TEMPERTURE= 1048.65PRESSURE D= 4.78170E-01

1-A	ACETYLENE	1.07432E-08	1.54454E-03
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	5.28809E-10	7.60265E-05
5-E	ETHANE	8.43896E-04	1.21326E 02
6-F	ETHYLENE	5.94512E-05	8.54723E 00
7-G	HYDROGEN	5.81388E-05	8.35856E 00
8-H	METHANE	2.67433E-06	3.84486E-01
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	4.87828E-04	7.01346E 01
12-L	CARBON	1.22073E-10	0.00000E-01
13-M	CARBON MONOXIDE	2.48565E-12	3.57360E-07

CONVERSION OF ETHANE TO ETHYLENE IS 6.58%

SYSTEM 1 820 TO 1050 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 14400.HOURS OF RUN

SYSTEM 1 820 TO 1050 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.21468E 01(1048.65, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.33349E-01(1048.65, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13617E 03(1048.65, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.13002E-08(1048.65, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.44133E 01(1048.65, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.70039E 00(1048.65, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.28340E 00(1048.65, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.18575E-02(1048.65, 8)

FUNCTION PRR(IS)
PR= 5.94928E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 6.60260E 05 VIS= 2.58054E-05 DEN= 1.06074E-01
FRICTION FACTOR= 1.24653E-02 V1,V2,VA= 1.02381E 03 3.44027E 02 6.83918E 02
TEMPERTURE= 1048.65PRESSURE D= 5.87065E-01

1-A	ACETYLENE	1.05628E-08	1.54208E-03
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	5.32238E-10	7.77026E-05
5-E	ETHANE	8.31139E-04	1.21340E 02
6-F	ETHYLENE	5.84837E-05	8.53816E 00
7-G	HYDROGEN	5.71891E-05	8.34917E 00
8-H	METHANE	2.63848E-06	3.85197E-01
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	4.80418E-04	7.01373E 01
12-L	CARBON	1.12438E-10	0.00000E-01
13-M	CARBON MONOXIDE	2.43515E-12	3.55514E-07

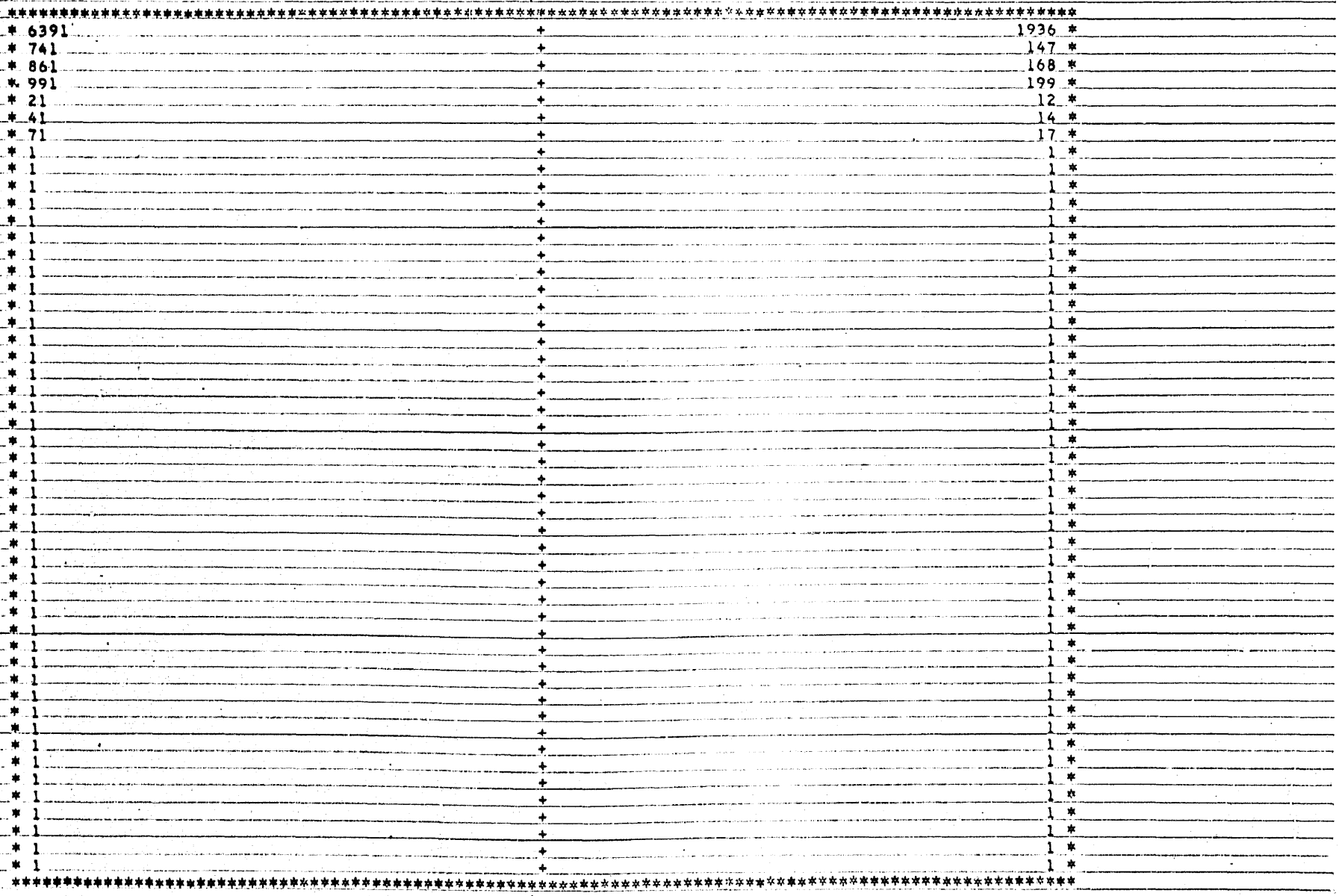
CONVERSION OF ETHANE TO ETHYLENE IS 6.57%

System 1 820 - 1050°K

CONVERSION OF Ethane to Ethylene Time Increment - 800 Hours

400.00 FT

CL



0. FT

CL

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reaction (R)
Temperature (T) 820-1090°K
Pressure (P) 8 -2 AT.
After 0 hours of Run
SYSTEM 2 820 TO 1090 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 0.HOURS OF RUN

SYSTEM 2 820 TO 1090 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.16896E 01(1087.75, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41663E-01(1087.75, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.51980E 02(1087.75, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12721E-08(1087.75, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42883E 01(1087.75, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.10960E 01(1087.75, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.25831E 00(1087.75, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.21013E-02(1087.75, 8)

FUNCTION PRR(IS)
PR= 5.85000E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 6.23836E 05 VIS= 2.65284E-05 DEN= 1.01286E-01
FRICTION FACTOR= 1.25911E-02 V1,V2,VA= 9.66857E 02 3.40258E 02 6.53570E 02
TEMPERTURE= 1087.75PRESSURE D= 4.95925E-01

1-A	ACETYLENE	7.35133E-08	1.17724E-02
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	4.59769E-09	7.36270E-04
5-E	ETHANE	6.58048E-04	1.05379E 02
6-F	ETHYLENE	1.52962E-04	2.44952E 01
7-G	HYDROGEN	1.50389E-04	2.40831E 01
8-H	METHANE	5.52751E-06	8.85169E-01
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	4.39198E-04	7.03327E 01
12-L	CARBON	2.32199E-09	0.00000E-01
13-M	CARBON MONOXIDE	4.99023E-11	7.99129E-06

CONVERSION OF ETHANE TO ETHYLENE IS 18.85%

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
Temperature (T) 820 - 1090° K
Pressure (P) 8-2 AT.
After 800. Hours of Run
283
SYSTEM 2 820 TO 1090 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 800.HOURS OF RUN

SYSTEM 2 820 TO 1090 DEG K

```
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.16896E 01(1087.75, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.41663E-01(1087.75, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.51980E 02(1087.75, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.12721E-08(1087.75, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.42883E 01(1087.75, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.10960E 01(1087.75, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.25831E 00(1087.75, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.21013E-02(1087.75, 8)

 FUNCTION PRR(IS)
 PR= 5.97498E 00    RADI(1)= 1.25001E-01    VOL= 0.00000E-01
 FUNCTION PRESD(T)
 RENU= 6.66289E 05    VIS= 2.65284E-05    DEN= 1.02449E-01
 FRICTION FACTOR= 1.24454E-02    V1,V2,VA= 1.08865E 03    3.92536E 02    7.40590E 02
 TEMPERTURE= 1087.75PRESSURE D= 6.17736E-01
  1-A  ACETYLENE          8.06998E-08    1.22797E-02
  2-B  ISO BUTANE         0.00000E-01    0.00000E-01
  3-C  N-BUTANE           0.00000E-01    0.00000E-01
  4-D  ISO-BUTENE         5.53991E-09    8.42979E-04
  5-E  ETHANE             6.89104E-04    1.04857E 02
  6-F  ETHYLENE           1.64378E-04    2.50125E 01
  7-G  HYDROGEN           1.61608E-04    2.45910E 01
  8-H  METHANE            5.96274E-06    9.07318E-01
  9-I  PROPANE            0.00000E-01    0.00000E-01
 10-J  PROPENE            0.00000E-01    0.00000E-01
 11-K  WATER              4.62250E-04    7.03381E 01
 12-L  CARBON             2.36740E-09    0.00000E-01
 13-M  CARBON MONOXIDE    5.76037E-11    8.76524E-06

 CONVERSION OF ETHANE    TO ETHYLENE    IS 19.25%
```

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
Temperature (T) 820-1090°K
Pressure (P) 8 - 2 AT.
After 2800. Hours of Run
285
SYSTEM 2 820 TO 1090 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER

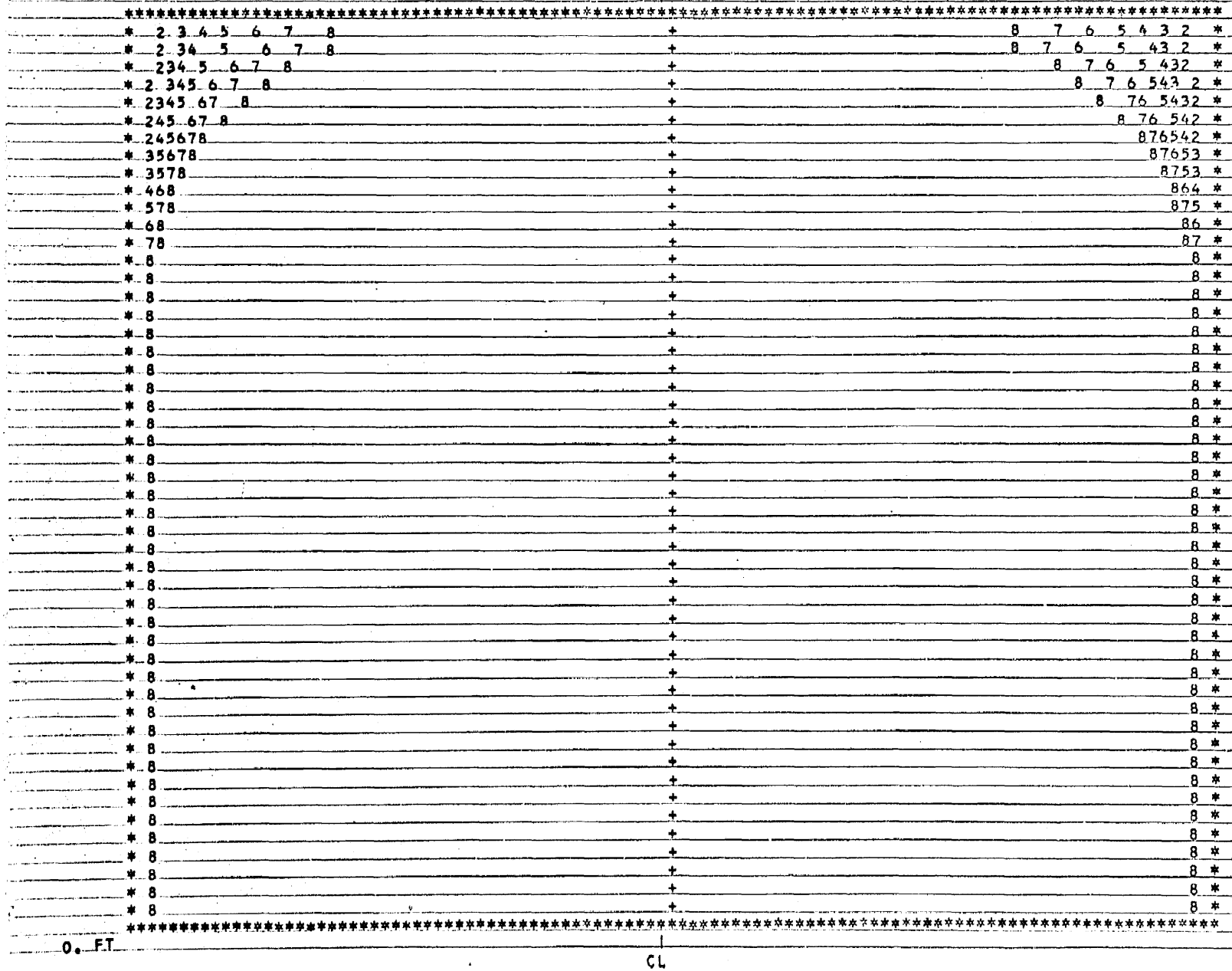
SYSTEM 2 820 TO 1090 DEG K

```
 FUNCTION REQC(T,I)
 REQC(T,I)=  0.16896E 01(1087.75, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=  0.41663E-01(1087.75, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=  0.51980E 02(1087.75, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=  0.12721E-08(1087.75, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=  0.42883E 01(1087.75, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=  0.10960E 01(1087.75, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=  0.25831E 00(1087.75, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=  0.21013E-02(1087.75, 8)

 FUNCTION PRR(IS)
 PR=  7.57496E 00    RAD1(1)=  1.25001E-01     VOL=  0.00000E-01
 FUNCTION PRESD(T)
 RENU=  7.33016E 05    VIS=  2.65284E-05     DEN=  1.32648E-01
 FRICTION FACTOR=  1.22395E-02    V1,V2,VA=  1.17383E 03     6.37380E 02     9.05613E 02
 TEMPERTURE= 1087.75PRESSURE D=  4.77038E-01
  1-A  ACETYLENE              2.93942E-07     2.23858E-02
  2-B  ISO BUTANE             0.00000E-01     0.00000E-01
  3-C  N-BUTANE               0.00000E-01     0.00000E-01
  4-D  ISO-BUTENE             4.55975E-08     3.47258E-03
  5-E  ETHANE                 1.25894E-03     9.58775E 01
  6-F  ETHYLENE               4.43229E-04     3.37551E 01
  7-G  HYDROGEN               4.35964E-04     3.32018E 01
  8-H  METHANE                1.62951E-05     1.24099E 00
  9-I  PROPANE                0.00000E-01     0.00000E-01
 10-J  PROPENE                0.00000E-01     0.00000E-01
 11-K  WATER                  9.23845E-04     7.03574E 01
 12-L  CARBON                 8.72880E-09     0.00000E-01
 13-M  CARBON MONOXIDE        4.41284E-10     3.36069E-05

 CONVERSION OF ETHANE          TO  ETHYLENE          IS 25.98%
```

System 2 820 - 1090°K

CONVERSION OF Ethane to Ethylene Time Increment - 400. Hours

400.00 FT



0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 0. Hours of Run
Temperature (T) 820-1100°K,
Pressure (P) 8 - 2 AT.
SYSTEM 3 820 TO 1100 DEG K

SYSTEM 3 820 TO 1100 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 0.HOURS OF RUN

SYSTEM 3 820 TO 1100 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.15790E 01(1099.33, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.44379E-01(1099.33, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.39589E 02(1099.33, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12639E-08(1099.33, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42525E 01(1099.33, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12439E 01(1099.33, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.25164E 00(1099.33, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.21764E-02(1099.33, 8)

FUNCTION PRR(IS)
PR= 5.85000E 00 RADI(1)= 1.25001E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 6.44918E 05 VIS= 2.67408E-05 DEN= 9.91257E-02
FRICTION FACTOR= 1.25172E-02 V1,V2,VA= 1.02508E 03 3.66747E 02 6.95909E 02
TEMPERTURE= 1099.33PRESSURE D= 6.18569E-01

1-A	ACETYLENE	1.26812E-07	2.21844E-02
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	8.05898E-09	1.40983E-03
5-E	ETHANE	5.48245E-04	9.59096E 01
6-F	ETHYLENE	1.93515E-04	3.38533E 01
7-G	HYDROGEN	1.90571E-04	3.33383E 01
8-H	METHANE	6.58295E-06	1.15162E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	4.02325E-04	7.03824E 01
12-L	CARBON	2.29484E-09	0.00000E-01
13-M	CARBON MONOXIDE	9.67245E-11	1.69209E-05

CONVERSION OF ETHANE TO ETHYLENE IS 26.05%

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
Temperature (T) 820-1100°K
Pressure (P) 8 - 2 ATM
After 600. Hours of Run
290
SYSTEM 3 820 TO 1100 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 600.HOURS OF RUN

SYSTEM 3 820 TO 1100 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.15783E 01(1099.41, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.44397E-01(1099.41, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.39522E 02(1099.41, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12639E-08(1099.41, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42523E 01(1099.41, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12448E 01(1099.41, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.25160E 00(1099.41, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.21769E-02(1099.41, 8)

FUNCTION PRR(IS)
PR= 6.34999E 00 RADI(1)= 1.25001E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.98597E 05 VIS= 2.67421E-05 DEN= 1.09679E-01
FRICTION FACTOR= 1.26841E-02 V1,V2,VA= 9.07750E 02 4.44542E 02 6.76144E 02
TEMPERTURE= 1099.41PRESSURE D= 4.37916E-01

1-A	ACETYLENE	2.52607E-07	2.93898E-02
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	2.41362E-08	2.80815E-03
5-E	ETHANE	7.79315E-04	9.06699E 01
6-F	ETHYLENE	3.34410E-04	3.89072E 01
7-G	HYDROGEN	3.29452E-04	3.83304E 01
8-H	METHANE	1.13902E-05	1.32521E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	6.04735E-04	7.03585E 01
12-L	CARBON	4.98883E-09	0.00000E-01
13-M	CARBON MONOXIDE	2.46665E-10	2.86985E-05

CONVERSION OF ETHANE TO ETHYLENE IS 29.94%

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 1200. Hours of Run
Temperature (T) 820-1100°K.
Pressure (P) 8 - 2 AT.
292
SYSTEM 3 820 TO 1100 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 1200.HOURS OF RUN

SYSTEM 3 820 TO 1100 DEG K

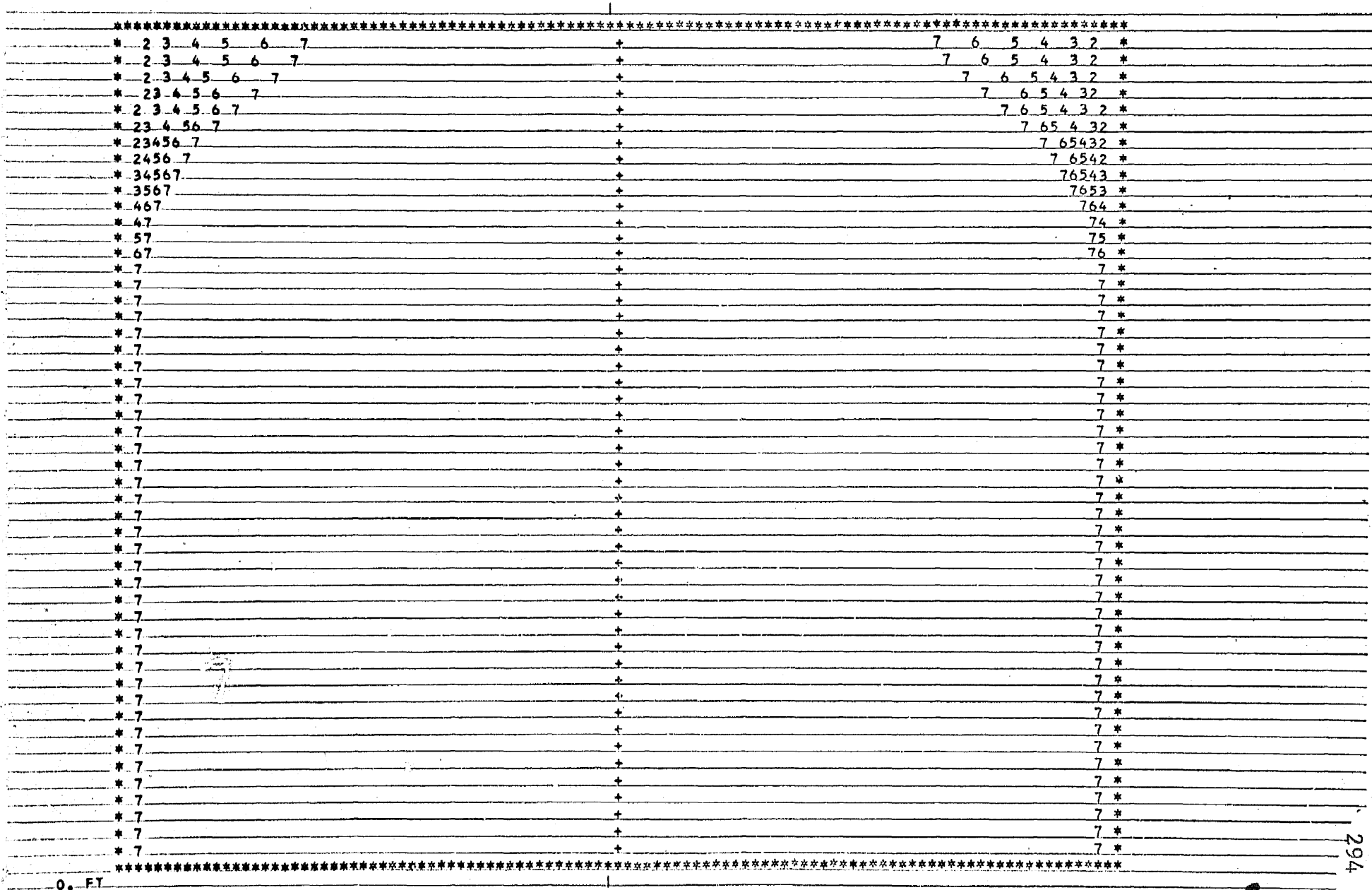
```
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.15835E 01(1098.84, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.44262E-01(1098.84, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.40043E 02(1098.84, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.12643E-08(1098.84, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.42540E 01(1098.84, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.12373E 01(1098.84, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.25191E 00(1098.84, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)= 0.21732E-02(1098.84, 8)

 FUNCTION PRR(IS)
 PR= 7.74997E 00    RAD1(1)= 1.25001E-01    VOL= 0.00000E-01
 FUNCTION PRESD(T)
 RENU= 7.00546E 05    VIS= 2.67318E-05    DEN= 1.34434E-01
 FRICTION FACTOR= 1.23364E-02    V1,V2,VA= 1.05652E 03    6.55824E 02    8.56175E 02
 TEMPERTURE= 1098.84PRESSURE D= 4.77855E-01
  1-A  ACETYLENE          5.61184E-07    4.22059E-02
  2-B  ISO BUTANE         0.00000E-01    0.00000E-01
  3-C  N-BUTANE           0.00000E-01    0.00000E-01
  4-D  ISO-BUTENE         9.18276E-08    6.90623E-03
  5-E  ETHANE             1.10141E-03    8.28352E 01
  6-F  ETHYLENE           6.18298E-04    4.65014E 01
  7-G  HYDROGEN           6.09387E-04    4.58312E 01
  8-H  METHANE            2.15144E-05    1.61807E 00
  9-I  PROPANE            0.00000E-01    0.00000E-01
 10-J  PROPENE            0.00000E-01    0.00000E-01
 11-K  WATER              9.35229E-04    7.03372E 01
 12-L  CARBON             1.04289E-08    0.00000E-01
 13-M  CARBON MONOXIDE    7.48683E-10    5.63073E-05

 CONVERSION OF ETHANE          TO  ETHYLENE          IS 35.79%
```

System 3 820 - 1100°K

CONVERSION OF Ethane to Ethylene Time Increment - 200. Hours

400.00 FT

CL



0. FT

CL

System 4 820 - 1110°K

CONVERSION OF Ethane to Ethylene   Time Increment - 100 Hours

```
     400.00 FT                                         CL
                                                       |
         ****************************************************************************************
         *  2  3    4     5                             +                         5    4   3  2   *
         *   2 3    4 5                                 +                            5  4   3 2   *
         *  2  3   4 5                                  +                             5 4  3  2   *
         *   23   4 5                                   +                              5 4  32    *
         *  23 4 5                                      +                               5 4 32    *
         * 2 3 45                                       +                                54 3 2   *
         * 234 5                                        +                                 5 432   *
         * 2345                                         +                                  5432   *
         * 2345                                         +                                  5432   *
         * 345                                          +                                   543   *
         * 35                                           +                                    53   *
         * 45                                           +                                    54   *
         * 45                                           +                                    54   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         * 5                                            +                                     5   *
         ****************************************************************************************
   0. FT                                                |
                                                       CL
```

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 0. Hours of Run
Temperature (T) 820-1115° K
Pressure (P) 8 - 2 AT.
296
SYSTEM 5 820. TO 1115. DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 0.HOURS OF RUN

SYSTEM 5 820. TO 1115. DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.14468E 01(1114.67, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.48158E-01(1114.67, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.27851E 02(1114.67, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12534E-08(1114.67, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42059E 01(1114.67, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.14648E 01(1114.67, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24328E 00(1114.67, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.22778E-02(1114.67, 8)

FUNCTION PRR(IS)
PR= 5.79999E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 6.73864E 05 VIS= 2.70204E-05 DEN= 9.66144E-02
FRICTION FACTOR= 1.24207E-02 V1,V2,VA= 1.08356E 03 4.24147E 02 7.53847E 02
TEMPERTURE= 1114.67PRESSURE D= 6.48700E-01

1-A	ACETYLENE	4.13905E-07	7.65848E-02
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	2.73525E-08	5.06103E-03
5-E	ETHANE	3.62656E-04	6.71020E 01
6-F	ETHYLENE	3.36698E-04	6.22992E 01
7-G	HYDROGEN	3.32943E-04	6.16044E 01
8-H	METHANE	1.02583E-05	1.89810E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	3.81377E-04	7.05661E 01
12-L	CARBON	1.04717E-08	0.00000E-01
13-M	CARBON MONOXIDE	5.11157E-10	9.45793E-05

CONVERSION OF ETHANE TO ETHYLENE IS 47.94%

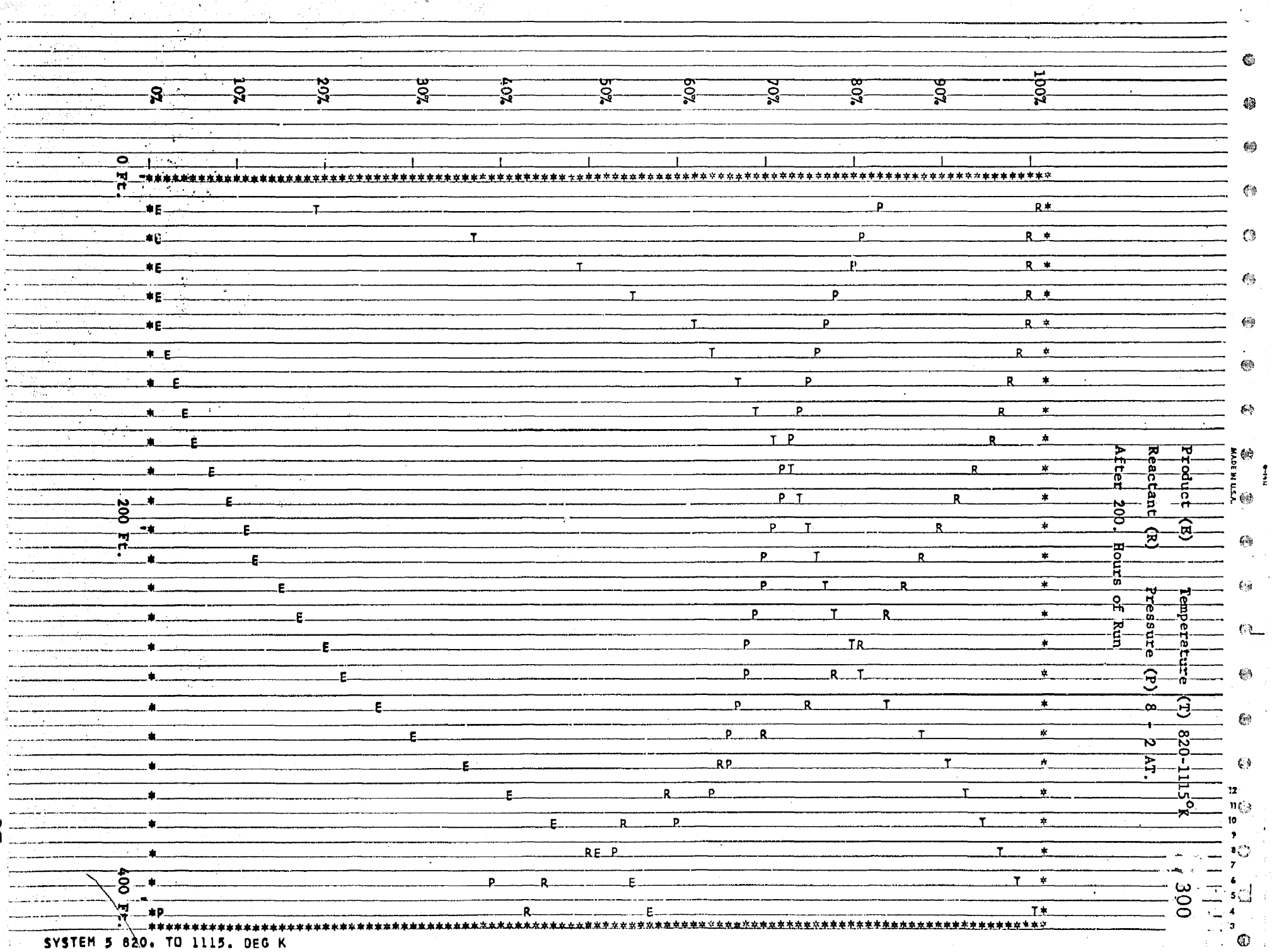
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 100. Hours of Run
Temperature (T) 820-1115 °K
Pressure (P) 8 - 2 AT.
SYSTEM 5 820. TO 1115. DEG K

SYSTEM 5 820. TO 1115. DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 100. HOURS OF RUN

SYSTEM 5 820. TO 1115. DEG K

```
 FUNCTION REQC(T,I)
REQC(T,I)= 0.14465E 01(1114.70, 1)
 FUNCTION REQC(T,I)
REQC(T,I)= 0.48166E-01(1114.70, 2)
 FUNCTION REQC(T,I)
REQC(T,I)= 0.27831E 02(1114.70, 3)
 FUNCTION REQC(T,I)
REQC(T,I)= 0.12534E-08(1114.70, 4)
 FUNCTION REQC(T,I)
REQC(T,I)= 0.42058E 01(1114.70, 5)
 FUNCTION REQC(T,I)
REQC(T,I)= 0.14653E 01(1114.70, 6)
 FUNCTION REQC(T,I)
REQC(T,I)= 0.24327E 00(1114.70, 7)
 FUNCTION REQC(T,I)
REQC(T,I)= 0.22780E-02(1114.70, 8)

 FUNCTION PRR(IS)
PR= 6.19998E 00    RADI(1)= 1.25000E-01    VOL= 0.00000E-01
 FUNCTION PRESD(T)
RENU= 6.31483E 05    VIS= 2.70210E-05    DEN= 1.04927E-01
FRICTION FACTOR= 1.25639E-02    V1,V2,VA= 9.64302E 02    4.87060E 02    7.25677E 02
TEMPERTURE= 1114.70PRESSURE D= 5.06068E-01
 1-A  ACETYLENE        6.76840E-07    9.14025E-02
 2-B  ISO BUTANE       0.00000E-01    0.00000E-01
 3-C  N-BUTANE         0.00000E-01    0.00000E-01
 4-D  ISO-BUTENE       6.02082E-08    8.13068E-03
 5-E  ETHANE           4.55308E-04    6.14861E 01
 6-F  ETHYLENE         5.01102E-04    6.76703E 01
 7-G  HYDROGEN         4.95826E-04    6.69579E 01
 8-H  METHANE          1.53378E-05    2.07126E 00
 9-I  PROPANE          0.00000E-01    0.00000E-01
10-J  PROPENE          0.00000E-01    0.00000E-01
11-K  WATER            5.22044E-04    7.04984E 01
12-L  CARBON           9.17796E-09    0.00000E-01
13-M  CARBON MONOXIDE  8.44405E-10    1.14031E-04

CONVERSION OF ETHANE        TO  ETHYLENE        IS 52.08%
```


0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 200. Hours of Run
Temperature (T) 820-1115°K
Pressure (P) 8 - 2 AT.
300
SYSTEM 5 820. TO 1115. DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 200.HOURS OF RUN

SYSTEM 5 820. TO 1115. DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.14453E 01(1114.85, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.48204E-01(1114.85, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.27739E 02(1114.85, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12533E-08(1114.85, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.42054E 01(1114.85, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.14675E 01(1114.85, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24319E 00(1114.85, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.22790E-02(1114.85, 8)

FUNCTION PRR(IS)
PR= 6.99997E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 7.49695E 05 VIS= 2.70237E-05 DEN= 1.16410E-01
FRICTION FACTOR= 1.21918E-02 V1,V2,VA= 1.20843E 03 6.63983E 02 9.36220E 02
TEMPERTURE= 1114.85PRESSURE D= 8.02283E-01

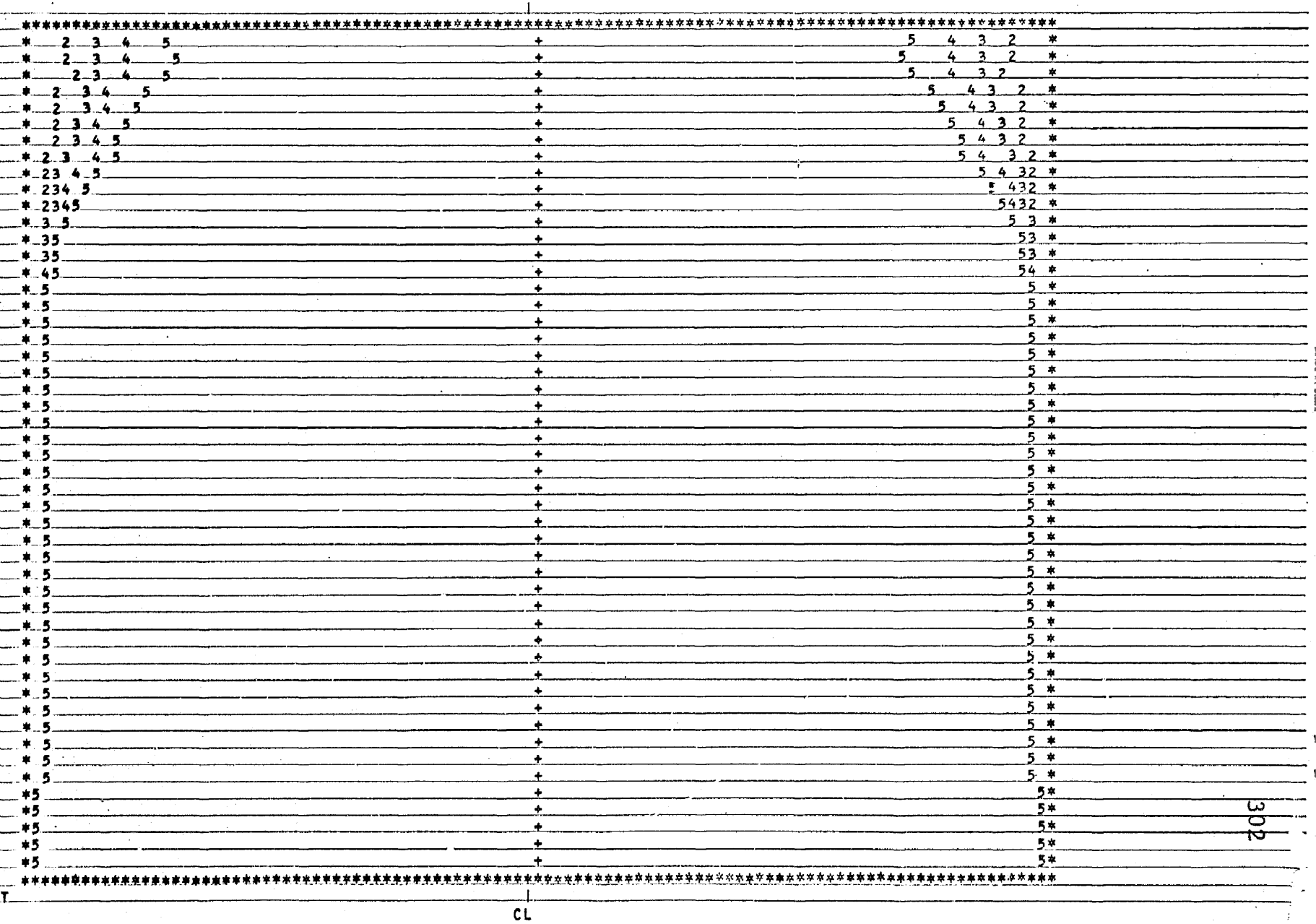
1-A	ACETYLENE	9.44364E-07	1.08446E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	1.10031E-07	1.26354E-02
5-E	ETHANE	4.84797E-04	5.56720E 01
6-F	ETHYLENE	6.38168E-04	7.32843E 01
7-G	HYDROGEN	6.31855E-04	7.25595E 01
8-H	METHANE	1.98661E-05	2.28134E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	6.13818E-04	7.04881E 01
12-L	CARBON	1.06108E-08	0.00000E-01
13-M	CARBON MONOXIDE	1.36979E-09	1.57300E-04

CONVERSION OF ETHANE TO ETHYLENE IS 56.40%

System 5 820 - 1115°K

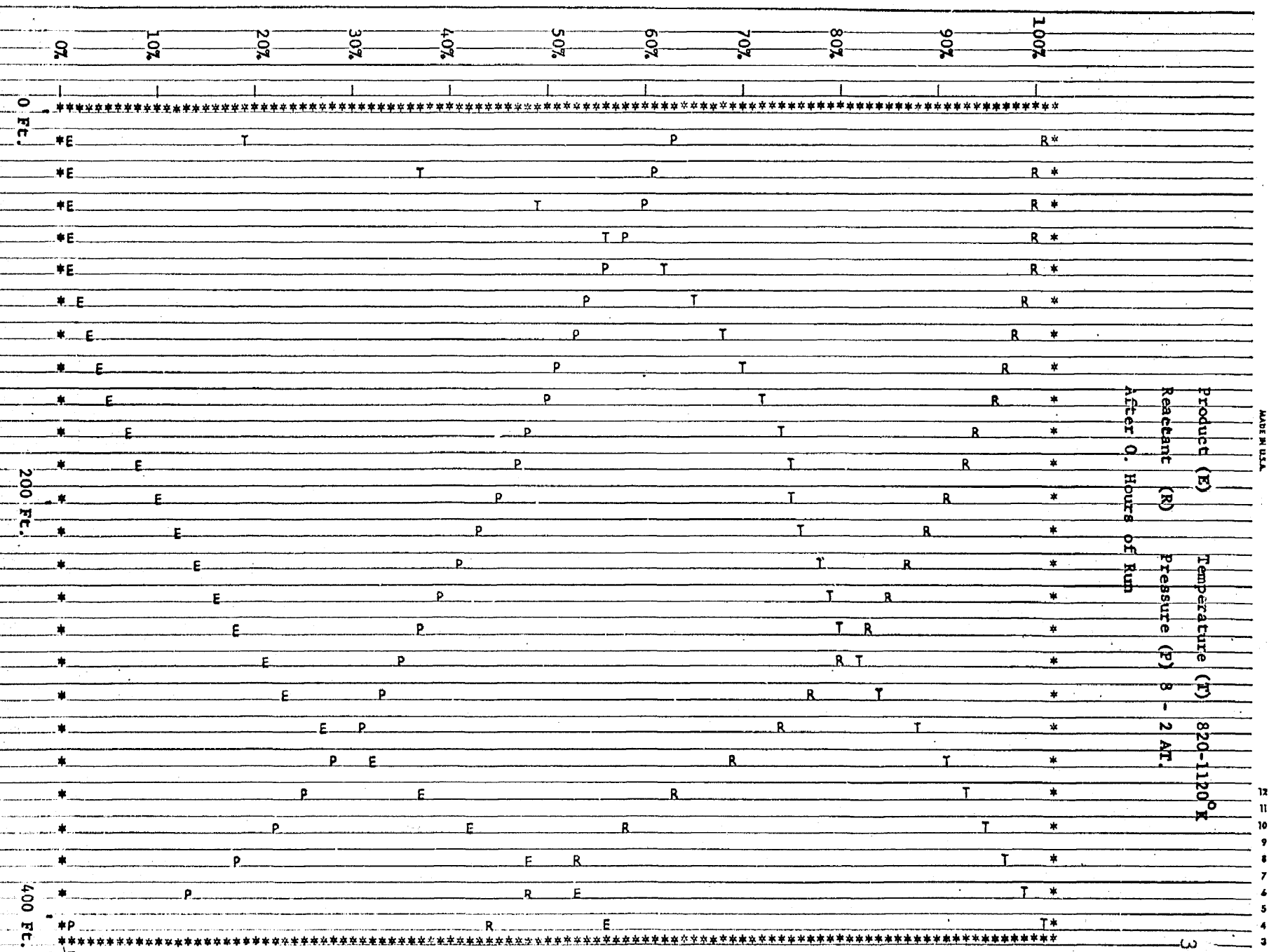
CONVERSION OF Ethane to Ethylene Time Increment - 50. Hours

400.00 FT



SYSTEM 6 820 TO 1120 DEG K

```
FUNCTION REQC(T,I)
REQC(T,I)=   0.14050E 01(1119.91, 1)
FUNCTION REQC(T,I)
REQC(T,I)=   0.49497E-01(1119.91, 2)
FUNCTION REQC(T,I)
REQC(T,I)=   0.24755E 02(1119.91, 3)
FUNCTION REQC(T,I)
REQC(T,I)=   0.12498E-08(1119.91, 4)
FUNCTION REQC(T,I)
REQC(T,I)=   0.41902E 01(1119.91, 5)
FUNCTION REQC(T,I)
REQC(T,I)=   0.15473E 01(1119.91, 6)
FUNCTION REQC(T,I)
REQC(T,I)=   0.24055E 00(1119.91, 7)
FUNCTION REQC(T,I)
REQC(T,I)=   0.23129E-02(1119.91, 8)

 FUNCTION PRR(IS)
PR=   5.84999E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
FUNCTION PRESD(T)
RENU=   6.10596E 05     VIS=   2.71156E-05     DEN=   9.86432E-02
FRICTION FACTOR=   1.26393E-02     V1,V2,VA=   9.19750E 02      4.22967E 02      6.71375E 02
TEMPERTURE= 1119.91PRESSURE D=   4.65656E-01
  1-A  ACETYLENE          6.53945E-07      1.05104E-01
  2-B  ISO BUTANE         0.00000E-01      0.00000E-01
  3-C  N-BUTANE           0.00000E-01      0.00000E-01
  4-D  ISO-BUTENE         4.75505E-08      7.64244E-03
  5-E  ETHANE             3.54534E-04      5.69815E 01
  6-F  ETHYLENE           4.49031E-04      7.21694E 01
  7-G  HYDROGEN           4.44716E-04      7.14759E 01
  8-H  METHANE            1.33184E-05      2.14058E 00
  9-I  PROPANE            0.00000E-01      0.00000E-01
 10-J  PROPENE            0.00000E-01      0.00000E-01
 11-K  WATER              4.38917E-04      7.05439E 01
 12-L  CARBON             1.06738E-08      0.00000E-01
 13-M  CARBON MONOXIDE    7.45954E-10      1.19892E-04

CONVERSION OF ETHANE          TO  ETHYLENE          IS 55.54%
```

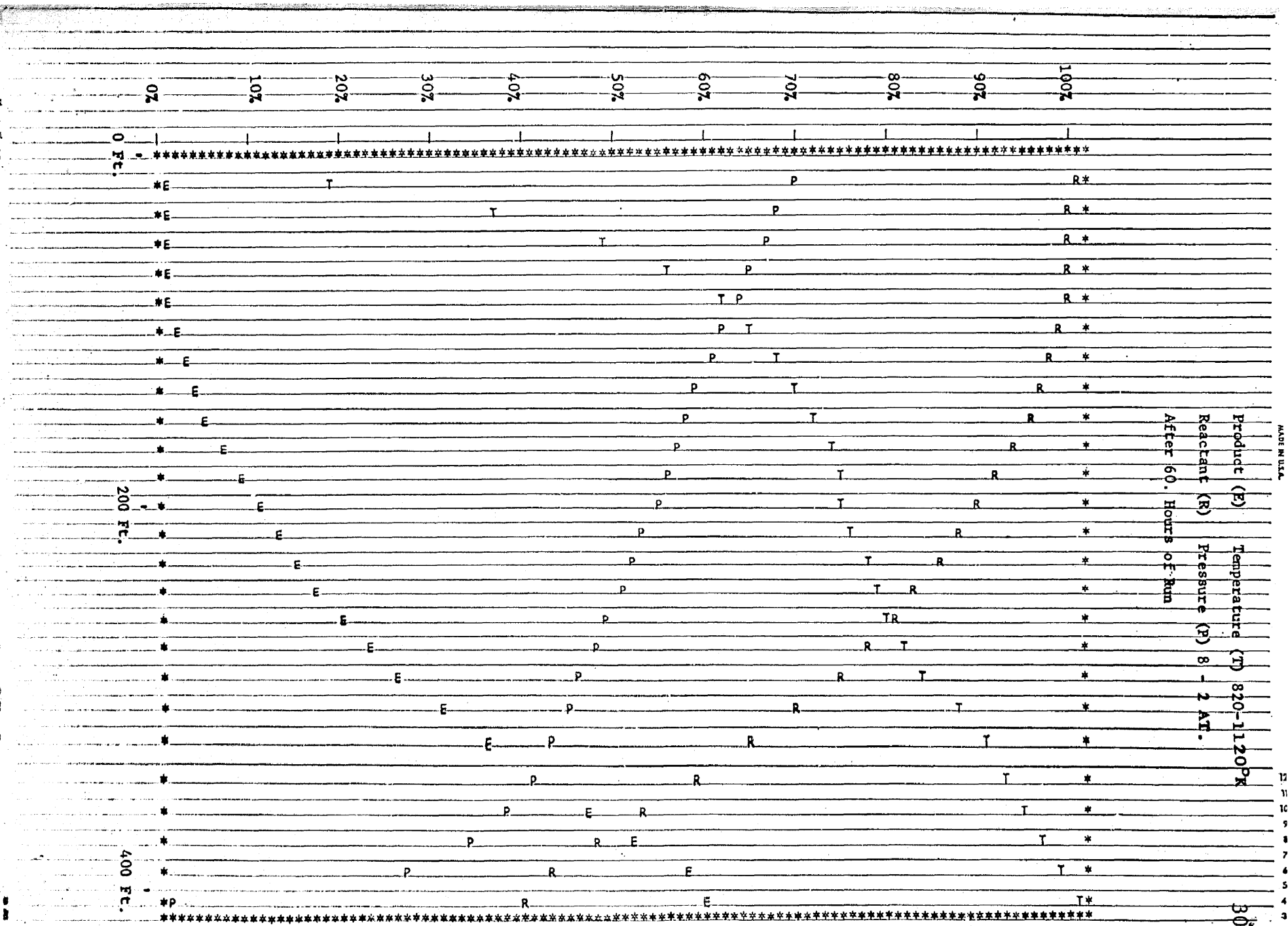


SYSTEM 6 820 TO 1120 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 0.HOURS OF RUN

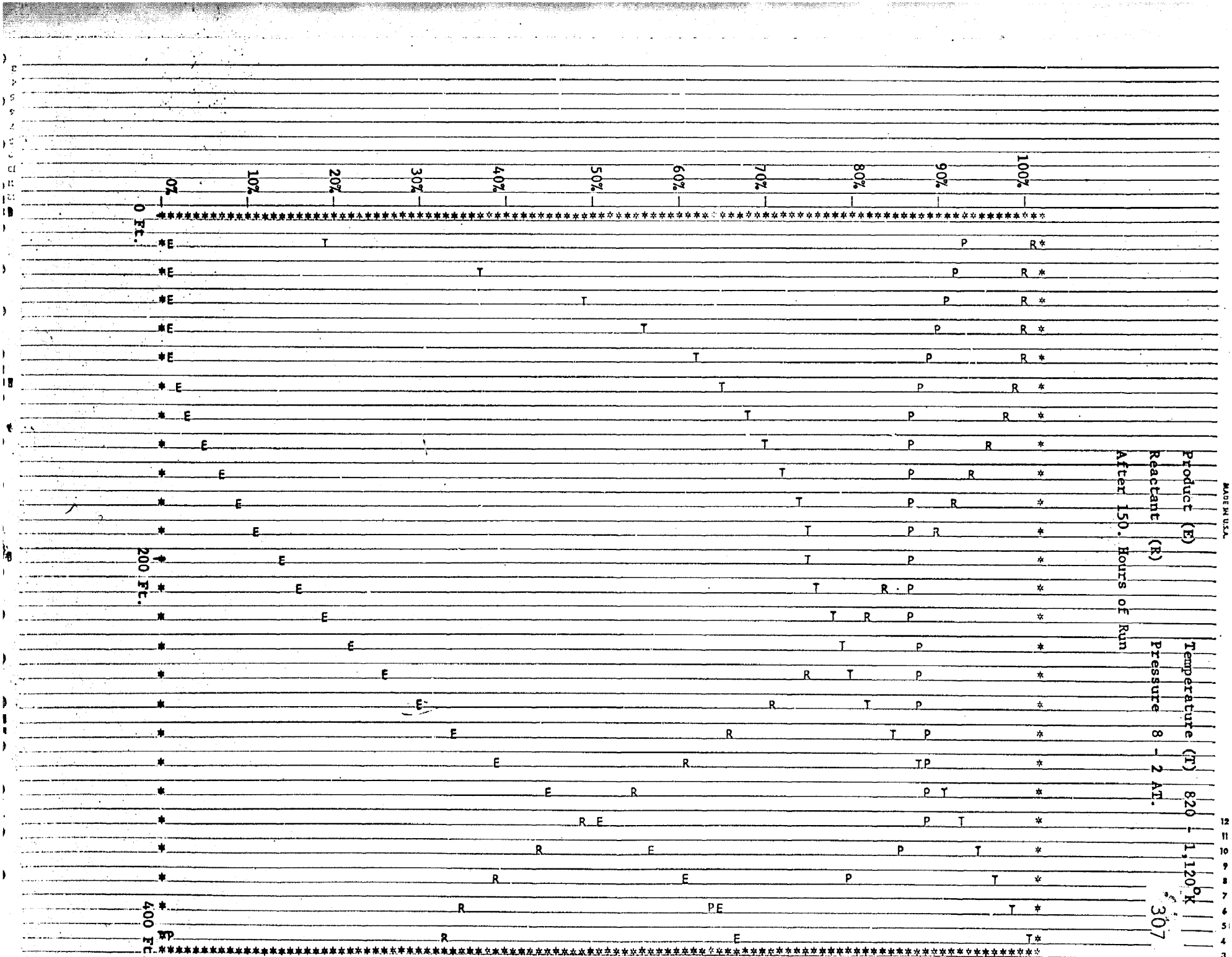
SYSTEM 6 820 TO 1120 DEG K

```
 FUNCTION REQC(T,I)
REQC(T,I)=   0.14053E 01(1119.86, 1)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.49486E-01(1119.86, 2)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.24779E 02(1119.86, 3)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.12499E-08(1119.86, 4)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.41904E 01(1119.86, 5)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.15466E 01(1119.86, 6)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.24057E 00(1119.86, 7)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.23126E-02(1119.86, 8)

  FUNCTION PRR(IS)
PR=   6.24999E 00     RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
RENU=   6.02925E 05     VIS=   2.71148E-05     DEN=   1.06391E-01
FRICTION FACTOR=   1.26678E-02     V1,V2,VA=   8.81027E 02      4.97107E 02      6.89065E 02
TEMPERTURE= 1119.86PRESSURE D=   3.84182E-01
  1-A  ACETYLENE          9.96890E-07      1.22141E-01
  2-B  ISO BUTANE         0.00000E-01      0.00000E-01
  3-C  N-BUTANE           0.00000E-01      0.00000E-01
  4-D  ISO-BUTENE         9.47991E-08      1.16149E-02
  5-E  ETHANE             4.21674E-04      5.16642E 01
  6-F  ETHYLENE           6.30941E-04      7.73040E 01
  7-G  HYDROGEN           6.25368E-04      7.66212E 01
  8-H  METHANE            1.88371E-05      2.30795E 00
  9-I  PROPANE            0.00000E-01      0.00000E-01
 10-J  PROPENE            0.00000E-01      0.00000E-01
 11-K  WATER              5.75646E-04      7.05291E 01
 12-L  CARBON             1.71810E-08      0.00000E-01
 13-M  CARBON MONOXIDE    1.32108E-09      1.61861E-04

CONVERSION OF ETHANE          TO ETHYLENE          IS 59.49%
```



SYSTEM 6 820 TO 1120 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 60.HOURS OF RUN


0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 150. Hours of Run
Temperature (T) 820 - 1,120° K
Pressure 8 - 2 AT.
307
SYSTEM 6 820 TO 1120 DEG K

SYSTEM 6 820 TO 1120 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 150.HOURS OF RUN

SYSTEM 6 820 TO 1120 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.14070E 01(1119.65, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.49431E-01(1119.65, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24895E 02(1119.65, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12500E-08(1119.65, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41910E 01(1119.65, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.15433E 01(1119.65, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24068E 00(1119.65, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23112E-02(1119.65, 8)

FUNCTION PRR(IS)
PR= 7.64997E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 7.04669E 05 VIS= 2.71110E-05 DEN= 1.30731E-01
FRICTION FACTOR= 1.23238E-02 V1,V2,VA= 9.97125E 02 6.91321E 02 8.44205E 02
TEMPERTURE= 1119.65PRESSURE D= 4.15535E-01

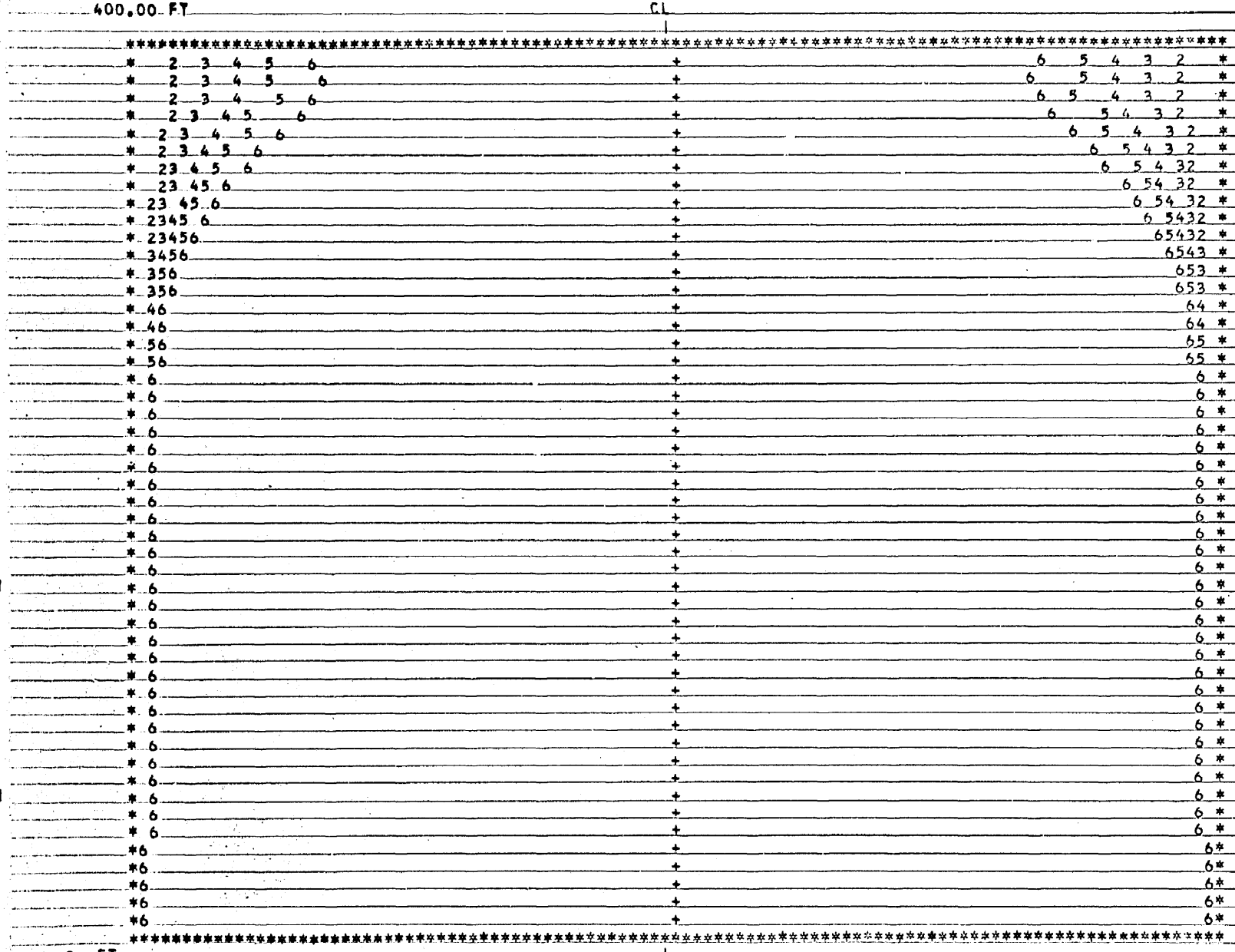
1-A	ACETYLENE	1.88742E-06	1.56755E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	2.79039E-07	2.31749E-02
5-E	ETHANE	5.06610E-04	4.20753E 01
6-F	ETHYLENE	1.04224E-03	8.65607E 01
7-G	HYDROGEN	1.03460E-03	8.59261E 01
8-H	METHANE	3.20098E-05	2.65849E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	8.49430E-04	7.05473E 01
12-L	CARBON	2.84832E-08	0.00000E-01
13-M	CARBON MONOXIDE	3.63621E-09	3.01996E-04

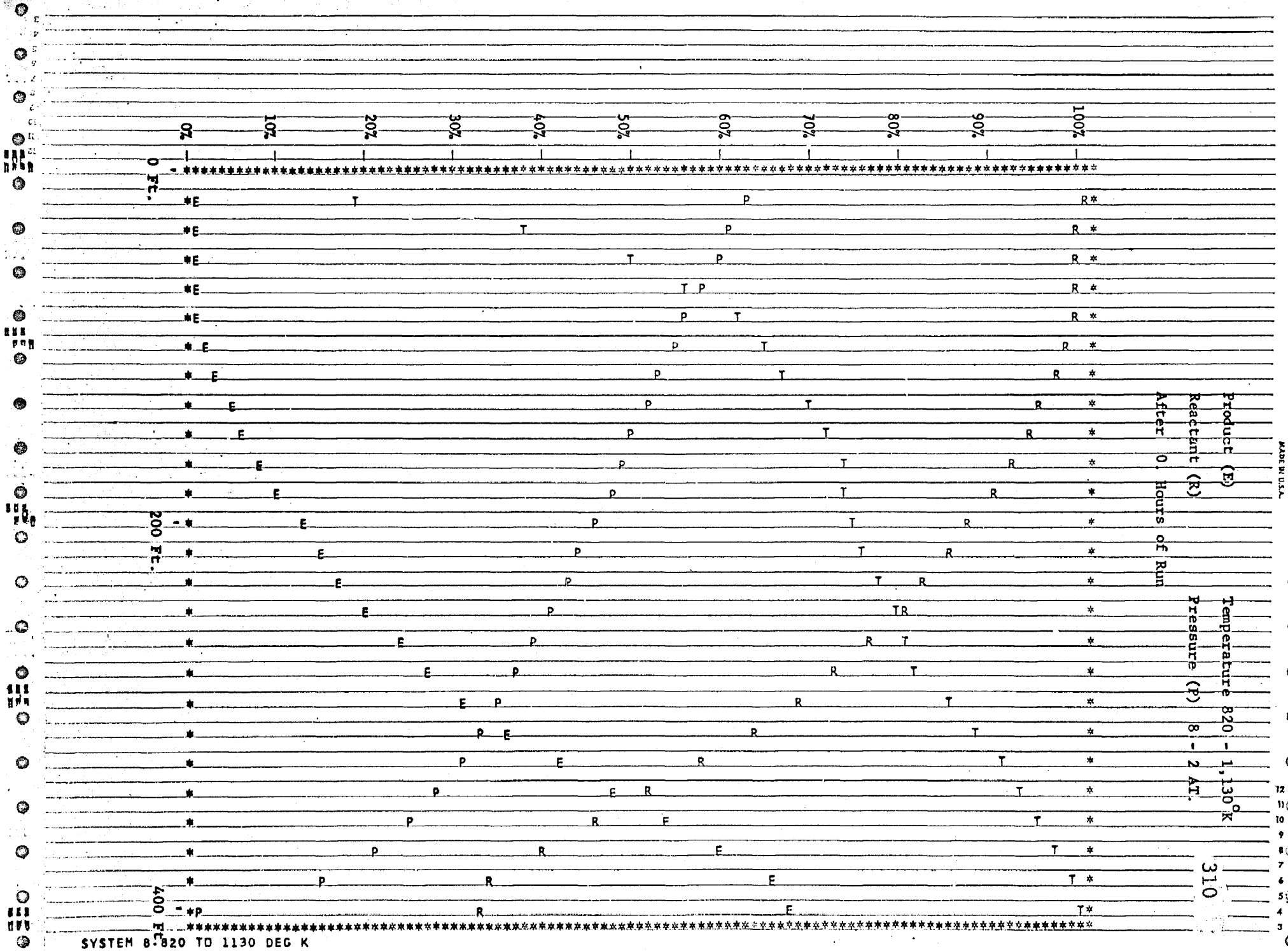
CONVERSION OF ETHANE TO ETHYLENE IS 66.62%

System 6—820 to 1,120°K

CONVERSION OF Ethane to Ethylene Time Increment - 30 Hours

400.00 FT




0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 0 Hours of Run
Temperature 820 - 1,130°K
Pressure (P) 8 - 2 AT.
310
SYSTEM 8.820 TO 1130 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 0.HOURS OF RUN

SYSTEM 8 820 TO 1130 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.13314E 01(1129.65, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.52056E-01(1129.65, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.19939E 02(1129.65, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12433E-08(1129.65, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41613E 01(1129.65, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.17111E 01(1129.65, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23561E 00(1129.65, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23789E-02(1129.65, 8)

FUNCTION PRR(IS)
PR= 5.84999E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.93554E 05 VIS= 2.72921E-05 DEN= 9.84756E-02
FRICTION FACTOR= 1.27033E-02 V1,V2,VA= 8.71775E 02 4.44210E 02 6.58005E 02
TEMPERTURE= 1129.65PRESSURE D= 3.87296E-01

1-A	ACETYLENE	1.05678E-06	1.61268E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	7.79846E-08	1.19006E-02
5-E	ETHANE	2.72974E-04	4.16566E 01
6-F	ETHYLENE	5.71635E-04	8.72330E 01
7-G	HYDROGEN	5.67819E-04	8.66507E 01
8-H	METHANE	1.62171E-05	2.47477E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	4.62869E-04	7.06350E 01
12-L	CARBON	2.37100E-08	0.00000E-01
13-M	CARBON MONOXIDE	1.44325E-09	2.20243E-04

CONVERSION OF ETHANE TO ETHYLENE IS 67.13%

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 20. Hours of Run
Temperature 820 - 1,130°K (T)
Pressure (P) 8 - 2 AT.
313
SYSTEM 8 820 TO 1130 DE

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 20.HOURS OF RUN

SYSTEM 8 820 TO 1130 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.13301E 01(1129.82, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.52101E-01(1129.82, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.19864E 02(1129.82, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12432E-08(1129.82, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41608E 01(1129.82, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.17140E 01(1129.82, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23553E 00(1129.82, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23801E-02(1129.82, 8)

FUNCTION PRR(IS)
FR= 6.04998E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.95313E 05 VIS= 2.72952E-05 DEN= 1.02186E-01
FRICTION FACTOR= 1.26966E-02 V1,V2,VA= 8.65936E 02 4.86969E 02 6.76450E 02
TEMPERTURE= 1129.82PRESSURE D= 3.59632E-01

1-A	ACETYLENE	1.29185E-06	1.73119E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	1.08193E-07	1.44989E-02
5-E	ETHANE	2.89946E-04	3.88553E 01
6-F	ETHYLENE	6.71100E-04	8.99332E 01
7-G	HYDROGEN	6.67016E-04	8.93860E 01
8-H	METHANE	1.91202E-05	2.56228E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	5.27161E-04	7.06442E 01
12-L	CARBON	2.89197E-08	0.00000E-01
13-M	CARBON MONOXIDE	1.94351E-09	2.60447E-04

CONVERSION OF ETHANE TO ETHYLENE IS 69.21%

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
Temperature (T) 820 - 1,130° K
Pressure 8 - 2 AT.
After 40. Hours of Run
315
SYSTEM 8 820 TO 1130 DEG K

SYSTEM 8 820 TO 1130 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 40.HOURS OF RUN

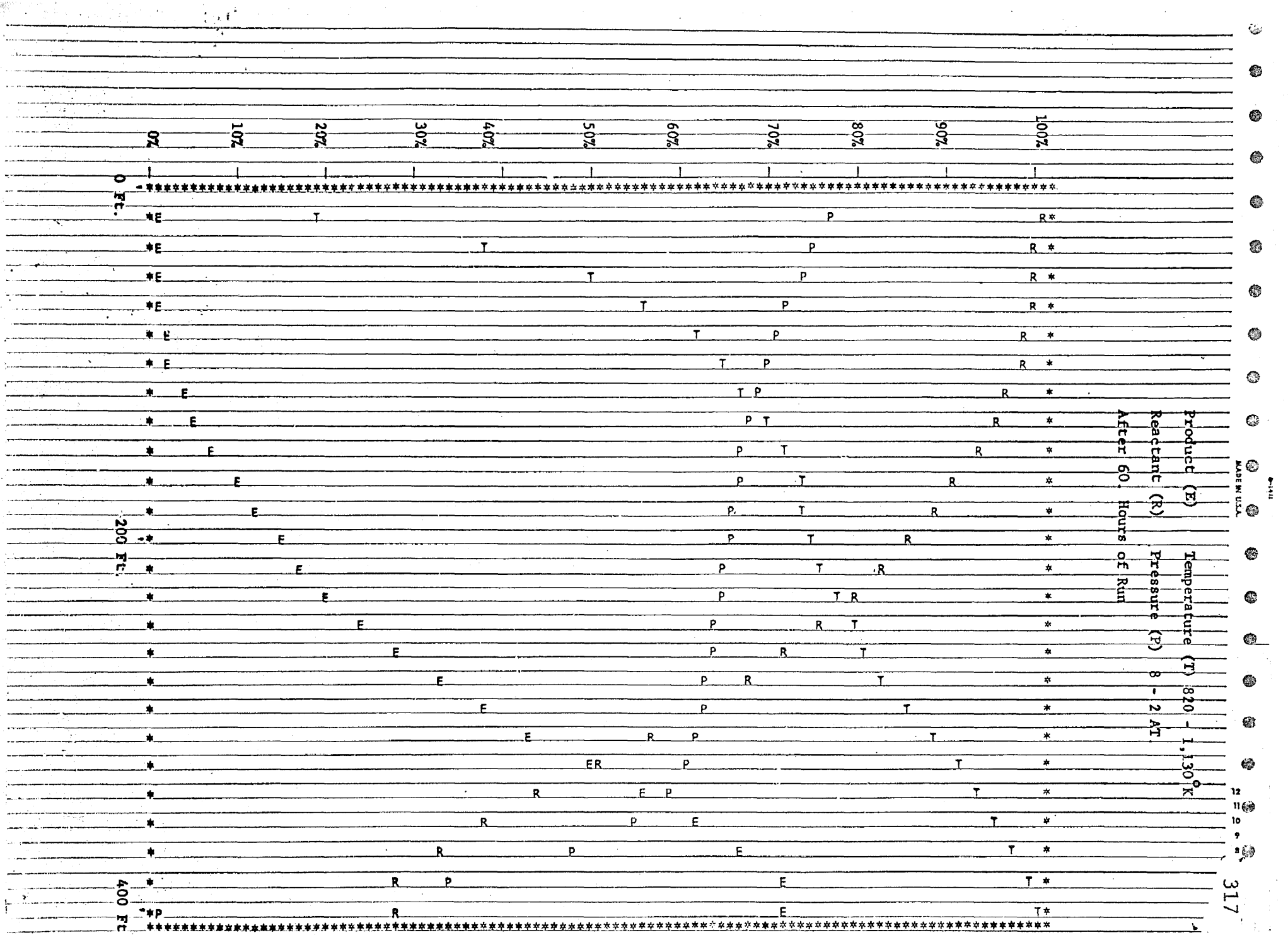
SYSTEM 8 820 TO 1130 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.13290E 01(1129.97, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.52141E-01(1129.97, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.19799E 02(1129.97, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12431E-08(1129.97, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41604E 01(1129.97, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.17166E 01(1129.97, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23546E 00(1129.97, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23811E-02(1129.97, 8)

FUNCTION PRR(IS)
PR= 6.24997E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 6.43134E 05 VIS= 2.72979E-05 DEN= 1.04751E-01
FRICTION FACTOR= 1.25233E-02 V1,V2,VA= 9.78020E 02 5.55756E 02 7.66881E 02
TEMPERTURE= 1129.97PRESSURE D= 4.63412E-01

1-A	ACETYLENE	1.35765E-06	1.76994E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	1.19764E-07	1.56134E-02
5-E	ETHANE	2.91053E-04	3.79440E 01
6-F	ETHYLENE	6.96474E-04	9.07978E 01
7-G	HYDROGEN	6.92330E-04	9.02576E 01
8-H	METHANE	1.99850E-05	2.60541E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	5.41815E-04	7.06355E 01
12-L	CARBON	2.63970E-08	0.00000E-01
13-M	CARBON MONOXIDE	2.07637E-09	2.70692E-04

CONVERSION OF ETHANE TO ETHYLENE IS 69.88%



317

SYSTEM 8 820 TO 1130 DEG K

SYSTEM 8 820 TO 1130 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 60.HOURS OF RUN

SYSTEM 8 820 TO 1130 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.13312E 01(1129.67, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.52061E-01(1129.67, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.19929E 02(1129.67, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12433E-08(1129.67, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41613E 01(1129.67, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.17114E 01(1129.67, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23560E 00(1129.67, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23791E-02(1129.67, 8)

FUNCTION PRR(IS)
PR= 6.64997E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 6.83693E 05 VIS= 2.72925E-05 DEN= 1.11424E-01
FRICTION FACTOR= 1.23891E-02 V1,V2,VA= 1.05074E 03 6.49466E 02 8.50081E 02
TEMPERTURE= 1129.67PRESSURE D= 5.00304E-01

1-A	ACETYLENE	1.67021E-06	1.89261E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	1.72698E-07	1.95693E-02
5-E	ETHANE	3.10223E-04	3.51531E 01
6-F	ETHYLENE	8.24950E-04	9.34795E 01
7-G	HYDROGEN	8.20531E-04	9.29787E 01
8-H	METHANE	2.39291E-05	2.71154E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	6.23476E-04	7.06494E 01
12-L	CARBON	3.16117E-08	0.00000E-01
13-M	CARBON MONOXIDE	3.01506E-09	3.41653E-04

CONVERSION OF ETHANE TO ETHYLENE IS 71.94%

Product (E)
Reactant (R)
After 80. Hours of Run
Temperature (T) 820 - 1,130°K
Pressure (P) 8 - 2 AT.
319
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
SYSTEM 8 820 TO 1130 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 80.HOURS OF RUN

SYSTEM 8 820 TO 1130 DEG. K

FUNCTION REQC(T,I)
REQC(T,I)= 0.13292E 01(1129.94, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.52134E-01(1129.94, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.19810E 02(1129.94, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12431E-08(1129.94, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41605E 01(1129.94, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.17162E 01(1129.94, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23547E 00(1129.94, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23809E-02(1129.94, 8)

FUNCTION PRR(IS)
PR= 7.44996E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 7.35213E 05 VIS= 2.72974E-05 DEN= 1.25442E-01
FRICTION FACTOR= 1.22331E-02 V1,V2,VA= 1.09030E 03 7.50084E 02 9.20201E 02
TEMPERTURE= 1129.94PRESSURE D= 4.85847E-01

1-A	ACETYLENE	2.35869E-06	2.15433E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	3.04831E-07	2.78419E-02
5-E	ETHANE	3.24966E-04	2.96810E 01
6-F	ETHYLENE	1.08120E-03	9.87522E 01
7-G	HYDROGEN	1.07696E-03	9.83651E 01
8-H	METHANE	3.18725E-05	2.91110E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	7.73853E-04	7.06805E 01
12-L	CARBON	4.26280E-08	0.00000E-01
13-M	CARBON MONOXIDE	5.46271E-09	4.98941E-04

CONVERSION OF ETHANE TO ETHYLENE IS 76.00%

System 8 820 to 1,130°K

```
CONVERSION OF  Ethane to Ethylene     Time Increment  - 10 Hours
     400.00 FT                                            CL
                                                           |
        *******************************************************************************************************
        *  23 4 5 6 7 8  9                                 +                                 9  8 7 6 5 4 32  *
        *  23 4 5 6 7 8  9                                 +                                 9  8 7 6 5 4 32  *
        *  23 45 6 7 8  9                                  +                                  9  8 7 6 54 32  *
        *  234 56 7 8  9                                   +                                   9  8 7 65 432  *
        *  2345 67  8 9                                    +                                    9 8  76 5432  *
        * 234 567 8 9                                      +                                      9 8 765 432 *
        * 23456 78 9                                       +                                       9 87 65432 *
        * 235 6789                                         +                                         9876 532 *
        * 2456789                                          +                                          9876542 *
        * 346789                                           +                                           987643 *
        * 35689                                            +                                            98653 *
        * 3679                                             +                                             9763 *
        * 4789                                             +                                             9874 *
        * 589                                              +                                              985 *
        * 69                                               +                                               96 *
        * 79                                               +                                               97 *
        * 89                                               +                                               98 *
        * 89                                               +                                               98 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        * 9                                                +                                                9 *
        *39                                                +                                                93*
        *9                                                 +                                                 9*
        *9                                                 +                                                 9*
        *9                                                 +                                                 9*
        *9                                                 +                                                 9*
        *9                                                 +                                                 9*
        *******************************************************************************************************
  0. FT                                                    |
                                                          CL
```

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 0 Hours of Run
Temperature (T) 820 - 1,140°K
Pressure (P) 8 - 2 AT.
322
SYSTEM 9 820 TO 1140 DEG K

SYSTEM 9 820 TO 1140 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 0.HOURS OF RUN

SYSTEM 9 820 TO 1140 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.12588E-01(1139.97, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.54862E-01(1139.97, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.15918E 02(1139.97, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12364E-08(1139.97, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41311E 01(1139.97, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.18999E 01(1139.97, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23059E 00(1139.97, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24499E-02(1139.97, 8)

FUNCTION PRR(IS)
PR= 5.84999E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.71734E 05 VIS= 2.74785E-05 DEN= 9.82519E-02
FRICTION FACTOR= 1.27890E-02 V1,V2,VA= 8.10474E 02 4.68698E 02 6.39595E 02
TEMPERTURE= 1139.97PRESSURE D= 3.09964E-01

1-A	ACETYLENE	1.75562E-06	2.50507E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	1.28877E-07	1.83893E-02
5-E	ETHANE	1.71303E-04	2.44429E 01
6-F	ETHYLENE	7.29314E-04	1.04065E 02
7-G	HYDROGEN	7.28052E-04	1.03885E 02
8-H	METHANE	2.00016E-05	2.85400E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	4.95805E-04	7.07456E 01
12-L	CARBON	2.68196E-08	0.00000E-01
13-M	CARBON MONOXIDE	2.68757E-09	3.83485E-04

CONVERSION OF ETHANE TO ETHYLENE IS 80.09%

SYSTEM 9 820 TO 1140 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 10.HOURS OF RUN

SYSTEM 9 820 TO 1140 DEG K

FUNCTION REQC(T,I)
REQC(T,I)= 0.12591E 01(1139.92, 1)
FUNCTION REQC(T,I)
REQC(T,I)= 0.54851E-01(1139.92, 2)
FUNCTION REQC(T,I)
REQC(T,I)= 0.15933E 02(1139.92, 3)
FUNCTION REQC(T,I)
REQC(T,I)= 0.12364E-08(1139.92, 4)
FUNCTION REQC(T,I)
REQC(T,I)= 0.41312E 01(1139.92, 5)
FUNCTION REQC(T,I)
REQC(T,I)= 0.18991E 01(1139.92, 6)
FUNCTION REQC(T,I)
REQC(T,I)= 0.23061E 00(1139.92, 7)
FUNCTION REQC(T,I)
REQC(T,I)= 0.24496E-02(1139.92, 8)

FUNCTION PRR(IS)
PR= 6.04998E 00 RADI(1)= 1.25000E-01 VOL= 0.00000E-01
FUNCTION PRESD(T)
RENU= 5.89074E 05 VIS= 2.74777E-05 DEN= 1.01651E-01
FRICTION FACTOR= 1.27206E-02 V1,V2,VA= 8.42546E 02 5.23113E 02 6.82828E 02
TEMPERTURE= 1139.92PRESSURE D= 3.16652E-01

1-A	ACETYLENE	2.01457E-06	2.59881E-01
2-B	ISO BUTANE	0.00000E-01	0.00000E-01
3-C	N-BUTANE	0.00000E-01	0.00000E-01
4-D	ISO-BUTENE	1.63693E-07	2.11164E-02
5-E	ETHANE	1.77148E-04	2.28523E 01
6-F	ETHYLENE	8.18407E-04	1.05575E 02
7-G	HYDROGEN	8.17481E-04	1.05455E 02
8-H	METHANE	2.25896E-05	2.91407E 00
9-I	PROPANE	0.00000E-01	0.00000E-01
10-J	PROPENE	0.00000E-01	0.00000E-01
11-K	WATER	5.48320E-04	7.07337E 01
12-L	CARBON	2.94898E-08	0.00000E-01
13-M	CARBON MONOXIDE	3.30073E-09	4.25796E-04

CONVERSION OF ETHANE TO ETHYLENE IS 81.25%

SYSTEM 9 820 TO 1140 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 30.HOURS OF RUN

SYSTEM 9 820 TO 1140 DEG K

```
 FUNCTION REQC(T,I)
REQC(T,I)=   0.12587E 01(1139.99, 1)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.54869E-01(1139.99, 2)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.15910E 02(1139.99, 3)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.12364E-08(1139.99, 4)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.41310E 01(1139.99, 5)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.19004E 01(1139.99, 6)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.23058E 00(1139.99, 7)
 FUNCTION REQC(T,I)
REQC(T,I)=   0.24501E-02(1139.99, 8)

  FUNCTION PRR(IS)
PR=   6.64927E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
RENU=   6.76480E 05     VIS=   2.74789E-05     DEN=   1.10855E-01
FRICTION FACTOR=    1.24122E-02     V1,V2,VA=   1.01716E 03      6.77111E 02      8.47114E 02
TEMPERTURE= 1139.99PRESSURE D=   4.47788E-01
  1-A  ACETYLENE              2.46985E-06      2.76317E-01
  2-B  ISO BUTANE             0.00000E-01      0.00000E-01
  3-C  N-BUTANE               0.00000E-01      0.00000E-01
  4-D  ISO-BUTENE             2.37965E-07      2.66226E-02
  5-E  ETHANE                 1.79596E-04      2.00925E 01
  6-F  ETHYLENE               9.66924E-04      1.08176E 02
  7-G  HYDROGEN               9.66943E-04      1.08178E 02
  8-H  METHANE                2.71818E-05      3.04100E 00
  9-I  PROPANE                0.00000E-01      0.00000E-01
 10-J  PROPENE                0.00000E-01      0.00000E-01
 11-K  WATER                  6.32064E-04      7.07129E 01
 12-L  CARBON                 2.93477E-08      0.00000E-01
 13-M  CARBON MONOXIDE        4.63480E-09      5.18525E-04

CONVERSION OF ETHANE              TO  ETHYLENE          IS 83.25%
```

0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
0 Ft.
200 Ft.
400 Ft.
Product (E)
Reactant (R)
After 40. Hours of Run
Temperature (T) 820 - 1140°K
Pressure (P) 8 - 2 AT.
SYSTEM 9 820 TO 1140 DEG K
REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 40. HOURS OF RUN

SYSTEM 9 820 TO 1140 DEG K

```
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.12591E 01(1139,93, 1)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.54853E-01(1139,93, 2)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.15931E 02(1139,93, 3)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.12364E-08(1139,93, 4)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.41312E 01(1139,93, 5)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.16992E 01(1139,93, 6)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.23061E 00(1139,93, 7)
 FUNCTION REQC(T,I)
 REQC(T,I)=   0.24496E-02(1139,93, 8)

  FUNCTION PRR(IS)
 PR=   7.24926E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
 FUNCTION PRESD(T)
 RENU=   7.42135E 05      VIS=   2.74778E-05      DEN=   1.20414E-01
 FRICTION FACTOR=   1.22133E-02      V1,V2,VA=   1.12288E 03      7.81735E 02      9.52323E 02
 TEMPERTURE= 1139.93PRESSURE 0=   5.39792E-01
  1-A  ACETYLENE          2.93686E-06      2.92000E-01
  2-B  ISO BUTANE         0.00000E-01      0.00000E-01
  3-C  N-BUTANE           0.00000E-01      0.00000E-01
  4-D  ISO-BUTENE         3.25328E-07      3.23460E-02
  5-E  ETHANE             1.77117E-04      1.76100E 01
  6-F  ETHYLENE           1.11169E-03      1.10531E 02
  7-G  HYDROGEN           1.11313E-03      1.10674E 02
  8-H  METHANE            3.17107E-05      3.15287E 00
  9-I  PROPANE            0.00000E-01      0.00000E-01
 10-J  PROPENE            0.00000E-01      0.00000E-01
 11-K  WATER              7.11395E-04      7.07310E 01
 12-L  CARBON             3.09526E-06      0.00000E-01
 13-M  CARBON MONOXIDE    6.45205E-09      6.41501E-04

 CONVERSION OF ETHANE          TO  ETHYLENE          IS 85.06%
```

SYSTEM 9 820 TO 1140 DEG K

REACTOR PRODUCT (E) REACTANT(R) TEMPERATURE(T) PRESSURE(P) AFTER 45.HOURS OF RUN

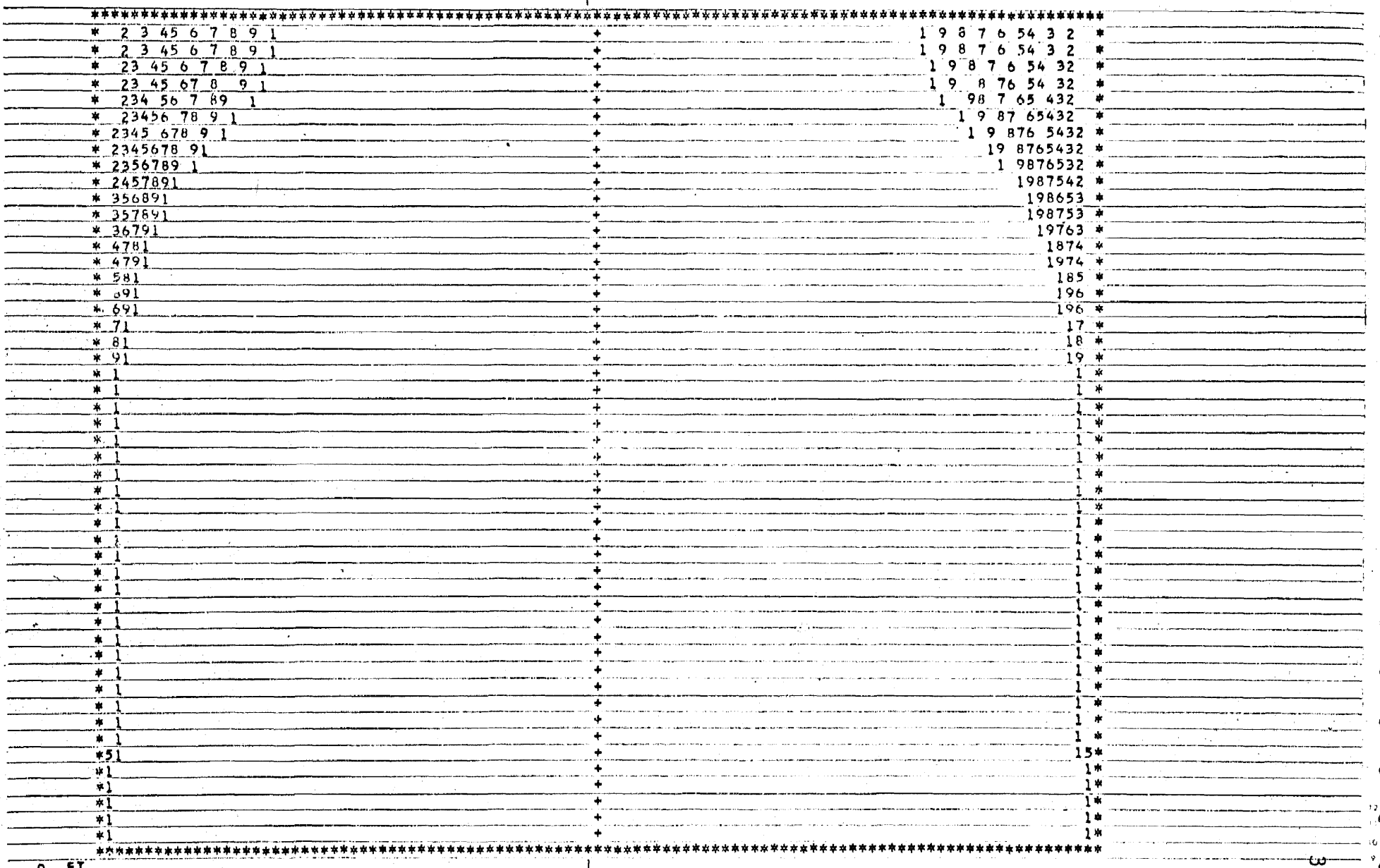
SYSTEM 9 820 TO 1140 DEG K

```
FUNCTION REQC(T,I)
REQC(T,I)=   0.12587E 01(1139.98, 1)
FUNCTION REQC(T,I)
REQC(T,I)=   0.54868E-01(1139.98, 2)
FUNCTION REQC(T,I)
REQC(T,I)=   0.15913E 02(1139.98, 3)
FUNCTION REQC(T,I)
REQC(T,I)=   0.12364E-08(1139.98, 4)
FUNCTION REQC(T,I)
REQC(T,I)=   0.41311E 01(1139.98, 5)
FUNCTION REQC(T,I)
REQC(T,I)=   0.19002E 01(1139.98, 6)
FUNCTION REQC(T,I)
REQC(T,I)=   0.23058E 00(1139.98, 7)
FUNCTION REQC(T,I)
REQC(T,I)=   0.24500E-02(1139.98, 8)

 FUNCTION PRR(IS)
PR=   7.84925E 00      RADI(1)=   1.25000E-01      VOL=   0.00000E-01
FUNCTION PRESD(T)
RENU=   7.56376E 05      VIS=   2.74787E-05      DEN=   1.31628E-01
FRICTION FACTOR=    1.21732E-02      V1,V2,VA=   1.08204E 03      8.16480E 02      9.49272E 02
TEMPERTURE= 1139.98PRESSURE D=   4.39163E-01
 1-A  ACETYLENE                3.71278E-06      3.11269E-01
 2-B  ISO BUTANE               0.00000E-01      0.00000E-01
 3-C  N-BUTANE                 0.00000E-01      0.00000E-01
 4-D  ISO-BUTENE               4.78404E-07      4.01081E-02
 5-E  ETHANE                   1.77037E-04      1.48423E 01
 6-F  ETHYLENE                 1.34991E-03      1.13173E 02
 7-G  HYDROGEN                 1.35403E-03      1.13518E 02
 8-H  METHANE                  3.89664E-05      3.26684E 00
 9-I  PROPANE                  0.00000E-01      0.00000E-01
10-J  PROPENE                  0.00000E-01      0.00000E-01
11-K  WATER                    8.43966E-04      7.07558E 01
12-L  CARBON                   4.22950E-08      0.00000E-01
13-M  CARBON MONOXIDE          9.58926E-09      8.03938E-04

CONVERSION OF ETHANE              TO  ETHYLENE          IS 87.10%
```

REACTOR RADIUS PROFILE FROM START TO CLOSE DOWN — Conversion of Ethane to Ethylene — Time Increment = 5 Hours

400.00 FT

CL



0. FT

CL

Appendix H

Explanation of How to Use PYRO

A. Data

The data given on the last two pages of this appendix shows the entire input of PYRO. It is best to break the data into card sets. This procedure simplifies the understanding of the data. It is also a great aid in setting up different data sets.

B. The reaction system chosen to prove this program was the pyrolysis of ethane. Six independent equations were set up with a combined total of 13 components and interts.

The six equations were: (48)

		Order Forward	Order Reverse
(1)	$C_2H_6 \rightarrow C_2H_4 + H_2$	1	1-1
(2)	$C_2H_6 \rightarrow CH_4 + \frac{1}{2}C_2H_4$	1	1-1
(3)	$C_2H_4 \rightarrow C_2H_2 + H_2$	1	1-1
(4)	$C_2H_2 \rightarrow 2C + H_2$	2	1-1
(5)	$2C_2H_2 \rightarrow C_4H_4$ (i.e.) C_4	1	1
(6)	$C + H_2O \rightarrow CO + H_2$	1-0	1-1

A number designation was arbitarily assigned to each

component. The computer assigned the letter designation.

1.	$CH \equiv CH$	Acetylene	(A)
2.	$CH_3(CH_3)CH\text{-}CH_3$	Iso-Butane	(B)
3.	$CH_4\text{-}(CH_2)_2\text{-}CH_4$	Butane	(C)
4.	$CH_3(CH_3)C{=}CH_2$	Iso-Butene	(D)
5.	$CH_3\text{-}CH_3$	Ethane	(E)
6.	$CH_2{=}CH_2$	Ethene	(F)
7.	H_2	Hydrogen	(G)
8.	CH_4	Methane	(H)
9.	$CH_3\text{-}CH_2\text{-}CH_3$	Propane	(I)
10.	$CH_2{=}CH\text{-}CH_3$	Propene	(J)
11.	H_2O	Water	(K)
12.	C	Carbon	(L)
13.	CO	Carbon Monoxide	(M)

The six equations were rewritten using the following conventions:

A value was assigned to IA corresponding to the value assigned to the component for each position in each equation (i.e.) in Equation 1.

$$\underset{(5)}{C_2H_6} \longrightarrow \underset{(6)}{C_2H_4} + \underset{(7)}{H_2}$$

Therefore

IA(1,1)=5 IA(1,2)=6 IA(1,3)=7

Using this system, it was possible to set up values for each of the equations with the restriction of 10 components per equation and 25 equations and 25 components per system.

The coefficient of each equation was read in in a similar manner:

Equation 1.

$$\underset{(1)}{C_2H_6} \longrightarrow \underset{(1)}{C_2H_4} + \underset{(1)}{H_2}$$

B(1,1)=1 B(1,2)=1 B(1,3)=1

or

Equation 5.

$$2C_2H_2 \longrightarrow C_4H_4$$
(2) (1)

B(5,1)=2 B(5,2)=1

The order of reaction of each component was read in in a similar manner:

Reaction 4.

$$C_2H_2^{\ 2} \longrightarrow 2C^1 + H_2^{\ 1}$$

BB(4,1)=2 BB(4,2)=1 BB(4,3)=1

If an equation is irreversible the most probably value was assigned to BB).

In all of the above examples, several things became apparent.

The first subscription in each subscripted variable referred to the equation number. The second subscript referred to the position in the equation. There was no need to fill blanks for positions or equations not used.

It was now necessary to tell the computer which components were reactants and which were products. This was done by counting the total number of each and reporting the results.

(i.e.) SF(1)=1 SR(1)=2

SF(5)=1 SR(5)=1

SF(6)=2 SR(6)=2

The first equation had one forward and two reverse components. The fifth had one each. The sixth had two each etc.

The foregoing conventions were used to set up the card sets used in PYRO.

Card Set 1 (Cards 1-2) Read (5,935),ID,F(ID) Format (I2,E8.0) Any changes in the Arrhenius Frequency Factor were made here. The factor F(I) was assumed to be (1.) unless a different value was found here. The changes were multiplied by the existing Arrhenius factor. The computer continued to read values until the 25th value was read in. The first variable was I and referred to the factor in which change was desired. The second value was the factor itself. The last card in this set had to contain a value of ID equal to 25 whether or not 25 equations were employed or the 25 equations remained unchanged. If either of these latter were the case, the following was used:

25 1.00E 00.

Card Set 2 (Card 3) Read (5,900)IR,IS Format (2I2)

This card set read in IR total number of reactants and and IS, the total number of chemical compounds and inerts.

Card Set 3 (4-6 cards) This card set read in the

temperature profile and instructions on the size of the time increment and total number of increments used in carbon deposition and instructions on how data was presented.

(Card 4) Read (5,943)IGOW,(Z(II),II=1,II) Format (I3,11F7.0)

IGOW was a computer internal control.

If: IGOW = 1 computer disregarded this data set and read in new data set.

IGOW = 2 computer continued on this data set.

IGOW = 3 computer stopped.

Z was the temperature taken at 10% intervals along the reactor length (there were a total of eleven values since both 0% and 100% values were included.)

(Card 5) Read (5,950) Card Format (80A1)

This card was used to identify the temperature profile. Any valid punch could have been used. This card was printed at the top of each new page.

(Card 6) Read (5,958)IB,IZZ,IPLOT

IB = number of hours comprising increment of carbon deposition.

IZZ = total number of increment before force out i.e. computer goes to new case.

IPLOT = 1	Plot results	Do not write out detailed calculation
IPLOT = 2	Plot results	Write out detailed calculation
IPLOT = 3	Do not plot results	Write out detailed calculation
IPLOT = 4	Do not plot results	Do not write out detailed calculation

Card Set 4 (Card 6) Read (5,919)T,PT,PRES,ZT,DL,POUT FORMAT (6E12.5).

T was the intial temperature at reactor inlet (^{o}K).

PT was the intial total pressure of all components (in atmospheres).

ZT was the total length of reactor (in feet).

DL was the intial reactor increment (in feet).

POUT was the minimum pressure at the outlet of the reactor (in atmospheres).

Card Set 5 (Card 8) Read (5,901) (SF(I),SR(I),I=1,IR) FORMAT (40I2)

SF(I) was the total number of reactants in equation I.

SR(I) was the total number of products in equation I.

Up to 20 reactions were read in per card.

Card Set 6 (Card 9-16) Read (5,901)ID,(IA(I,M)M=1,IT) FORMAT (40I2)

IA(IM) was the identification by position of each component.

The value of IT was equal to SF(I) + SR(I) (i.e.) the total number of reactants and products in the reaction (I). Only one equation was read per card.

ID was an identity check. It had to have the same value as the internally generated value of I or the program would stop after writing an appropriate error message.

Card Set 7 Read (5,903)ID,(B(I,M),M=1,IT),(BB(I,M) M=1,IT) Only values from one equation were read per card.

ID and IT were the same as in Card Set 6.

B(I,M) was the coefficient of the component in the Ith equation Mth position.

BB(I,M) was the order of reaction of the components of the Ith equation Mth position.

Card Set 8 Read (5,904)(C(J),J=1,IS) Cards (25-28) FORMAT (12F6.5)

C(J) was the partial pressure of component (J). The sum IS

C(J) had to equal PT. C(J) was in atmospheres. 12
J=1

values were read per card.

Card Set 9 (Cards 27 - 30) Read (5,905)(ENAME(J)J=1,IT) FORMAT (80A1)

ENAME(20*1) was the alphanumeric identification of each component IT=20*IS.

Any valid punch was acceptable. 20 spaces were allowed per identification. All unfilled spaces had to contain blanks. Four identifications were contained on a card.

Card Set 10 Cards (31 - 43) Read (5,906)(CP(J,M),M=1,4) ID Cards (31 - 43) FORMAT (4E16,8,17)

CP(J,M) was the heat capacity data for the Jth component of the form $CP(J)=CP(J,1)+CP(J,2)*T+CP(J,3)*T^2+CP(J,4)*T^3$

One card per component was read.

ID had to be equal to J or an error message was generated and the computer program was stopped.

The data used for heat capacity was generated by a second computer program Marquardt Non-Linear Regression Analysis adapted by the author and given in Appendix H of this study.

Card Set 11 (Cards 44 - 51) FORMAT (I2,E7.1,FI).4) Read (5,901)ID,EA(I),EE(I)

EA(I) was the Arrhenius Frequency Factor for the Ith equation.

EE(I) was the Arrhenius Activation Energy of the Ith equation. (23) (29) (33) (46) (55)

ID had to equal J or the program was stopped and the appropriate error message was printed.

Card Set 12 (Cards 52 - 64) Read (5,908)ID,DS,(J), DH(J),DF(J) FORMAT (I2,3F9.2)

ID (See Card Set (6))

DS(J) was the entropy of the Jth component BTU/lb mole $^{o}_{K}$(22).

DH(J) was the enthalpy of the Jth component BTU/lb mole $^{o}_{K}$

DF(J) was the Log (K_f) of the Jth component(44)

The data for each component was on a different card.

Card Set 13 (Cards 65 - 78) Read (5,911)ID,(CLJ(J,M), M=1,2),SMWT(J) If (CLJ(J,2).EQ.0) Read (5,940)DE(J)911 FORMAT(I2,3X3F5.2) 940 FORMAT(F10.0)

ID (see Card Set (6))

CLJ(J,1) was the constant of Lennard and Jones collision parameter (7).

CLJ(J,2) was the constant of Lennard and Jones /K (^{o}K)

SMWT(J) was the molecular weight of the Jth component.

DP(J) If the component was a solid under reaction conditions, the constants of Lennard and Jones were equal to zero and DE(J), the density of the component, was read in as the next card (lbs/ft^3). There was one card per gas component and two cards per solid component.

Card Set 14 Read (5,908)IJ,TT,FI(I) Cards (79 - 86) FORMAT (I2,3F9.2)

IJ was the same as ID (See Card Set (6))

TT was the temperature (^{o}K) at which the equilibrium constant (K_C) was known.

PI(I) was the equilibrium constant K_C for the Ith equation[48]. There was one card per equation.

Card Set 15 (Card 87) Read (5,902)RAD,TMPH FORMAT (2F10.5)

RAD was the radius of the reactor in feet.

TMPH was the total molar flow at the beginning of the reaction in pound moles per hour.

Card Set 16 (Card 89) Read (5,909) KEYR, KEYP FORMAT (2I2)

KEYR was the component number of the key reactant.

KEYP was the component number of the key product.

Card Set 17 (Cards 89 - 91) This card set was the same as Card Set (3). This card set could be repeated for as many new temperature profiles as desired. All other constants remained fixed at initial values.

```
Card Set 1   41.00E 02                                                                                                    1
             251.00E 00                                                                                                   2
Card Set 2   0813                                                                                                         3
Card Set 3   007 820.  970.  1020.  1045.  1060.  1067.  1080.  1090.  1105.  1125.  1140.                               4
             SYSTEM 9 820 TO 1140 DEG K                                                                                   5
             10 10  1                                                                                                     6
Card Set 4      820.E 00     4.0E 00     8.00E 00   400. E 00   .5000E 00   2.000E 00                                  7
Card Set 5   0102010201020102010201020201020102                                                                           8
Card Set 6   01 5 6 7                                                                                                     9
              2 5 8 6                                                                                                     10
             03060107                                                                                                     11
              4 112 7                                                                                                     12
              5 6 4                                                                                                       13
             06111213 07                                                                                                  14
              7 910 7                                                                                                     15
              8 9 8 6                                                                                                     16
Card Set 7   01 1. 1. 1. 1. 1. 1.                                                                                         17
             02 2. 2. 1. 1. 1. .5                                                                                         18
             03 1. 1. 1. 1. 1. 1.                                                                                         19
             04 1. 2. 1. 1. 1. 1.                                                                                         20
             05 2. 1. 2. 1.                                                                                               21
             06 1. 1. 1. 1. 0. 1. 1. 1.                                                                                   22
             07 1. 1. 1. 1. 1. 1.                                                                                         23
             08 1. 1. 1. 1. 1. 1.                                                                                         24
Card Set 8   0.     0.     .00   0.    3.80630.0   0.0   0.0   0.0   0.0   2.0490.0                                     25
             0.0                                                                                                          26
Card Set 9   ACETYLENE              ISO BUTANE             N-BUTANE               ISO-BUTENE                           27
             ETHANE                 ETHYLENE               HYDROGEN               METHANE                              28
             PROPANE                PROPENE                WATER                  CARBON                               29
             CARBON MONOXIDE                                                                                             30
Card Set 10   0.586720 09E 01  0.19574307E-01 -0.12957129E-04  0.34664522E-08  00001                                    31
             -0.190091 09E 01  0.99299729E-01 -0.54748874E-04  0.11818035E-07  00002                                    32
              0.911440 75E-01  0.92179775E-01 -0.47610869E-04  0.95772386E-08  00003                                    33
              0.709775 75E 00  0.82089603E-01 -0.45349472E-04  0.98367536E-08  00004                                    34
              0.906502 06E 00  0.44198409E-01 -0.18638693E-04  0.28561491E-08  00005                                    35
              0.984672 13E 00  0.37012149E-01 -0.19448082E-04  0.40415067E-08  00006                                    36
              0.700991 34E 01 -0.53663156E-03  0.10057875E-05 -0.24534463E-09  00007                                    37
              0.400967 72E 01  0.14933866E-01 -0.17271594E-06 -0.15927819E-08  00008                                    38
             -0.109255 67E 01  0.73140860E-01 -0.37875361E-04  0.76719720E-08  00009                                    39
              0.734198 42E 00  0.56630877E-01 -0.28379858E-04  0.55099498E-08  10                                       40
              0.771826 77E 01  0.12946531E-03  0.31513555E-05 -0.11503503E-08  00011                                    41
             -0.135590 93E 01  0.14472824E-01 -0.11009429E-04  0.30278435E-08  00012                                    42
              0.686305 62E 01 -0.40851929E-03  0.24804694E-05 -0.10177783E-08  00013                                    43
Card Set 11  016.04E16   67000.                                                                                         44
             02 1.6E12   67000.                                                                                         45
             03 1.8E13   76000.                                                                                         46
             04 9.7E10   67000.                                                                                         47
             05 2.6E13   60000.                                                                                         48
             069.255E3   21300.                                                                                         49
             07 2.9E13   63300.                                                                                         50
             08 3.2E13   63000.                                                                                         51
Card Set 12  01 47.997  54194.   -8.8738                                                                                52
             02 70.42   -31452.  -14.5973                                                                               53
             03 74.10   -29012.  -14.1427                                                                               54
             04 73.48   280.     -13.669                                                                                55
             05 54.85   -20236.  -5.7014                                                                                56
             06 52.45   12496.   -6.1738                                                                                57
             07 31.211  0.       0.                                                                                     58
             08 44.50   -17869.  -1.0075                                                                                59
             09 64.51   -24820.  -9.9839                                                                                60
```

```
10 63.80   4879.     -9.4909
11 45.106  -57797.9 10.05973
12 1.3069   0.        0.
13 47.301  -26415.7 10.47761
```

Card Set 13

```
01   4.221 185.26.04
02   5.341 313.58.12
03   5.333327.458.12
04   5.388314. 56.12
05   4.418 230.30.07
06   4.221 185.28.05
07   2.915 38. 2.016
08   3.822 137.16.04
09   5.061 254.44.09
10   4.757 281.42.08
11   3.216 499.18.02
12   0.0  0.0  12.00
135.
13   3.590 110.28.01
```

Card Set 14

```
1 800.    5.51
2 1000.   40.45
3 875.    .036
4 1000.   74.00000.
5 1000.   21643.
6 900.    33.8
7 1000.   3.196
8 900.    26.0
```

Card Set 15 .175 500.

Card Set 16 0506

Card Set 17 003 0.00E 00 0.0E 00 0.0E 00 0.0E 00

```
END OF JOB
```

```
$00 10 1
```

Appendix I

I Determination of Pipe Temperature on Outside Wall of Reactor

II Data Calculated by Computer

A. Equilibrium Constants

B. Enthalpy of Reaction BTU/Lb Mole ^{o}K

C. Heat Capacity BTU/Lb Mole ^{o}K

I Determination of Pipe Temperature on Outside Wall of Reactor Optimum Case Worst Conditions

A. Heat Flux due to Reaction

$$Q = \sum_{J=1}^{I=IR} \Delta H_{ri} \; -\Delta X_i \quad TMPH_{J_I} \qquad (1)$$

I or J	$TMPH_J$ LB moles / Hour	H_{ri} Cal / gm moles	J_i	$TMPHJ_I$ Gm moles / Hour	X_i Lb Moles / Lb Moles 46' Reactor	$(X_i)(TMPH)H_{ri}$ Cal / gm mole* Lb mole* Hour / Lb mole .464 ft.
1	.1165	12093	5	53.34	4.109E-3	2650.472
2	0	-14333	5	53.34	9.156E-5	-69.985
3	0	53024	6	75.51	1.83E-3	82.781
4	.0191	1492	2	.1165	5.237E-3	.910
5	53.34	1847	6	75.51	1.24E-7	.173
6	75.51	-27601	11	70.49	7.39E-9	-1.438
7	74.83	3391	9	0		0
8	2.26	-8277	9	0		0
9	0					
10	0					
11	70.44					
12	0					
13	$1.234X10^{-4}$					

$$\frac{Total*2662.838*Hours*1.8\ BTU}{.46\ Foot\ Reactor}$$

4793.01BTU/(Hours-.464 ft. reactor)

B. Heat Flux due to Heating

$$Q_{TR} \sum_{J=1}^{IS} (C_{P_J})(TMPH_J)(\Delta T/.464 \text{ ft. reactor}) \qquad (2)$$

373.9 ft. into reactor T was 1115.14°K

390.0 ft. into reactor T is 1121.24°K

$$\frac{\Delta T}{\Delta L} = \frac{1121.24-1115.14}{390.0-373.7} = \frac{6.10}{16.3} = \frac{.3742^{\circ}K}{\text{ft}} = \frac{.1736^{\circ}K \text{ temp. rise}}{.464 \text{ ft reactor}} \qquad (3)$$

J	CP_J BTU Lb Mole °R	$TMPH_J$ Lb Moles Hr	$TMPH_J$ CP_J T/.464 BTU/Hr/ .46 ft reactor
1	16.40	.1165	.5970
2	57.24	0	0
3	57.07	0	0
4	49.58	.091	.2959
5	31.04	53.34	517.398
6	23.72	75.51	559.72
7	7.33	74.83	171.41
8	18.28	2.26	12.91
9	44.41	0	0
10	36.30	0	0
11	10.20	70.44	224.68
12	5.29	0	0
13	8.09	1.234×10^{-4}	.00831
		TOTAL	487.01

Total heat flux = 4793.01 + 1487.01 = 6280.02 BTU/Hr. .464 ft. reactor)

$$\overline{C_P} = \frac{C_{PJ}TMPH_J}{TMPH_J} = \frac{17.83 \text{ BTU}}{\text{Lb Mole } ^{\circ}R} \quad (4)$$

$$\overline{MW} = \frac{MW_J TMPH_J}{TMPH_J} = \frac{18.74 \text{ Lb moles}}{\text{Lb}} \quad (5)$$

$$\text{Average heat capacity} = \frac{\overline{CP}}{\overline{MW}} = \frac{17.83}{18.74} = .9514 \frac{\text{BTU}}{\text{LB}^{\circ}R}$$

$$.9514 \frac{\text{BTU}}{\text{Lb}^{\circ}R} * \frac{1.8^{\circ}R}{^{\circ}K} = 1.713 \frac{\text{BTU}}{\text{Lb}^{\circ}K} \quad (6)$$

$$K = \left[C_P + \frac{5}{4}\frac{R}{M}\right] U \quad (6)$$

$$K = .9514 \frac{\text{BTU}}{\text{Lb}^{\circ}R} + \frac{\frac{1.987 \text{ BTU}}{1.25 * \text{Lb mole } ^{\circ}R}}{1.875 \text{Lb/Lb mole}} \quad 2.705 \text{ X } 10^{-5} \frac{\text{Lb}}{\text{ft sec}} * \frac{3600 \text{ sec}}{\text{hour}} \quad (7)$$

$$K = \frac{\text{BTU}}{.1055^{\circ}R \text{ hour ft}^2/\text{ft}} = \frac{\text{BTU}}{1900 \ ^{\circ}K \text{ hour ft}^2/\text{ft}} \quad (8)$$

$$Pr_N = \frac{C_P U}{K} \quad \frac{(.9514)(2.7139 \text{ X } 10^{-5})}{.1075} * \frac{3600}{\text{ft}} \quad (9)$$

$Pr_{NU} = 0.8811$

$$\frac{H_o D^o}{K} = (0.026)\,(RE)^{.8}\,(Pr)^{.33}\left(\frac{U_o}{U_i}\right)^{.14} \tag{10}$$

$$\frac{H_o D}{K} = (.026)(5.582\ E5)^{.8}(.8811)^{.33}\left(\frac{2.701\ E-5}{2.705\ E-5}\right)^{.14} \tag{11}$$

$$H_o = 978 * \frac{K}{D} = 978 * \frac{(1900)}{.141} = 1318\ \frac{BTU}{Hr\ {}^oK\ ft^2} \tag{12}$$

$$q = \frac{2\pi\Delta L(T_a - T_b)}{\frac{1}{r_o h_o} + \frac{Ln(r_1/r_0)}{K_{carbon}} + \frac{Ln(r_2/r_1)}{K_{steel}}} \tag{13}$$

$$K_{carbon} = .55\ \frac{BTU}{{}^oR\ hour\ ft^2/ft} * \frac{1.8\ {}^oR}{1.0\ {}^oK} = .990\ \frac{BTU}{{}^oK\ hour} \tag{14}$$

$$K_{steel} = 26\ \frac{BTU_2}{{}^oR\ hour\ ft^2/ft} * \frac{1.8\ {}^oR}{1.0\ K} = 46.8\ \frac{BTU}{{}^oK\ hour} \tag{15}$$

Using the value calulated in equation (14) and (15) and a heat flux of 6280 BTU/hour the following is obtained:

$$6280 = \frac{2 \quad (.464) \quad (1200 - T_b)}{\frac{1}{(.0705)\ 1318} + \frac{\ln \frac{.125}{.0705}}{1.0800} + \frac{\ln \frac{.150}{.125}}{46.8}} \qquad (16)$$

$$6280 = \frac{2.915(1200-T_b)}{.01076 + .5784 + .003995} \qquad (17)$$

$$T_b = 1120 + \frac{6280(.01076 + .5784 + .003895)}{2.915} = 1120 +$$

$$1270 = 2390^{o}K \qquad (18)$$

Clean Tube

$$T_b = 1120 + \frac{6280 \frac{1}{.125h_o} + \frac{\ln \frac{.150}{.125}}{46.8}}{2.915} = \frac{6280(.006069+.003895}{2.915} \qquad (19)$$

$$T_b = 2.47 + 1120 = 1141.47^{o}K \qquad (20)$$

The safe operating temperature was $1480^{o}K$.

$$q = \frac{2L(T_a - T_b)}{\frac{1}{r_o h_o} + \frac{Ln(r_1/r_0)}{K \text{ carbon}} + \frac{Ln(r_2/r_1)}{K \text{ steel}}} \qquad (21)$$

$$-6280 = \frac{2\ (.464)(1120-T_b)\ ^{o}K}{\frac{1}{(0.700)1318} + \frac{LN\left(\frac{.125}{.0705}\right)}{10.8} + \frac{LN\left(\frac{.150}{.125}\right)}{46.8}} \qquad (22)$$

$T_b = 1267.4^{o}K$

Incornell (25% Cr 20% Ni 55%Fe) is safe to work with up to $2200^{o}F$ or $1477.^{o}K$.

This means that it would be both safe and possible to operate the reactor with this optimum temperature profile without melting the pipes or exposing the reactor to unsafe conditions.

R_o Ft.	$T^{o}K$	Temperature Skin ^{o}K	Thickness of Carbon Layer (ft)
.125	21.48	1141.48	0
.120	30.15	1150.15	.005
.110	48.25	1168.	.015
.095	80.34	1200.	.030
.080	117.8	1238.	.045
.070	147.0	1267.	.055
.060	182.0	1302.	.065
.030	347.0	1467.	.095

Data Calculated by Computer

Reactor Position 390.00 ft.

Reynolds Number 5.672×10^{5}

VIS = 2.7139×10^{-5} Lb/ft. sec.

Reactor Increment of Conversion .469 feet

Thermo conduction steel = $26.0 \times 1.8 = 46.8$ BTU/^{o}K Hour ft^{2}/ft

Thermo conduction coke = $6.0 \times 1.8 = 10.8$ BTU/^{o}K Hour ft^{2}/ft

Appendix J

Nomenclature PYRO

AMWT Average molecular weight of reacting system

B(I,K) Coefficient of component in K^{th} position I^{th} reaction

BB(I,K) Order of reaction of component in I^{th} position K^{th} reaction

C(J) Concentration of J^{th} component (lb. moles/$ft.^3$)

Card(80) Alphanumeric identification of reaction system

CF Temporary constant used in calculating the product of concentration raised to order of reaction components in the forward direction

CLJ(J,1) Constant of Lennard and Jones - collision diameter $(\text{Å})_{J^{th}}$ component

CLJ(J,2) Constant of Lennard and Jones - ϵ/K - $(^oK)_{J^{th}}$ component

CP(J,1-4) Heat capacity data for J^{th} component C_p=CP(J,1) + CP(J,2)*T+CP(J,3)*T^2+CP(J,4)*T^3 (BTU/lb.mole ^oF)

CR Temporary constant used in calculating the products of concentration raised to the order of reaction of each reaction component in the reverse direction

CT $=\Sigma$C(J) (lb.moles/ft^3)

D =MAX(ABS(DXA(I))) i.e. the max of the absolute incremental change of reaction

$$DCP(I,1\text{-}4) = \sum_{K=SF(I)+1}^{SR(I)} \frac{B(I,K)}{B(I,1)} CP(I,1\text{-}4) - \sum_{K=1}^{SF(I)} \frac{B(I,K)}{B(I,1)} CP(I,1\text{-}4) \quad \text{(BTU/lb.mole } ^{o}F) \qquad (1)$$

(i.e.) Summation of heat capacity of products - heat capacity of reactants

DF(I) Summation of free energy of products - free energy of reactants I^{th} reaction (BTU/lb.mole)

DH(I) Summation of heat of formation of products - heat of formation of reactants (BTU/lb.mole)

DS(I) Summation of entropy of products - entropy of reactants (BTU/lb.mole)

EA(I) Arrhenius frequency factor of I^{th} reaction

EE(I) Arrhenius activation energy of I^{th} reaction (cal/m)

ENAME(20J) Alphanumeric identification of the J^{th} component (maximum 20 characters)

F(J) Factor by which the Arrhenius frequency factor is changed - assumed to be one

FI(I) Constant of integration used in calculating the equilibrium constant

GC Gas constant = 1.341 At/lb mole ^{o}K

HR Number of hours in which carbon has been accumulating

HT(J) Heat of reaction of the (J) component (BTU/lb.mole)

I Temporary storage to denote I^{th} reaction

IA(I,K) Used to identify J in the reaction species in the I^{th} reaction the K^{th} position (i.e. J=IA(J,K)

IB Number of increments the reactor will calculate before it is forced off

ID Temporary storage

IDATA(K) Used in printing information on reaction systems

IDATB(K) Used in printing information on reaction systems

IDATP(K) Used in plotting subroutines

IGO Used in print-out as control variable

IGOTO Used as control in determining whether to continue calculation or to read in new data

IGOW Used as control

II Temporary

IIN Temporary

IJ Temporary

IJK Temporary

IM Temporary

IPLOT Used to determine form of print-out

IR Total number of reactions

IS Total number of chemical species

ISS Temporary

IT Temporary

ITEST	Used as program control
IWMZ	Used in print-out
IX	Temporary
IZZ	Temporary
I1	Temporary
I2	Temporary
I3	Temporary
J	Temporary
JJ	Temporary
JJ1	Temporary
JJ2	Temporary
J1	Temporary
J2	Temporary
J3	Temporary
J4	Temporary
K	Temporary - usually refers to position in reaction
KEYP	Key product identification. Used by computer in yield calculation as well as plotting.
KEYR	Key reactant identification. Used by computer in yield calculation as well as plotting
KK	Temporary
L	Temporary - usually used to denote particular heat capacity term

M	Temporary
MA	Used as computer control. Limits total number of iterations.
MAZE	Used as computer control in pressure calculation
MB	Used to determine size of the step
MI	Temporary
MM	Temporary
MMM	Temporary
MT	Temporary
MY	Computer control number of small iterations between print-out
MZ	Computer control number of print-outs desired
M10	Computer control
N	Temporary
NO	Temporary number of solid components
P(J)	Pressure of J component (at)
PD	Pressure drop increment (in At.)
PDIP	Initial incremental pressure change used in convergence (At)
PI	Pressure into reactor (At)
POUT	Pressure out of reactor (At)
PPI(J)	Initial pressure of J^{th} component (At)
PRES	Max. allowable pressure in reactor (At)
PRETT	Pressure used if valocity of sound is exceeded (At)

PSAVE	Pressure in previous increment (At)
PT	Total pressure in reactor at any point (At)
PTI	Initial total pressure (At)
PTTE	Temporary pressure storage (At)
PT2	Temporary pressure storage (At)
R	Gas constant 1,987 cal/gram mole ^{o}K
RA	Rate of reaction
RAD	Radius of the reactor (Ft)
RADD(I)	Radius of reactor at I% temporary storage (Ft)
RADF(I)	Radius of reactor at I% previously calculated (Ft)
RADI(I)	Radius of reactor at I% presently being calculated
RADU	Original radius of clean reactor (Ft)
RAF	Original radius of clean reactor (Ft)
RATE	Total rate of reaction
REQ	Reciprocal of equilibrium constant
REQTT	Reciprocal of equilibrium constant
RIJ	Used to calculate percent position in reactor
RJ	Used to calculate percent position in reactor
RN1	Moles before reaction segment DL (lb.moles)
RN2	Moles after reaction segment DL (lb.moles)
RI	Temporary
SF(I)	(Integer) Number of components in I^{th} forward reaction
SMWT(J)	Molecular weight of J^{th} component

SR(I)	(Integer) number of components in I^{th} reverse reaction
ST	Temporary
T	Temperature of reactor (any point) (^{o}F)
TIN	Temperature of inlet conditions (^{o}F)
TM	Temporary temperature storage (^{o}F)
TMPH	Total moles per hour (lb moles/hour)
TMPHI	Initial molar flow rate (lb.moles/hour)
TR	Temporary storage - temperature (^{o}F)
TT	Temporary temperature storage (^{o}F)
VEL1	Velocity of gas at any point in reactor (ft/sec)
VI(I)	Viscosity of component (I) (lb/ft sec)
VIS	Viscosity of reaction system (lb/ft sec)
VC(J,L)	Concentration of component J at L% into reactor
WDZA(I,L)	Rate of reaction I at distance L% into reactor
WPJ(L)	Pressure L% into reactor (At)
WT(L)	Temperature L% into reactor (^{o}F)
WTM(J,L)	Total mole/hour of component J, L% into reactor
WTMPH(L)	Total mole/hour L% into reactor
WVEL1(L)	Velocity ft/sec L% into reactor
WZIC(L)	Length ft, L% into reactor
X	Used as temporary in calculating heat of reaction, heat capacity
XN	Used to calculate temperature profile in reactor

XXN	Used to calculate temperature profile in reactor
YIELD	WTM(KEYR,100)/WTM(KEYR,0)*100
Z(L)	Temperature profiles at 10% distance along reactor (^{o}F)