A STUDY OF AN ADIABATIC TUBULAR REACTOR FOR THE MULTIPLE CHLORINATION OF METHANE

BY

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FACULTY COMMITTEE

APPROVEL. ______________________

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ABSTRACT

A computer program has been developed which simulates the multiple chlorination of methane in an adiabatic, tubular reactor. Euler's method is used to approximate the solutions of the programs differential equations.

The program is designed to determine the amount of an inert diluent required in the feed stream to attain some specified conversion of methane in a safe and efficient temperature range. Particular emphasis is put on determining the amount of diluent required to attain 98% conversion of methane at an outlet temperature of 723°K. The program also determines the reactor volume necessary to achieve the specified conversion, and the product distribution at the reactor outlet.

The three diluents investigated were CCl_4, HCl, and N_2. Relationships between reactor volume required to attain 98% conversion of methane at an outlet temperature of 723°K and reactant feed temperature are presented for each diluent. The use of elevated pressure to reduce the reactor volume of the HCl inerted system is also discussed.

The developed program is readily adaptable to any set of operating data and should provide a useful tool for designing adiabatic, tubular reactors for exothermic, competitive, consecutive reactions.

ACKNOWLEDGEMENTS

The author wishes to express his gratitude to Dr. Deran Hanesian for his guidance and encouragement in this endeavor.

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INTRODUCTION

Series reactions such as the successive chlorination of methane or benzene, are industrially important type reactions. The general representation of such a reaction is

$$A \xrightarrow{+B,k_1} R \xrightarrow{+B,k_2} S \xrightarrow{+B,k_3} T. \quad (10)$$

The thermal chlorination of methane in the vapor phase follows this reaction pattern and may be represented as follows

$$CH_4 \xrightarrow{+Cl_2,k_1} CH_3Cl \xrightarrow{+Cl_2,k_2} CH_2Cl_2 \xrightarrow{+Cl_2,k_3} CHCl_3 \xrightarrow{+Cl_2,k_4} CCl_4.$$

The industrial importance of this reaction is indicated by the 1972 U. S. production statistics

Methyl chloride	- 200 million pounds [17]
Methylene chloride	- 300 million pounds
Chloroform	- 200 million pounds
Carbon Tetrachloride	- 1 billion pounds.

These quantities are expected to double in the next decade.

Because the exothermic process is extremely temperature sensitive, and there is a close correlation between temperature, reaction time, and product distribution, careful control of the reaction temperature is imperative to product quality and safe operation. Various methods have been employed to control reaction temperature. Reaction moderating catalysts have been used as well as various light sources.[13] On the laboratory scale McBee, Hass, Nether and Strickland[14] designed a multiple feed port reactor for feeding chlorine into a flowing stream of methane. Johnson, Parsons, and Roberts [6] used a fluid bed reactor to moderate the reaction temperature of the vapor phase reaction.

While all these techniques have merit, a more practical method for controlling the temperature of the vapor phase reaction in an industrial reactor appears to be recycling an inert diluent along with the reactants. The unreactive inert would act as a heat sink for the heat generated by the four exothermic reactions. By using the proper amount of inert a simple adiabatic, tubular, reactor, of proper volume, could be used to produce the chlorinated methanes over a safe and efficient temperature range. Product degradation would be minimized and the problem of flaming in the reactor avoided. Such a reaction system would also avoid the scale up complications, which might be associated with scaling complex fluid bed reactors and multiple feed reactors from laboratory and pilot plant size to industrial scale.

The purpose of this present work is to simulate the multiple chlorination of methane in an industrial size, adiabatically operated, tubular reactor. The reactor model will be used to determine

1) The amount of inert diluent required in the feed stream to properly moderate the reaction temperature over a safe and efficient operating range.

2) The reactor volume necessary to achieve a specified conversion of the methane.

3) The variation in product distribution with reactor operating conditions.

Based on these results optimum operating conditions will be discussed.

LITERATURE SEARCH

Reaction Kinetics

The reaction kinetics of the thermal chlorination of methane has been studied by a number of investigators. Pease and Walz[16] established that the rate of chlorination of methane in the vapor state without the presence of oxygen is proportional to the concentrations of methane and chlorine. This observation has been confirmed by other authors[12],[18] who found the successive chlorinations of methane to be bimolecular, irreversible and hence kinetically second order.

We can then state that the successive chlorination of methane fits into a class of homogeneous, competitive, consecutive reactions which can be represented by the following set of equations.

$$CH_4 + Cl_2 \xrightarrow{k_1} CH_3Cl + HCl \quad (1)$$

$$CH_3Cl + Cl_2 \xrightarrow{k_2} CH_2Cl_2 + HCl \quad (2)$$

$$CH_2Cl_2 + Cl_2 \xrightarrow{k_3} CHCl_3 + HCl \quad (3)$$

$$CHCl_3 + Cl_2 \xrightarrow{k_4} CCl_4 + HCl \quad (4)$$

The rate constants for the four reactions have been studied by various authors. Pease and Walz determined rate constants in terms of $sec.^{-1} \cdot atm.^{-1}$ for reactions (1) and (2) run in glass tubes in the temperature range of 225 to

245°C. Johnson, Parsons, and Roberts obtained rate constants for all four reactions also in terms of $sec.^{-1} \cdot atm.^{-1}$. These experiments were carried out in a fluid bed reactor. Arai[1] studied the rate constants of all four reactions in the temperature range of 275 to 370°C in electrically heated tubes. His data are presented in terms of $gm\ mole \cdot hr^{-1} \cdot ml^{-1} \cdot atm^{-2}$.

The data of these investigators is presented in Figures 1 to 4. For the purposes of this study all rate constant data is presented in terms of $ft^3 \cdot lb\ mole^{-1} \cdot hr^{-1}$. The following conversions were used to convert the data of the various authors to the desired units.

$$k(ft^3 \cdot lb\ mole^{-1} \cdot hr^{-1}) = k(gm\ mole \cdot hr^{-1} \cdot ml^{-1} \cdot atm^{-2})(T^2)(1.07 \times 10^2)$$
$$= k(sec^{-1} \cdot atm^{-1})(T)(4.73 \times 10^3) \qquad (5)$$

<u>Basic Data</u>

The literature was also searched for thermodynamic data necessary for the solution of the energy balance equation. The pertinent data, specific heats, free energies of reactions, and heats of formation were obtained from the JANAF Tables[5].

THEORY

The expressions necessary to develop a mathematical model for the thermal chlorination of methane in an adiabatic, plug flow reactor are considered below. The development which follows assumes ideal performance and neglects pressure drop in the reactor.

Determination of Reaction Temperature Range

As previously noted the reaction between chlorine and methane involves four successive, highly exothermic, reactions. Each generates approximately 45,000 BTU per lb mole of compound reacted. If this heat is not controlled the temperature of the reacting mass will rise to a point where other secondary reactions predominate and the formation of unwanted by-products becomes significant.

Various authors have found that if the temperature of the reaction is not carefully controlled, deleterious side reactions can occur which may result in product degradation at best and flaming in the reactor or violent explosions at worst. According to Jones, Allison, and Meighan[7] "if the temperature of the reaction rises above 500°C, the reaction may react explosively to form carbon according to the formula"

$$CH_4 + 2Cl_2 \longrightarrow C + 4HCl. \qquad (6)$$

Wilson and Howland[19] confirm this and show that the above reaction generates heat at a rate of over 100,000 BTU per lb mole of methane reacted. They also state that as carbon is formed it accelerates the reaction autocatalytically which leads to the production of additional carbon. Other factors studied by these authors show that while the chlorination reactions are moderate at 250°C, they are rapid at 400°C and all components present, except for carbon tetrachloride, are liable to decompose exothermally at temperatures above 450°C.

Pease and Walz in their chlorination study found that at reaction temperatures above 400°C when methane is in excess the reaction is rapid but not explosive; however, when chlorine is in excess the mixture may become explosive. According to Kirk and Othmer(8) all commercial processes for the manufacture of chloromethanes are operated in the temperature range of 350 to 500°C. Using this temperature range takes advantage of the high reaction rates without reaching decomposition temperatures.

Various techniques have been tried to moderate the reaction temperature. McBee, Hass, and Nether used a multiple feed port reactor for feeding chlorine into a flowing stream of methane. Johnson, Parsons, and Roberts used a fluid bed reactor to moderate the reaction temperature. They also found that when the reaction temperature reaches 450°C, unless the chlorine molar concentration is below 10 to 15%, ignition and pyrolysis can take place in the reactor.

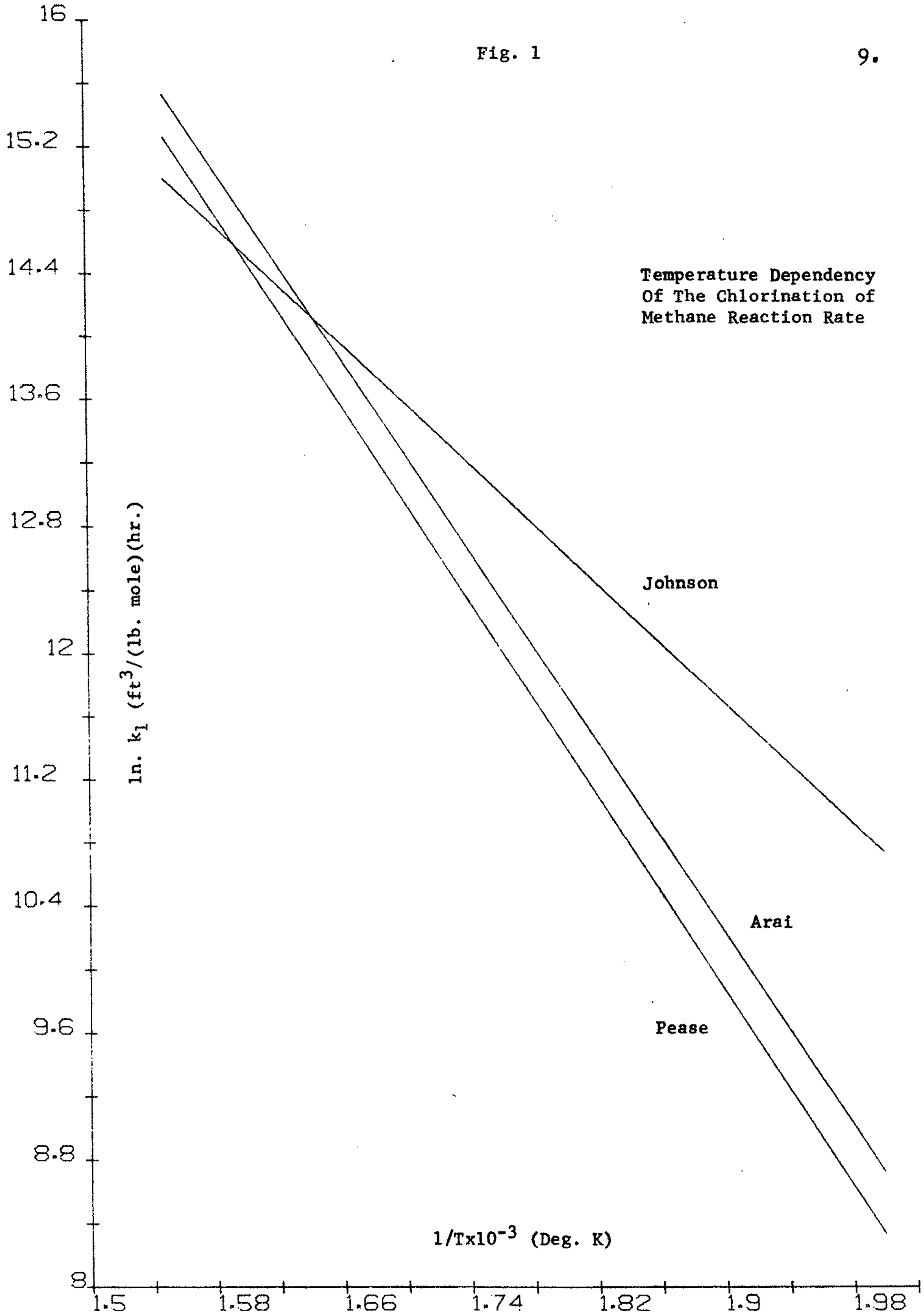
From the preceding discussion it is clear that when performing the multiple chlorination of methane it is important to make constructive use of the high heats of reactions without creating a temperature situation in the reactor which might cause uncontrollable reactions. The literature clearly stresses the fact that at temperatures below 250°C the thermal chlorination reactions are slow and sluggish, while at a temperature above 500°C product degradation is likely to occur because the rates of side reactions predominate. For the purposes of this work, it was therefore decided to study the reactions in the temperature range of 250°C (523°K) to 450°C (723°K). This range seems particularly desirable for industrial purposes as it achieves high rates of reaction without reaching temperatures which cause undesirable side reactions.

Establishment of Rate Constants

In establishing rate constant data for this study the literature search uncovered three major sources. Since some variation between the data existed, resolution was necessary.

As can be seen in Fig. 1 rate constants of Pease and Arai for the methane reaction, Eq. 1, are in agreement. Both authors also determined the activation energy of the reaction to be approximately 31,000 calories/gm mole. While the data of Johnson, Parsons, and Roberts differs from the other investigators, this is expected since they observed that the energy of activation of the methane reaction is significantly reduced

Fig. 1


Temperature Dependency
Of The Chlorination of
Methane Reaction Rate
Johnson
Arai
Pease
ln. k1 (ft3/(lb. mole)(hr.)
1/Tx10-3 (Deg. K)
16
15.2
14.4
13.6
12.8
12
11.2
10.4
9.6
8.8
8
1.5
1.58
1.66
1.74
1.82
1.9
1.98

to 20,000 calories/gm mole when the reaction is carried out in a fluid bed reactor. However, in a separate experiment performed in an empty tubular reactor, similar to that of Pease, they obtained an energy of activation in close agreement with that proposed by Arai and Pease.

The consistancy of the rate constant data for the methane chlorination in an empty plug flow reactor is apparent from the above data, and thus, for the purposes of this study the data of Arai were selected.

Figure 2 shows the rate constants of Johnson, Parsons, Roberts and Arai for the chlorination of methyl chloride. Both investigators found an activation energy for this reaction of approximately 18,000 calories/ gm mole. Johnson, Parsons and Roberts also observed that the ratio of k_2 to k_1 to be 2.0. This was confirmed by Pease and Natta[15], who found k_2/k_1 to be approximately 2 at a temperature of 315°C. The rate constant data were therefore determined by using an activation energy of 18,000 calories/gm mole and a value of k_2 at 315°C of $1.1 \times 10^6 ft^3 \cdot lb\ mole^{-1} \cdot hr^{-1}$ which represents a ratio for k_2/k_1 of 2.0.

As can be seen in Fig. 3 the data of both investigators are in excellent agreement for the methylene chloride chlorination. Resolution was therefore unnecessary.

Average values of the data presented in Fig. 4 were taken to obtain the relationship between rate constant (k_4) and

Fig. 2

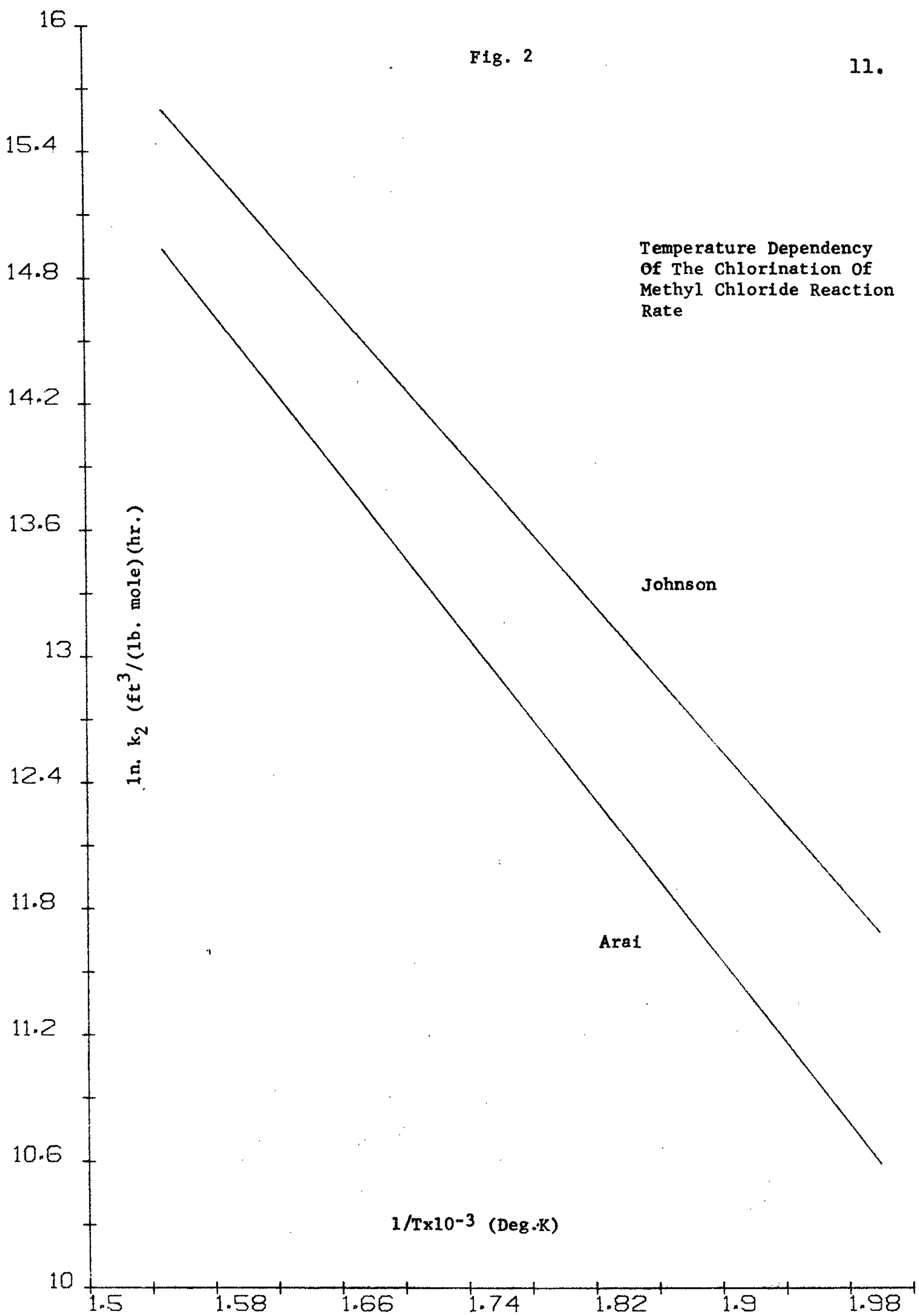

Temperature Dependency Of The Chlorination Of Methyl Chloride Reaction Rate
Johnson
Arai
ln. k_2 (ft^3/(lb. mole)(hr.)
1/Tx10^{-3} (Deg.K)
16
15.4
14.8
14.2
13.6
13
12.4
11.8
11.2
10.6
10
1.5
1.58
1.66
1.74
1.82
1.9
1.98

Fig. 3

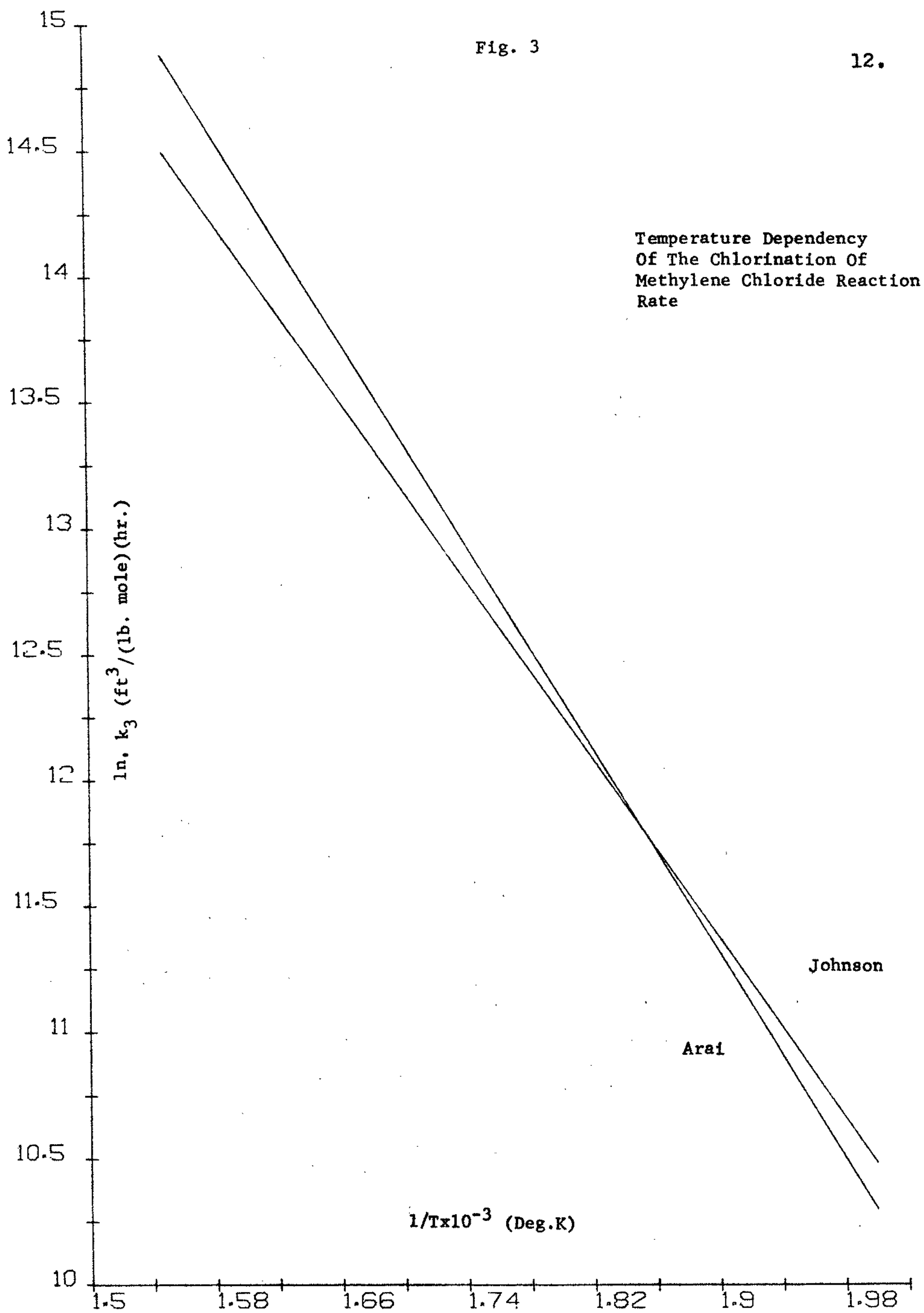
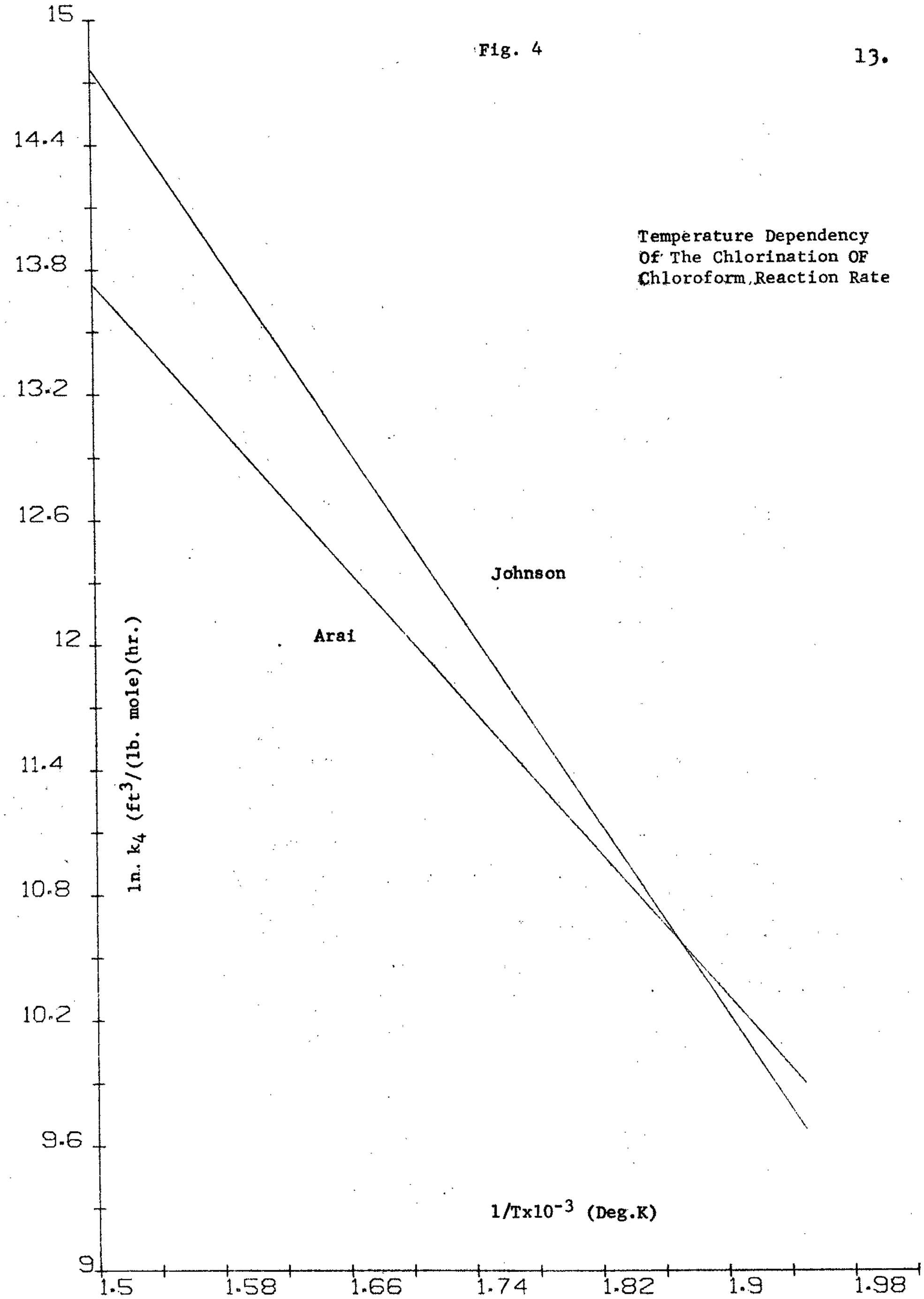

Temperature Dependency
Of The Chlorination Of
Methylene Chloride Reaction
Rate
ln, k3 (ft3/(lb. mole)(hr.)
1/Tx10-3 (Deg.K)
Johnson
Arai
15
14.5
14
13.5
13
12.5
12
11.5
11
10.5
10
1.5
1.58
1.66
1.74
1.82
1.9
1.98

Fig. 4


Temperature Dependency
Of The Chlorination OF
Chloroform Reaction Rate
Johnson
Arai
ln. k4 (ft3/(lb. mole)(hr.)
1/Tx10-3 (Deg.K)
15
14.4
13.8
13.2
12.6
12
11.4
10.8
10.2
9.6
9
1.5
1.58
1.66
1.74
1.82
1.9
1.98

temperature (T) for the chloroform reaction. The ratio of k_4/k_1 at 315°C obtained from the averaged data is 0.38. This value agrees with the k_4/k_1 ratio reported by Kobert and Troltenier(9).

Rate constants versus reciprocal of absolute temperature for the four successive chlorinations are presented in Fig. 5. The equations which represent these data according to the Arrhenius law are

$$k_1 = 7.980\times10^{16}\cdot\exp(-30036/RT) \quad (7)$$

$$k_2 = 5.479\times10^{16}\cdot\exp(-17962/RT) \quad (8)$$

$$k_3 = 5.894\times10^{12}\cdot\exp(-18930/RT) \quad (9)$$

$$k_4 = 3.480\times10^{12}\cdot\exp(-19415/RT) \quad (10)$$

Thermodynamic Considerations

Free Energy and Equilibrium Constants

Free energy data for the reactants and products of the four chlorination reactions was obtained from JANAF Tables. Free energy changes for each reaction were then calculated at temperatures of 500 and 700°K, the extremeties of the operating range. Equilibrium constants were calculated using the equation

$$K_{eq} = \exp(-\Delta F/RT) \quad (11)$$

Results are summarized in Table 1. These data were in close agreement with that of Wilson and Howland, also shown in Table 1.

Fig. 5

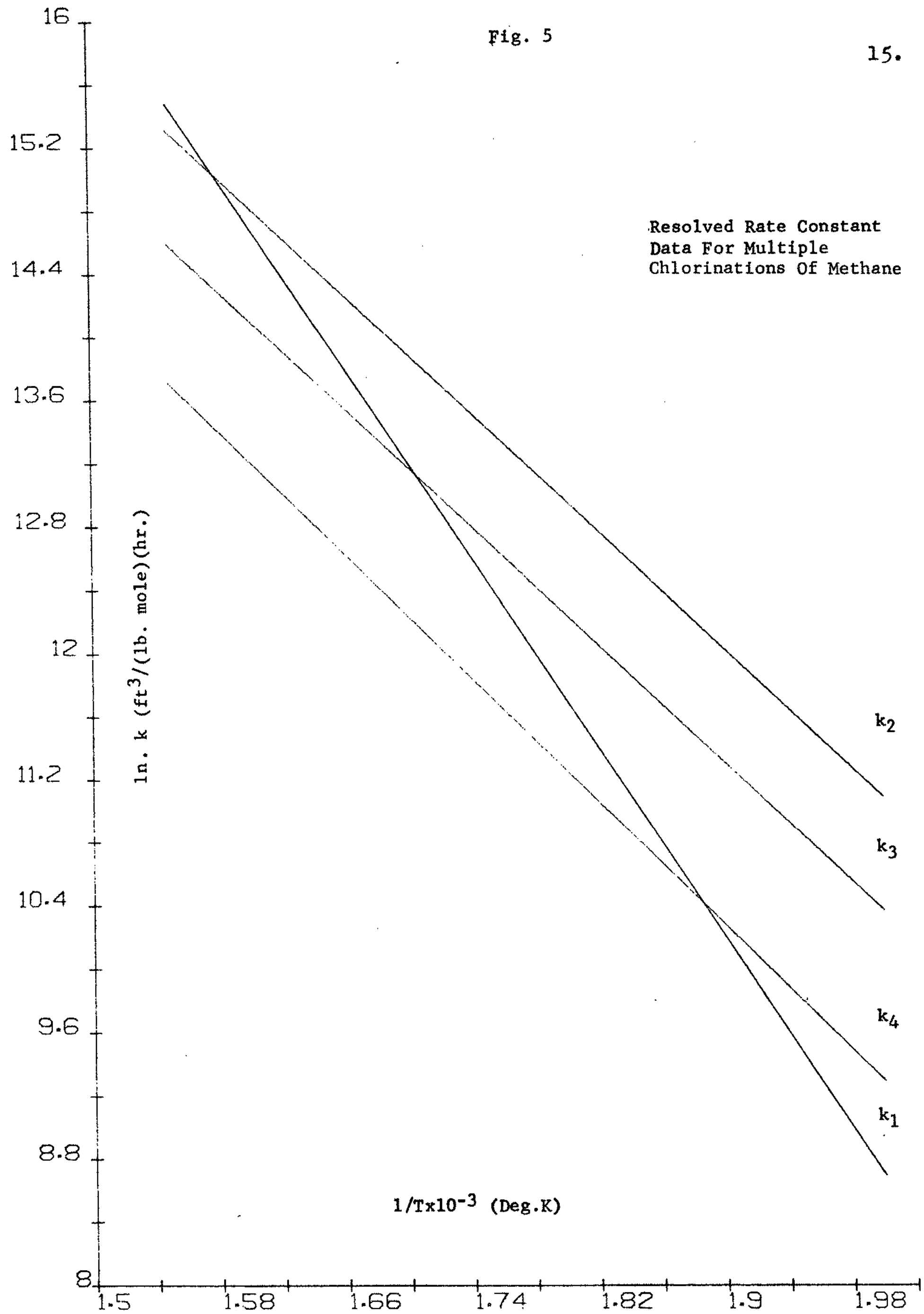

Resolved Rate Constant
Data For Multiple
Chlorinations Of Methane
ln. k (ft3/(lb. mole)(hr.)
1/Tx10-3 (Deg.K)
k2
k3
k4
k1
16
15.2
14.4
13.6
12.8
12
11.2
10.4
9.6
8.8
8
1.5
1.58
1.66
1.74
1.82
1.9
1.98

TABLE 1

Free Energy of Reaction and Equilibrium Constants for Chlorination Reactions

Reaction	ΔF 500°K	ΔF 700°K	K_{eq} 500°K	K_{eq} 700°K
Chlorination of CH_4	-26287 (-25308)	-26886 (-25928)	$3.4x10^{11}$ ($9.8x10^{10}$)	$2.66x10^{8}$ ($1.1x10^{8}$)
Chlorination of CH_3Cl	-23858 (-23691)	-24027 (-23912)	$2.93x10^{10}$ ($2.0x10^{10}$)	$3.38x10^{7}$ ($2.6x10^{7}$)
Chlorination of CH_2Cl_2	-23504 (-22719)	-23261 (-22548)	$2.05x10^{10}$ ($7.3x10^{9}$)	$1.94x10^{7}$ ($9.9x10^{6}$)
Chlorination of $CHCl_3$	-20521 (-21412)	-19799 -	$1.01x10^{9}$ ($4.2x10^{11}$)	$1.60x10^{6}$ -

1) ΔF in calories per gm mole

2) Wilson's data shown in parenthesis

As stated by Levenspiel[11] "$K_{eq} >> 1$ indicates that practically complete conversion is possible and the reaction can be considered to be irreversible". Since irreversibility exists and all reactions proceed essentially to completion, it was deemed unnecessary to calculate the equilibrium conversion.

Specific Heat and Heat of Reaction

The specific heat and heat of formation data obtained from the literature were used to derive the basic equations necessary for the solution of the energy balance. The heat of formation of the components was used to determine the heat of reaction of the four primary chlorinations at various temperatures using the following equation

$$\left[\Delta H_R = \Sigma\Delta H_F(\text{products}) - \Sigma\Delta H_F(\text{reactants})\right]_{T={}^{o}K} \qquad (12)$$

These data along with the specific heat were programed into the 1130 computer and using a International Business Machines regression analysis routine MULTR[4], based on least square polynomial fit, equations relating specific heat and heat of reaction as functions of temperature were obtained. These equations are shown in Tables 2 and 3. Values from the derived equations were checked with published data, and found to be in excellent agreement.

TABLE 2

Constants for Molal Specific Heats of Gases

Equation Form: $cp = a + b \cdot 10^{-2} T - c \cdot 10^{-5} T^2$

where T is in ^{o}K; BTU/(lb mole)(^{o}K)

Component	a	b	c
CH_4	7.826	2.40	-
CH_3Cl	5.372	4.50	1.684
CH_2Cl_2	9.143	5.112	2.365
$CHCl_3$	16.731	4.878	2.558
CCl_4	26.617	4.176	2.468
HCl	11.905	.1458	-
Cl_2	14.494	.1944	-
N_2	11.578	.2376	-

TABLE 3

Constants for Heat of Reaction of Chlorination Reactions

Equation Form: $\Delta H_R = a + b \cdot T + c \cdot 10^{-2} T^2 + d \cdot 10^{-6} \cdot T^3$

where T is in ^{o}K; BTU/lb mole

Reaction	a	b	c	d
Chlorination of CH_4	-44699	-0.7041	.2662	-1.5005
Chlorination of CH_3Cl	-43704	3.6186	-3.7152	-0.6007
Chlorination of CH_2Cl_2	-46135	7.2468	-0.0053	1.4998
Chlorination of $CHCl_3$	-43576	9.2448	-0.7250	0.0225

Establishment of the Mathematical Model

Mass Balance

The thermal chlorination of methane fits into a class of competitive-consecutive reactions which can be represented by equations 1 to 4. Since the reactions are irreversible, constant volume, and bimolecular, the rate expressions describing the above reactions are

$$r_{CH_4} = dC_{CH_4}/dt = -k_1C_{CH_4}C_{Cl_2} \quad (13)$$

$$r_{CH_3C_1} = dC_{CH_3Cl}/dt = k_1C_{CH_4}C_{Cl_2} - k_2C_{CH_3Cl}C_{Cl_2} \quad (14)$$

$$r_{CH_2Cl_2} = dC_{CH_2Cl_2}/dt = k_2C_{CH_3Cl_2} - k_3C_{CH_2Cl_2}C_{Cl_2} \quad (15)$$

$$r_{CHCl_3} = dC_{CHCl_3}/dt = k_3C_{CH_2Cl_2}C_{Cl_2} - k_4C_{CHCl_3}C_{Cl_2} \quad (16)$$

$$r_{CCl_4} = dC_{CCl_4}/dt = k_4C_{CHCl_3}C_{Cl_2} \quad (17)$$

$$r_{Cl_2} = dC_{Cl_2}/dt = -k_1C_{CH_4}C_{Cl_2} - k_2C_{CH_3Cl}C_{Cl_2} -k_3C_{CH_2Cl_2}C_{Cl_2} - k_4C_{CHCl_3}C_{Cl_2} \quad (18)$$

$$r_{HCl} = dC_{HCl}/dt = k_1C_{CH_4}C_{Cl_2} + k_2C_{CH_3Cl}C_{Cl_2} +k_3C_{CH_2Cl_2}C_{Cl_2} + k_4C_{CHCl_3}C_{Cl_2} \quad (19)$$

For purposes here the rate expressions will be written in terms of total pressure and component mole fractions. The mathematical manipulation for converting the methane rate expression is shown below and the other rate expressions are similar. Since the ideal gas law applies

$$C_{CH_4} = P_{CH_4}/RT \quad (20)$$

$$C_{Cl_2} = P_{Cl_2}/RT \quad (21)$$

and according to Dalton's law of partial pressures

$$P_{CH_4} = P_{TOT} \cdot y_{CH_4} \tag{22}$$

$$P_{Cl_2} = P_{TOT} \cdot y_{Cl_2} . \tag{23}$$

Combining equations 20 and 22 and equations 21 and 23 and substituting the results into Eq. 13, Eq. 24 results.

$$r_{CH_4} = \frac{-k_1 \cdot P_{TOT}^2 \cdot y_{CH_4} \cdot y_{Cl_2}}{(RT)^2} \tag{24}$$

The other rate expressions written in this form are:

$$r_{CH_3Cl} = \frac{P_{TOT}^2}{(RT)^2} \left(k_1 \cdot y_{CH_4} \cdot y_{Cl_2} - k_2 y_{CH_3Cl} \cdot y_{Cl_2}\right) \tag{25}$$

$$r_{CH_2Cl_2} = \frac{P_{TOT}^2}{(RT)^2} \left(k_2 \cdot y_{CH_3Cl_2} \cdot y_{Cl_2} - k_3 \cdot y_{CH_2Cl_2} \cdot y_{Cl_2}\right) \tag{26}$$

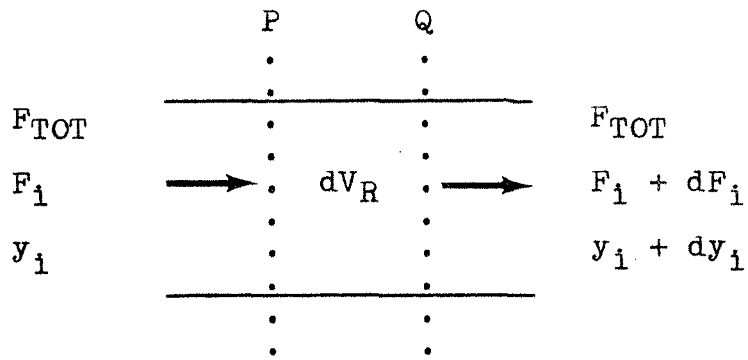
$$r_{CHCl_3} = \frac{P_{TOT}^2}{(RT)^2} \left(k_3 \cdot y_{CH_2Cl_2} \cdot y_{Cl_2} - k_4 \cdot y_{CHCl_3} \cdot y_{Cl_2}\right) \tag{27}$$

$$r_{CCl_4} = \frac{P_{TOT}^2}{(RT)^2} \left(k_4 \cdot y_{CHCl_3} \cdot y_{Cl_2}\right) \tag{28}$$

$$r_{Cl_2} = -\frac{P_{TOT}^2}{(RT)^2} \Big(k_1 \cdot y_{CH_4} \cdot y_{Cl_2} + k_2 \cdot y_{CH_3Cl} \cdot y_{Cl_2} + k_3 \cdot y_{CH_2Cl_2} \cdot y_{Cl_2} + k_4 \cdot y_{CHCl_3} \cdot y_{Cl_2}\Big) \tag{29}$$

$$r_{HC_1} = \frac{P_{TOT}^2}{(RT)^2} \Big(k_1 \cdot y_{CH_4} \cdot y_{Cl_2} + k_2 \cdot y_{CH_3Cl} \cdot y_{Cl_2} + k_3 \cdot y_{CH_2Cl_2} \cdot y_{Cl_2} + k_4 \cdot y_{CHCl_3} \cdot y_{Cl_2}\Big) \tag{30}$$

With all rate expressions properly defined, the component mass balances for all species involved in the reaction system are developed. In preparing the mass balances the plug flow assumption is made. It is further assumed that there is negligible diffusion relative to the bulk flow(3).



Let P and Q be two planes containing between them an infinitesimal part dV_R of the total reactor volume, V_R. Let F_{TOT} be the total molar flow rate across either of these planes. This is a valid restriction for the complex chloromethane system since the total moles in the system is fixed by the stociometry of the reaction and is constant at any point in the reactor. Further let y_i and $y_i + dy_i$ be the lb moles of any component per unit lb mole of the fluid at planes P and Q respectively. In accordance with the plug flow assumption these mole fractions are uniform over the cross section as is the reaction rate and the molar flow rate. Finally let r_i be the reaction rate of any component i. Then by mass balance,

$$F_{TOT}(y_i+dy) = F_{TOT}y_i + r_i dV_R \tag{31}$$

$$F_{TOT}dy_i = r_i dV_R \tag{32}$$

$$\frac{dy_i}{dV_R} = \frac{r_i}{F_{TOT}} \tag{33}$$

Based upon this analysis individual mass balance equations for all reacting species can be rewritten as:

$$dyCH_4/dV_R = r_{CH_4}/F_{TOT} \tag{34}$$

$$dyCH_3Cl/dV_R = r_{CH_3Cl}/F_{TOT} \tag{35}$$

$$dyCH_2Cl_2/dV_R = r_{CH_2Cl_2}/F_{TOT} \tag{36}$$

$$dyCH_3Cl/dV_R = r_{CHCl_3}/F_{TOT} \tag{37}$$

$$dyCCl_4/dV_R = r_{CCl_4}/F_{TOT} \tag{38}$$

$$dyCl_2/dV_R = r_{Cl_2}/F_{TOT} \tag{39}$$

$$dyHCl/dV_R = r_{HCl}/F_{TOT} \tag{40}$$

Energy Balance

Since the reaction takes place adiabatically and the system is an exothermic one, the temperature will rise as the reactor volume, V_R, increases. As the reactions take place the heat liberated in a differential volume, dV_R, due to the four simultaneous chlorinations must equal the gain in enthalpy of the following stream. Mathematically the heat generation terms may be expressed as

$$\text{Heat Generation} = \text{Molar Heat of Reaction} \cdot \text{Extent of Reaction}$$

or

$$\text{Heat Generation} = \Delta H_{R_1} \cdot F_{CH_4} \cdot X_{CH_4} + \Delta H_{R_2} \cdot F_{CH_3Cl} \cdot X_{CH_3Cl}$$

$$+ \Delta H_{R_3} \cdot F_{CH_2Cl} + X_{CH_2Cl_2} + \Delta H_{R_3} \cdot F_{CHCl_3} \cdot X_{CHCl_3} \quad (41)$$

The gain in enthalpy of the stream may be expressed as

$$\text{Enthalpy Gain} = \text{Molar Flow rate} \cdot \text{Specific Heat} \cdot \text{Temperature Change}$$

or

$$\text{Enthalpy Gain} = \Big(F_{CH_4} \cdot cp_{CH_4} + F_{CH_3Cl} \cdot cp_{CH_3Cl} + F_{CH_2Cl_2} \cdot cp_{CH_2Cl}$$

$$+ F_{CHCl_3} \cdot cp_{CHCl_3} + F_{CCl_4} \cdot cp_{CCl_4} + F_{Cl_2} \cdot cp_{Cl_2}$$

$$+ F_{HCl} \cdot cp_{HCl} + F_{N_2} \cdot cp_{N_2} \Big) \, dT \quad (42)$$

Since

$$F_{CH_4} \cdot X_{CH_4} = r_1 dV_R \quad (43)$$

$$F_{CH_3Cl} \cdot X_{CH_3Cl} = r_2 dV_R \quad (44)$$

$$F_{CH_2Cl_2} \cdot X_{CH_2Cl_2} = r_3 dV_R \quad (45)$$

$$F_{CHCl_3} \cdot X_{CHCl_3} = r_4 dV_R \quad (46)$$

and

$$F_{CH_4} = F_{TOT} \cdot y_{CH_4} \quad (47)$$

$$F_{CH_3Cl} = F_{TOT} \cdot y_{CH_3Cl} \quad (48)$$

$$F_{CH_2Cl_2} = F_{TOT} \cdot y_{CH_2Cl_2} \quad (49)$$

$$F_{CHCl_3} = F_{TOT} \cdot y_{CHCl_3} \tag{50}$$

$$F_{CCl_4} = F_{TOT} \cdot y_{CCl_4} \tag{51}$$

$$F_{Cl_2} = F_{TOT} \cdot y_{Cl_2} \tag{52}$$

$$F_{HCl} = F_{TOT} \cdot y_{HCl} \tag{53}$$

$$F_{N_2} = F_{TOT} \cdot y_{N_2} \tag{54}$$

the energy balance may be written in its final form:

$$\sum_{n=1}^{4} \Delta H_{R_n} \cdot r_n \cdot dV_R = \sum_{i=1}^{8} F_{TOT} \cdot y_i \cdot cp_i \cdot dT \tag{55}$$

or

$$\frac{dV_R}{dT} = \frac{F_{TOT} \sum_{i=1}^{8} y_i \cdot cp_i}{\sum_{n=1}^{4} \Delta H_{R_n} \cdot r_n} \tag{56}$$

<u>Computer Program</u>

A computer program was developed for solving the mass and energy balance equations previously described. For purposes of this study, temperature was used as the independent variable and component mole fraction and reactor volume as the dependent (solution) variables. The initial conditions are

$$T_0 = T(0) = \text{Inlet feed temperature}$$

$$V_R(T_0) = V_0 = 0$$

$$y_i(V_0) = y_{i_0} = \frac{F_{i_0}}{F_{TOT}} \quad .$$

The mass and energy equations are then solved by a technique known as Euler's method for the approximate solution of first order differential equations. This method is described in detail by Carnahan, Luther, and Wilkes[2].

If the step change is given by ΔT, then,

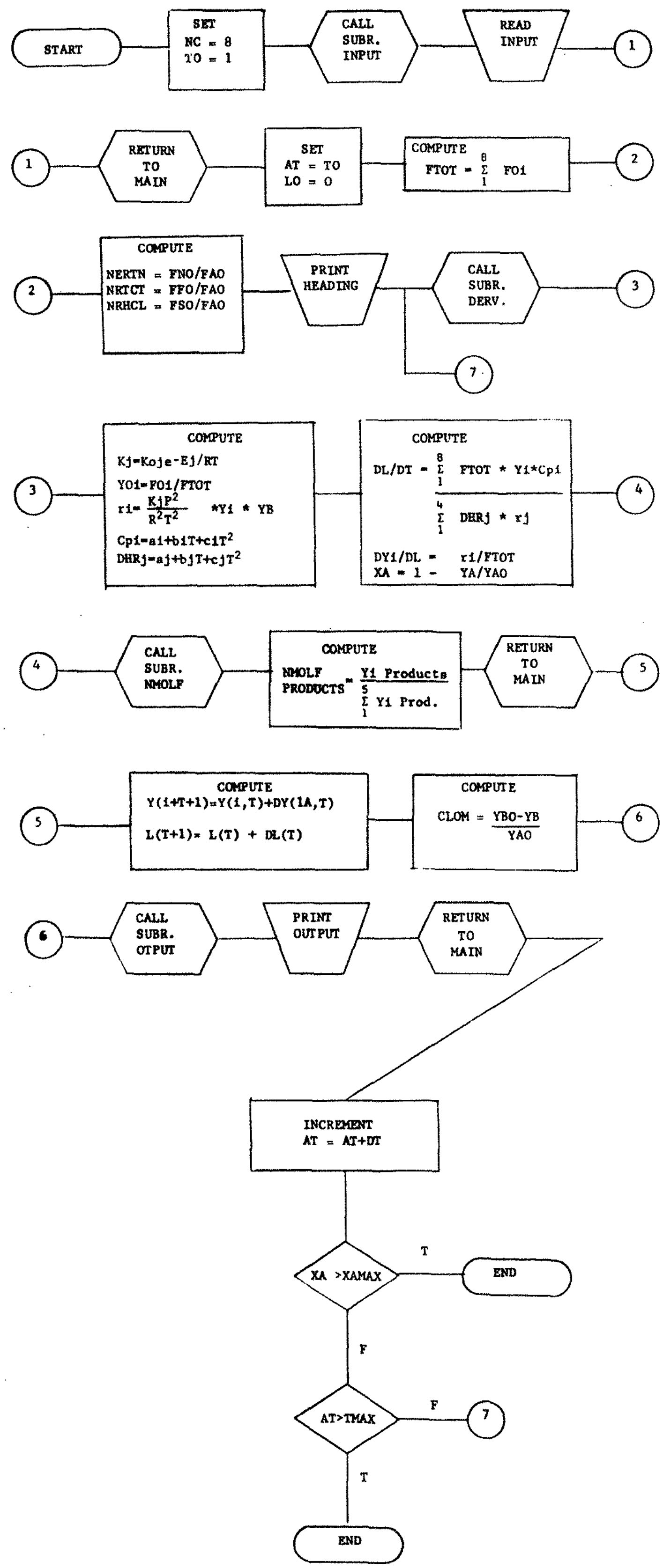
$$V_{R_m} = V_{R_{m-1}} + \Delta T \left(\frac{dV_R}{dT}\right)_{m-1} \tag{57}$$

$$y_{i_m} = y_{i_{m-1}} + \Delta V_R \left(\frac{dy_i}{dV_R}\right)_{m-1} \tag{58}$$

Here V_{R_m} and y_{i_m} are respectively the reactor volume and component mole fractions at $T = m\Delta T$. At the beginning of the m^{th} step the values of $y_{i_{m-1}}$ and $V_{R_{m-1}}$ have already been calculated. The values of dV_R/dT and dy_i/dV_R can be computed from equations 33 to 40 and Eq. 56. Then V_{R_m} and y_{i_m} can be computed from equations 57 and 58. The process is repeated for subsequent steps until the desired conversion of methane or the upper temperature limit is reached.

The program contains provision for printing values for temperature, reactor volume, conversion of methane, moles Cl_2 reacted/mole CH_4, and product distribution of specified values of m. The logic diagram for the program is shown in Figure 6, and the program is given in the Appendix.

FIG. 6 LOGIC DIAGRAM



DISCUSSION OF RESULTS

In this study, control of the reaction temperature of the multiple chlorination of methane by three inert diluents, carbon tetrachloride, CCl_4, hydrogen chloride, HCl, and nitrogen, N_2, was investigated. While each is compatible with the reaction system, the two former are available as reaction products.

The reactant feed rates chosen for the study were 10 lb moles/hr CH_4 and 42 lb moles/hr Cl_2. This feed stream was chosen since it is typical of the size used to feed a large reactor. A reactor or battery of reactors capable of handling this feed could produce several million pounds of chlorinated methanes per year. The reactant feed temperatures studied were 523°K (250°C), 543°K (270°C), 553°K (280°C), 563°K (290°C), and 573°K (300°C). The outlet temperature was set at 723°K (450°C).

For each feed temperature a set of three equations was developed relating conversion of methane as a function of lb moles of diluent in the feed stream per lb mole of CH_4. These equations, presented in Table 4, were obtained by making a number of runs at each inlet temperature for various values of the diluent ratios. Values of conversion so obtained from each run were then correlated with the diluent ratio used. A regression equation at each inlet temperature for each inert

TABLE 4

REGRESSION EQUATIONS FOR PREDICTING CONVERSION OF METHANE FOR VARIOUS DILUENT RATIOS

Equation Form: $X_A = A \cdot 10^{-1} + B \cdot 10^{-2} \cdot I + C \cdot 10^{-3} \cdot I^2$

	A	B	C
$T_0 = 523^oK$			
CCl_4	3.3671	10.007	3.82
HCl	7.5970	0.574	
N_2	7.8527	0.511	
$T_0 = 543^oK$			
CCl_4	3.7480	8.283	2.76
HCl	7.2074	0.610	
N_2	7.3810	0.588	
$T_0 = 553^oK$			
CCl_4	2.9865	9.048	2.95
HCl	7.3905	0.534	
N_2	7.2436	0.579	
$T_0 = 563^oK$			
CCl_4	7.4724	1.650	
HCl	7.3729	0.509	
N_2	7.1842	0.556	
$T_0 = 573^oK$			
CCl_4	2.5288	8.583	2.49
HCl	7.0787	0.539	
N_2	6.9019	0.582	

relating $X_A = f(I)$ was then obtained by using the International Business Machine regression analysis routine, MULTR, previously mentioned. (See page 17 and reference 4.) These equations were used to predict, at each inlet temperature, the amount of a particular inert required to achieve a conversion of 98% at an outlet temperature of 723°K. The predicted amount of inert was used to predict the reactor volume and product distribution.

Carbon Tetrachloride As An Inert Diluent

Results of using CCl_4 as an inert diluent and operating the reactor at 1 atmosphere are summarized in Table 5 and Figure 7. As T_0 is increased from 523 to 573°K the amount of CCl_4 necessary to achieve 98% conversion at an outlet temperature of 723°K increases from 11.3 lb moles/lb mole CH_4 to 15.0 lb moles/lb mole CH_4. Roughly for each 10° rise in inlet temperature one additional lb mole of CCl_4 per lb mole of CH_4 is required in the feed stream.

As the inlet temperature increases from 523 to 573°K the reactor volume required to achieve 98% conversion decreases from 5720 ft^3 to 990 ft^3. Closer inspection of these data show that as the inlet temperature decreases from 573 to 543°K, a 30° change, the reactor volume approximately doubles. Reactor volume doubles again upon reducing inlet temperature an additional 20°, from 543 to 523°K. As can be seen from Figure 7, lowering the inlet temperature to below 523°K causes

TABLE 5

RESULTS OF COMPUTER STUDY USING CCl_4 AS THE INERT DILUENT

Reactor Pressure - 1 Atm

T_0 (^oK)	I $\left(\frac{\text{Moles } CCl_4}{\text{Mole } CH_4}\right)$	V_R (ft^3)	Product Distribution (Mole Fraction) CH_3Cl	CH_2Cl_2	$CHCl_3$	CCl_4
523	11.3	3940	.0228	.4982	.1954	.2836
543	12.5	2060	.0232	.5218	.1913	.2637
553	13.3	1580	.0223	.5288	.1893	.2600
563	14.1	1230	.0227	.5403	.1870	.2499
573	15.0	990	.0225	.5525	.1848	.2397

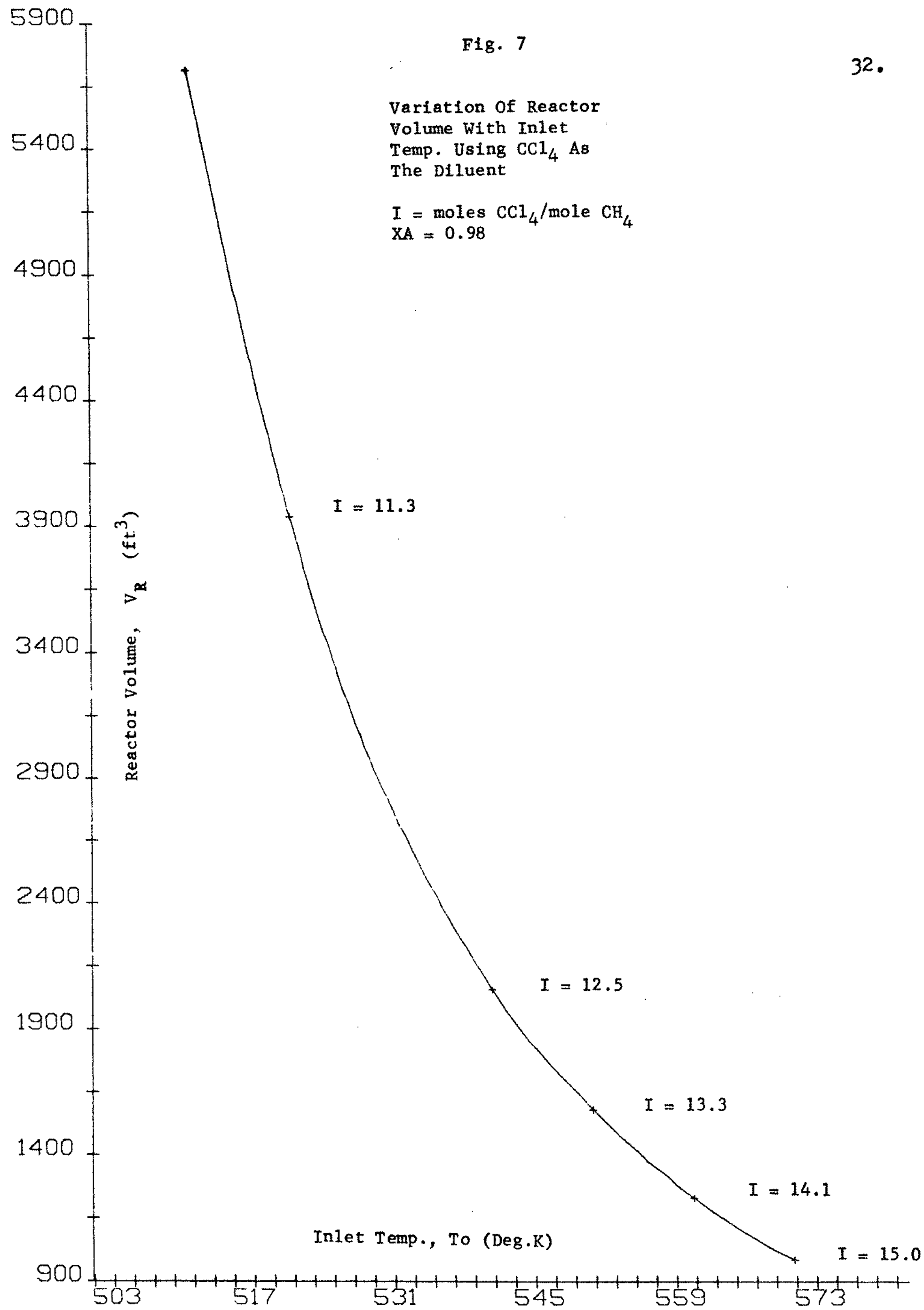


Fig. 7
Variation Of Reactor Volume With Inlet Temp. Using CCl4 As The Diluent
I = moles CCl4/mole CH4
XA = 0.98
I = 11.3
I = 12.5
I = 13.3
I = 14.1
I = 15.0
Reactor Volume, VR (ft3)
Inlet Temp., To (Deg.K)
5900
5400
4900
4400
3900
3400
2900
2400
1900
1400
900
503
517
531
545
559
573

even more substantial increases in the volume. Increasing the feed temperature beyond 573°K provides only minor reduction in the reactor volume. It was also determined that a reactor volume of 350 ft^3 is required to increase methane conversion from 50 to 98% and this volume is independent of inlet temperature and diluent ratio. However, Table 6 shows that the total reactor volume required to attain 50% conversion changes drastically with feed temperature and diluent ratio.

Product distribution at low inlet temperatures favors formation of CCl_4, ca. 30%, and lowers formation of CH_2Cl_2 ca. 49%. A high inlet temperature lowers formation of CCl_4, ca. 24%, and increases formation of CH_2Cl_2, ca. 55%. Formation of $CHCl_3$ remains relatively constant, ca. 19%. Only a slight amount of CH_3Cl, ca. 2%, is present at the exit of the reactor at these conditions. See Figure 8 for typical results.

<u>Hydrogen Chloride As An Inert Diluent</u>

Results of using HCl as an inert diluent and operating the reactor at 1 atmosphere are summarized in Table 7 and Figure 9. Increasing the inlet temperature from 523 to 573°K increases the amount of HCl from 38 to 51 lb moles/lb mole CH_4. An additional 3 lb moles HCl/lb mole CH_4 is required for each 10° increase in inlet temperature.

TABLE 6

REACTOR VOLUME REQUIRED FOR OBTAINING VARIOUS DEGREES OF CH_4 CONVERSION

T_0 (^oK)	V_R For X_A = 0 to 0.5 (ft^3)	V_R For X_A = 0.5 to 0.98 (ft^3)
CCl_4		
523	3510	430
543	1710	350
553	1230	350
563	910	320
573	690	300
HCl		
523	24200	3200
543	12900	3100
553	9200	2600
563	7000	2600
573	5300	2500
N_2		
523	24400	3400
543	11500	2500
553	8800	2500
563	6800	2400
573	5200	2300

Fig. 8

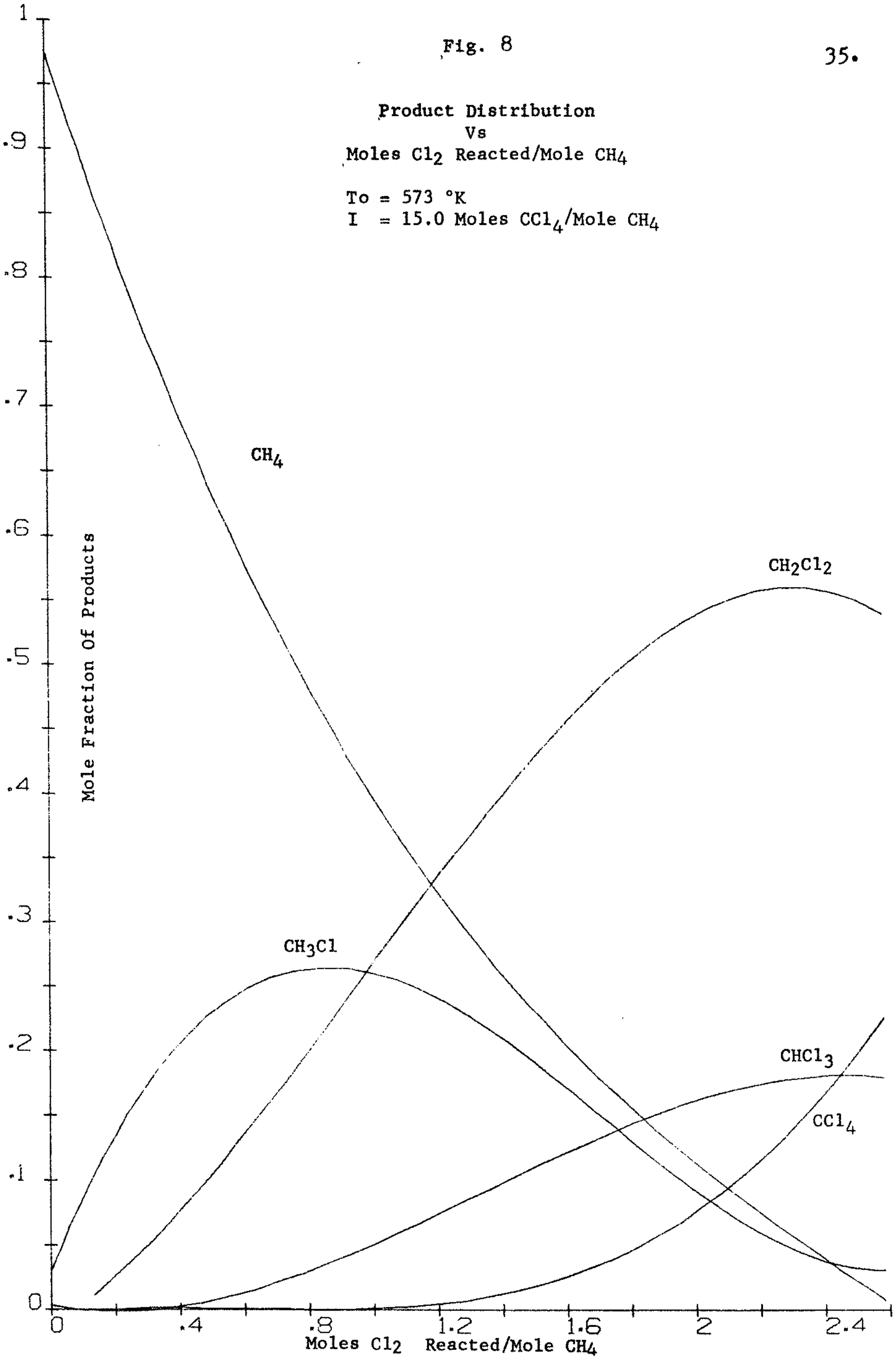

Product Distribution
Vs
Moles Cl_2 Reacted/Mole CH_4
To = 573 °K
I = 15.0 Moles CCl_4/Mole CH_4
CH_4
CH_2Cl_2
CH_3Cl
$CHCl_3$
CCl_4
Mole Fraction Of Products
Moles Cl_2 Reacted/Mole CH_4
1
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
0
.4
.8
1.2
1.6
2
2.4

TABLE 7

RESULTS OF COMPUTER STUDY USING HCl AS THE INERT DILUENT

Reactor Pressure - 1 Atm

T_0 (°K)	I $\left(\frac{\text{Moles HCl}}{\text{Mole } CH_4}\right)$	V_R (ft^3)	Product Distribution CH_3Cl	CH_2Cl_2	$CHCl_3$	CCl_4
523	38	27400	.0224	.4950	.1956	.2862
543	43	15800	.0194	.5051	.1919	.2861
553	45	11800	.0213	.5236	.1895	.2659
563	48	9600	.0207	.5318	.1876	.2607
573	51	7800	.0214	.5451	.1852	.2484

TABLE 8

RESULTS OF COMPUTER STUDY USING HCl AS THE INERT DILUENT

Reactor Pressure - 2.8 Atm

T_0 (°K)	I $\left(\frac{\text{Mole HCl}}{\text{Mole } CH_4}\right)$	V_R (ft^3)	Product Distribution CH_3Cl	CH_2Cl_2	$CHCl_3$	CCl_4
553	45	1510	.0213	.5234	.1893	.2658
563	48	1220	.0207	.5314	.1874	.2605
573	51	990	.0214	.5450	.1852	.2483

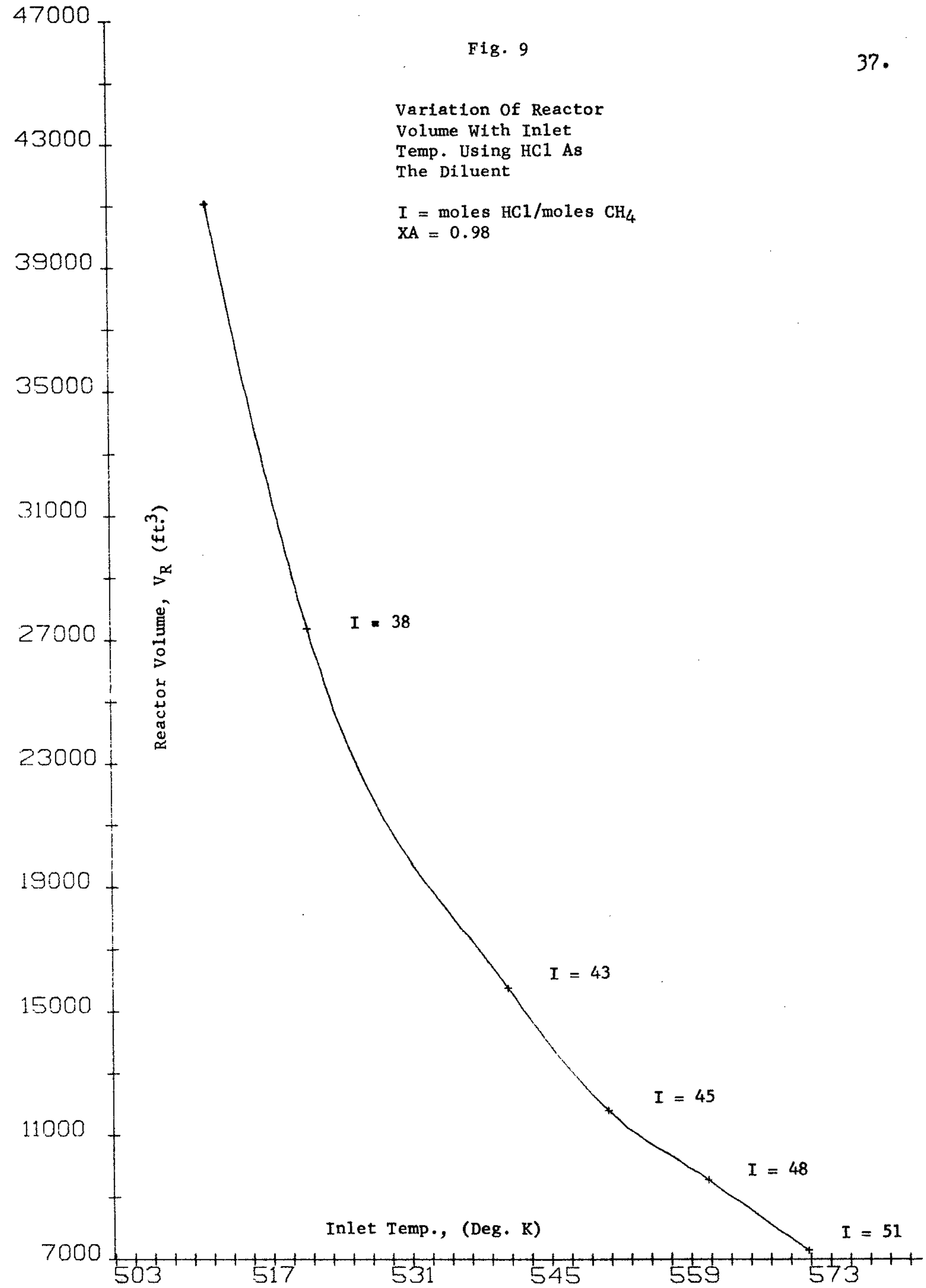


Fig. 9

Variation Of Reactor Volume With Inlet Temp. Using HCl As The Diluent

I = moles HCl/moles CH_4
XA = 0.98

The reactor volume decreases from 27,400 ft^3 to 7,800 ft^3 over the temperature range studied. It was observed that when the feed temperature is increased from 543 to 573°K, the reactor volume is approximately halved, from 15,800 ft^3 to 7800 ft^3. When feed temperature is decreased from 543 to 523°K, a 20° change, the reactor volume nearly doubles. As can be seen from Figure 9, lowering inlet temperature below 523°K causes even more substantial increases in reactor volume. Only minor reduction in volume is observed by increasing inlet temperature above 573°K.

The reactor volume required to increase methane conversion from 50 to 98% varies only slightly 2500 ft^3 to 3200 ft^3 regardless of the feed temperature. However, the reaction volume required to attain 50% conversion increases from 5300 ft^3 to 24,200 ft^3 as inlet temperature is decreased from 573 to 523°K. See Table 6.

As with CCl_4, low feed temperatures favor formation of CCl_4 while higher feed temperatures favor formation CH_2Cl_2. Formation of $CHCl_3$ remains relatively constant. See Figure 10, for typical results.

<u>Nitrogen As An Inert Diluent</u>

Results of using N_2 as an inert diluent and operating the reactor at 1 atmosphere are summarized in Table 9 and Figure 11, and closely parallel those of HCl. Increasing the feed temperature from 523 to 573°K increases the diluent ratio

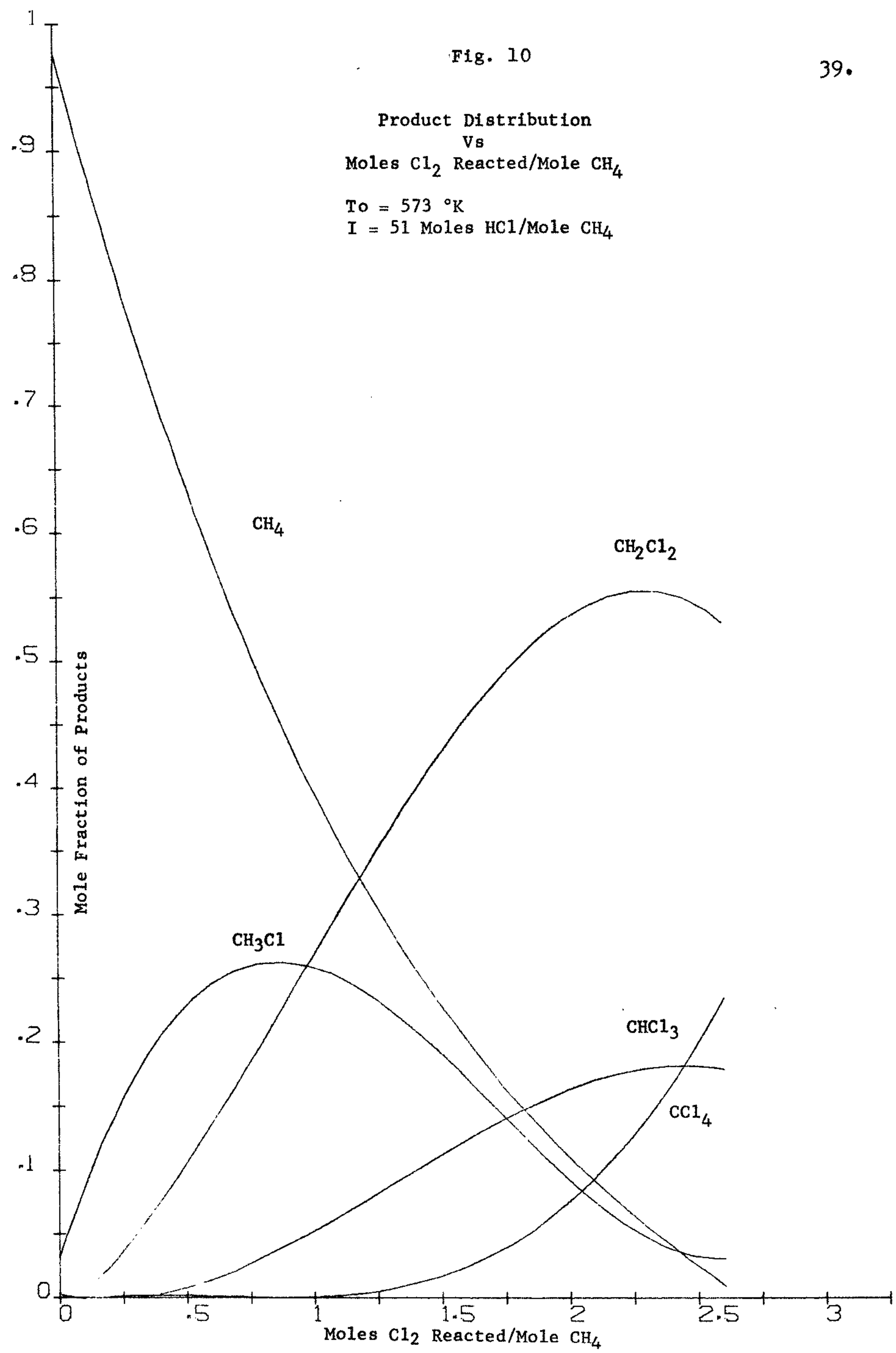


Fig. 10
Product Distribution
Vs
Moles Cl_2 Reacted/Mole CH_4
To = 573 °K
I = 51 Moles HCl/Mole CH_4
1
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
Mole Fraction of Products
CH_4
CH_2Cl_2
CH_3Cl
$CHCl_3$
CCl_4
0
.5
1
1.5
2
2.5
3
Moles Cl_2 Reacted/Mole CH_4

TABLE 9

RESULTS OF COMPUTER STUDY USING

N_2 AS THE INERT DILUENT

Reactor Pressure - 1 Atm

T_0	I	V_R	Product Distribution			
(^oK)	$\left(\frac{\text{Moles } N_2}{\text{Mole } CH_4}\right)$	(ft^3)	CH_3Cl	CH_2Cl_2	$CHCl_3$	CCl_4
523	38	27800	.0193	.4834	.1951	.3045
543	41	14000	.0240	.5233	.1909	.2595
553	44	11300	.0216	.5256	.1893	.2634
563	47	9200	.0208	.5328	.1873	.2599
573	50	7500	.0213	.5449	.1852	.2489

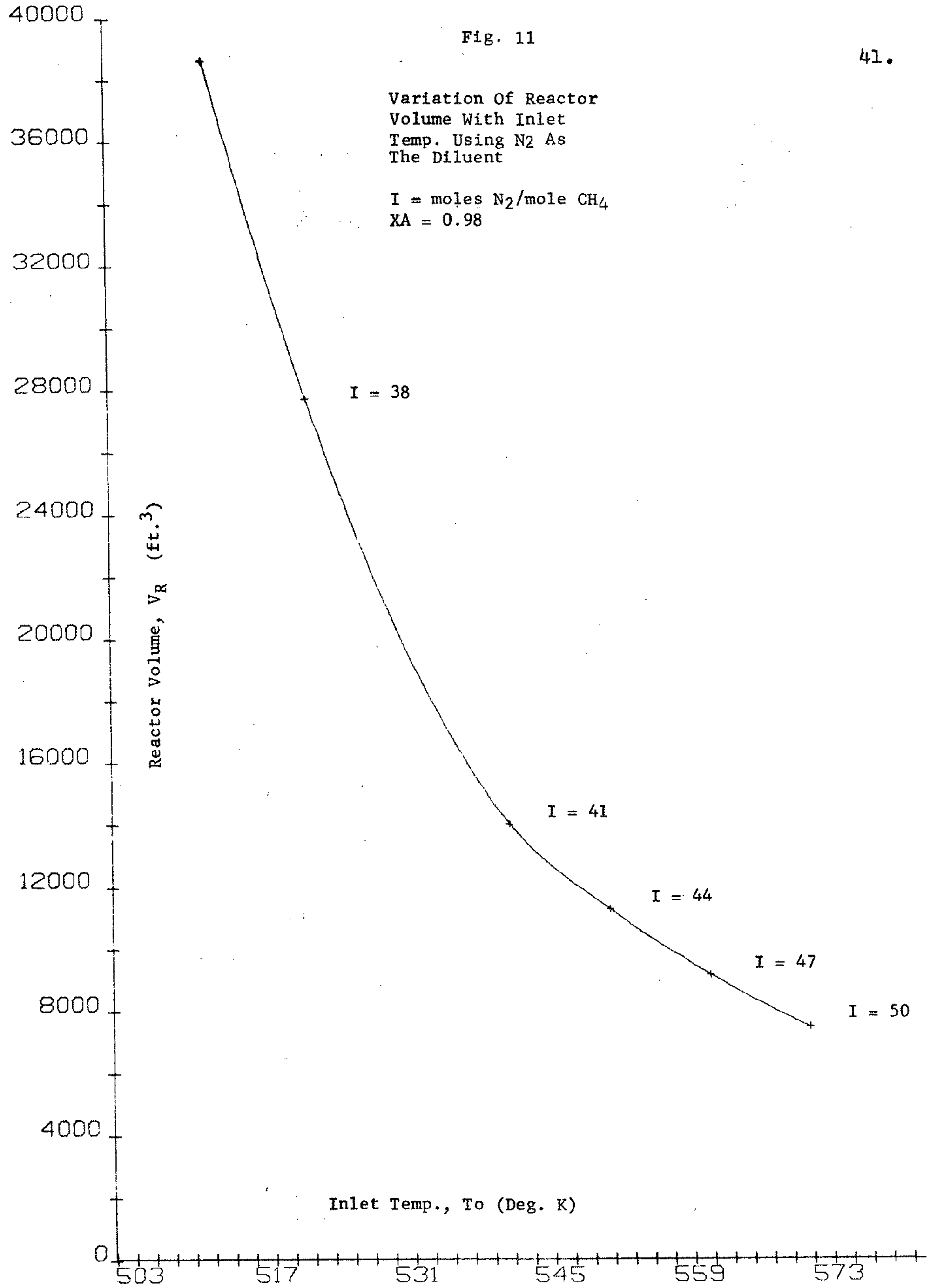


Fig. 11
Variation Of Reactor Volume With Inlet Temp. Using N2 As The Diluent
I = moles N2/mole CH4
XA = 0.98
I = 38
I = 41
I = 44
I = 47
I = 50
Reactor Volume, VR (ft.3)
Inlet Temp., To (Deg. K)
40000
36000
32000
28000
24000
20000
16000
12000
8000
4000
0
503
517
531
545
559
573

from 38 to 50 lb moles N_2/lb mole CH_4. As with HCl 3 lb moles N_2/lb mole CH_4 additional is required for each 10°C rise in inlet temperature.

The reactor volume decreases from 27,800 ft^3 to 7500 ft^3 over the temperature range studied. It was observed that when inlet temperature is increased from 543 to 573°K the reactor volume is approximately halved. When T_0 is decreased from 543 to 523°K, a 20° change, the volume doubles. The same observation can be made for N_2 as was made for CCl_4 and HCl. Lowering the feed temperature below 523°K causes a substantial increase in reactor volume, while increasing it above 573°K reduces the volume by only a minor amount.

The reactor volume required to increase methane conversion from 50 to 98% is nearly constant at 2500 ft^3 regardless of the feed temperature. However, the reactor volume required to attain 50% conversion increases from 5200 - 24,400 ft^3 as inlet temperature is decreased from 573 to 523°K. See Table 6.

Product distribution is nearly identical to the distribution obtained when CCl_4 and HCl is used. Low feed temperatures favor formation of CCl_4, while high feed temperatures favor formation of CH_2Cl_2. See Figure 12 for typical results.

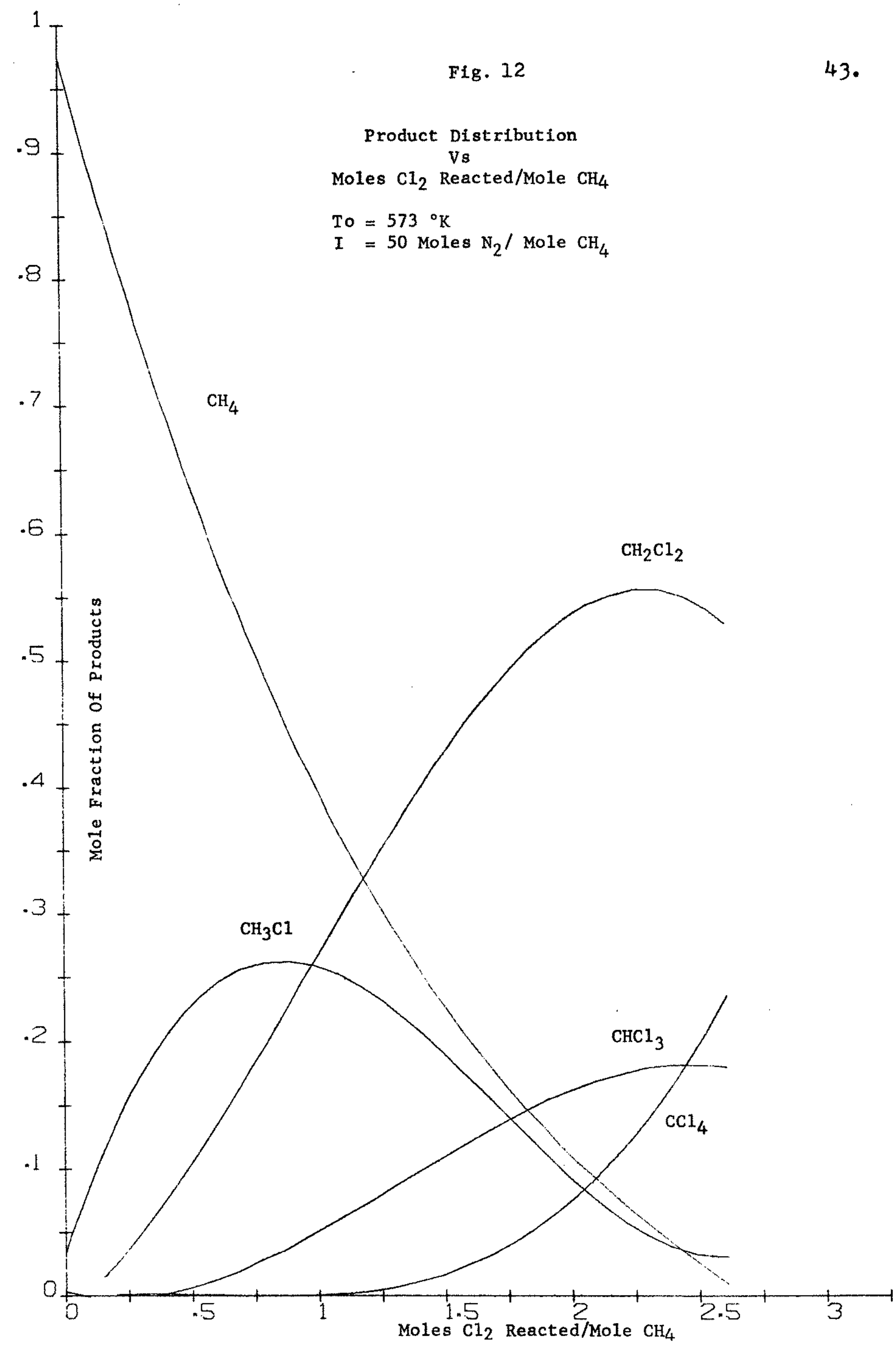


Fig. 12
Product Distribution
Vs
Moles Cl2 Reacted/Mole CH4
To = 573 °K
I = 50 Moles N2/ Mole CH4
CH4
CH2Cl2
CH3Cl
CHCl3
CCl4
Mole Fraction Of Products
Moles Cl2 Reacted/Mole CH4
1
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
.5
1.5
2
2.5
3

A Comparison of Three Diluents

When designing an adiabatic reactor capable of achieving 98% conversion of methane at an outlet temperature of 723°K, approximately 65% of the available Cl_2 is consumed. When fed with 10 lb moles/hr (160 lbs) of CH_4 and 42 lb moles (2982 lbs) of Cl_2, the reactor will produce approximately 1100 lb/hr of chlorinated product. The composition of this product stream varies slightly with inlet temperature and diluent ratio.

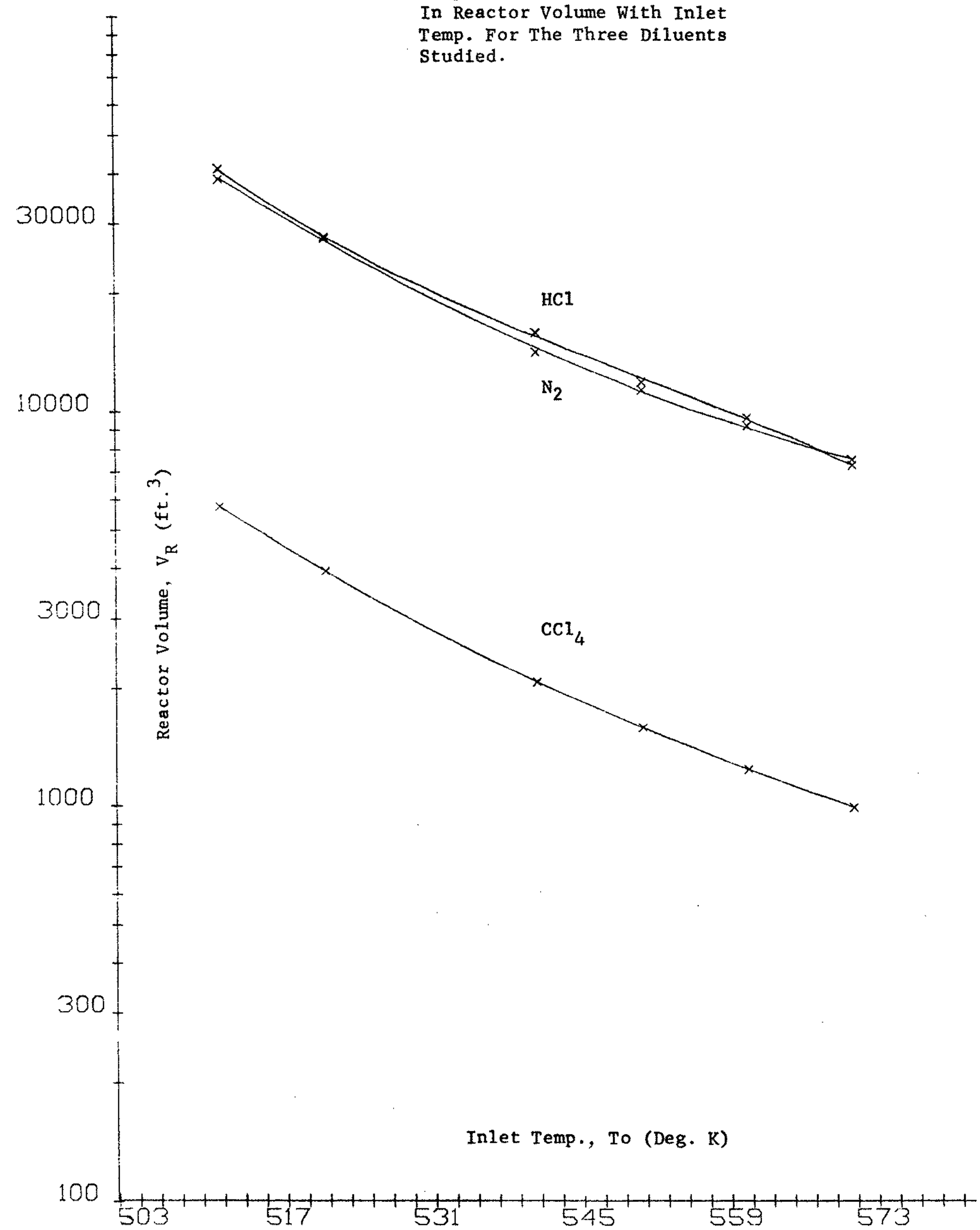
Because a large amount of heat is generated by the highly exothermic chlorinations, large amounts of inert are required to maintain a safe operating temperature of below 723°K. The correlation between feed temperature and diluent ratio shows the following masses of inerts are required as inlet temperature varies from 523 to 573°K:

CCl_4 - 17,600 to 23,400 lbs/hr
HCl - 14,000 to 18,900 lbs/hr
N_2 - 10,600 to 14,000 lbs/hr.

While more CCl_4 is required than either HCl or N_2, a reactor designed using CCl_4 as the inert is considerably smaller than one using either HCl or N_2. Figure 13 shows the volume of the CCl_4 reactor at inlet temperatures ranging from 523 to 573°K is approximately one-tenth that of the other inert gases at comparable inlet temperatures. Therefore, on a volumetric basis, one would choose the reactor with CCl_4

Fig. 13

Comparison Of The Variation In Reactor Volume With Inlet Temp. For The Three Diluents Studied.



as the inert. However, consideration must be given to the additional equipment and processing costs which would be incurred when vaporizing the large amount of the relatively high boiling CCl_4. It seems similar costs would not be encountered when using HCl or N_2 as the recycle gas instead of CCl_4.

It was also observed that as the reaction mass approaches the exit of the reactor with CCl_4 as the inert the reaction temperature is rising rapidly over a relatively small volumetric element, i.e., 5^o over 5 to 7 ft^3. In the case of using HCl or N_2 the temperature rise at the exit is more moderate, i.e., 3^o over 30 to 50 ft^3. This moderate temperature rise at the exit of the reactor is a definite advantage when quenching the product stream prior to purification.

While the volume of the reactors using HCl or N_2 are nearly equivalent, HCl would be preferred since it is available in large quantities as a reaction by-product and it could be removed from the product stream more easily than N_2.

Finally the study indicates regardless of which inert is used, the inlet temperature of the feed stream should be varied from 543 to 573°K. Feed temperatures below 543°K require too large a reactor volume, while temperatures above 573°K necessitate additional heating of the feed stream with little reduction in the reactor volume.

Effect of Pressure on The HCl System

While using the HCl inerted system has definite advantages over either the CCl_4 or N_2 systems, the reactor volume is considerably larger than the volume of a CCl_4 inerted system operated at comparable temperature and pressure. However, since reactor volume is directly proportional to the inverse of the total pressure squared, consideration was given to increasing the pressure on the HCl system in order to obtain a reduction in volume.

For inlet temperatures ranging from 553 to 573°K, it was determined that operating the HCl at approximately 3 atm. achieved reactor volumes comparable to those obtained on the CCl_4 system operated at 1 atm. See Table 8.

The quantity of HCl required and product distribution did not change with the increase in pressure. Figure 14 shows typical product distribution results which compare with Figure 10. Although only 3 atmospheres, is necessary to reduce the reactor volume to a size comparable to the CCl_4 recycle systems, further increases in pressure may be utilized for additional benefits.

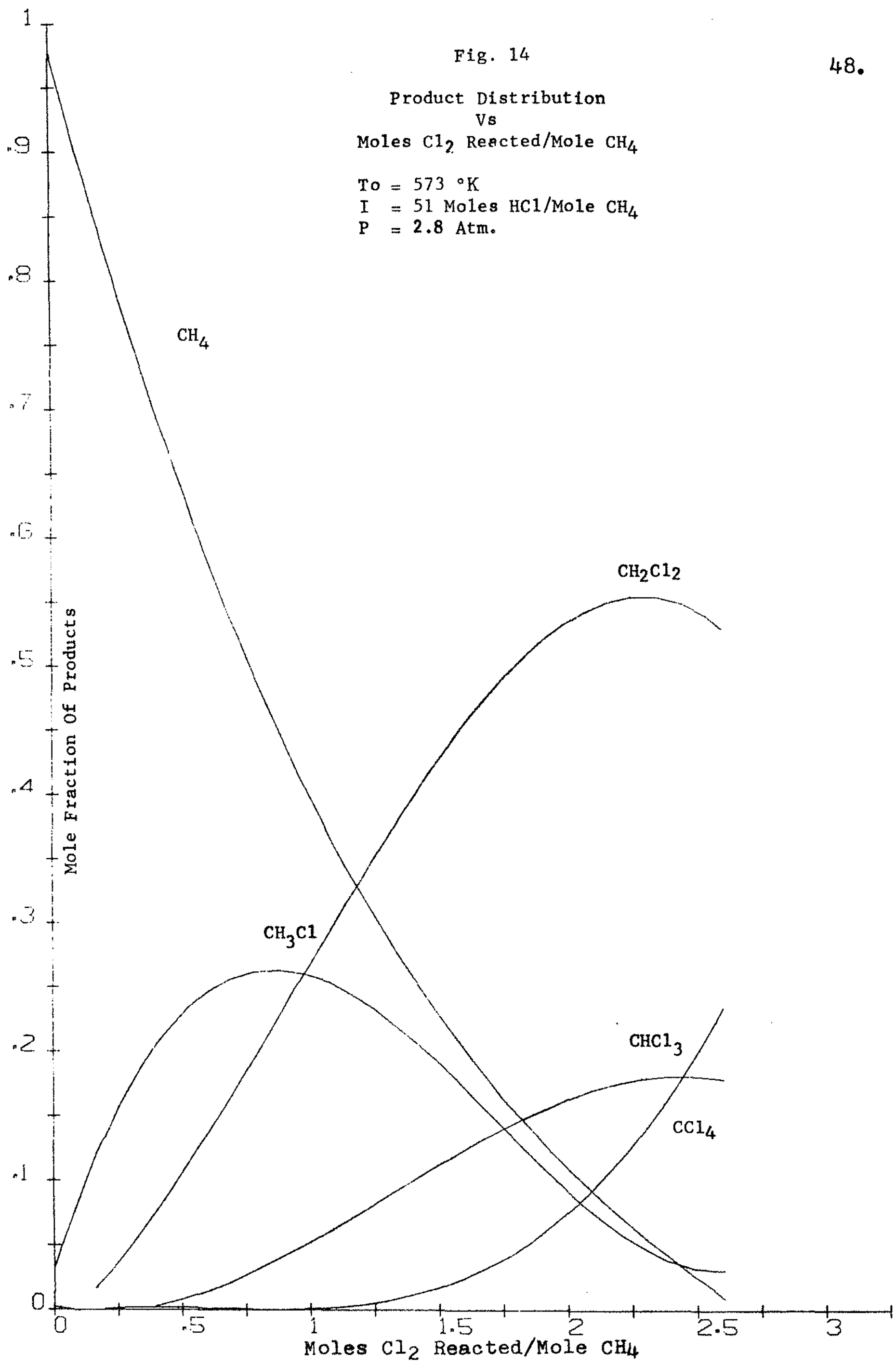


Fig. 14
Product Distribution
Vs
Moles Cl2 Reacted/Mole CH4
To = 573 °K
I = 51 Moles HCl/Mole CH4
P = 2.8 Atm.
CH4
CH2Cl2
CH3Cl
CHCl3
CCl4
Mole Fraction Of Products
Moles Cl2 Reacted/Mole CH4
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
.5
1.5
2
2.5
3

CONCLUSIONS

The conclusions made are:

1. The presence of inert diluents, such as CCl_4, HCl, or N_2, in the reactant feed stream of an adiabatic tubular reactor for the multiple chlorination of methane can effectively moderate the exothermic chlorination reactions so 98% conversion of methane is achieved at a maximum outlet temperature of $723^{o}K$.
2. The amount of any inert diluent required depends on the feed temperature of the reactants. Correlations between conversion of methane and amount inert at various feed temperatures were developed.
3. The reactor size is dependent on the total pressure of the system and the inlet temperature. The reactor volume is directly proportional to the reciprocal of the total pressure squared. A correlation between reactor volume and inlet feed temperature was developed for each inert.
4. When 98% conversion of the methane is obtained, product distribution at the outlet of the reactor varied slightly with the inlet temperature and the amount of diluent in the feed stream. Product distribution is essentially independent of total pressure.
5. To obtain 98% conversion, HCl is the recommended diluent. The feed temperature should range from 553 to $573^{o}K$ and the reactor should be operated at an elevated pressure. An HCl system operated at approximately 3 atm. and a

feed temperature of 573°K would require 51 lb moles HCl per lb mole of methane to achieve 98% conversion of the methane at an outlet temperature of 723°K. The volume of this reactor would be 990 ft^3 per 10 lb moles of CH_4 fed. This reactor system would produce the following product stream

CH_4 - 3 lb/hr

$CHCl_3$ - 10 lb/hr

CH_2Cl_2 - 450 lb/hr

$CHCl_3$ - 215 lb/hr

CCl_4 - 385 lb/hr .

RECOMMENDATIONS

The following recommendations are made:

1. While the use of HCl diluent in a reactor operated at elevated pressure is recommended, the optimum pressure was not found. This can only be accomplished by equating the cost of designing and installing a small high pressure reactor and the required accessories with the cost of a larger lower pressure reactor and its accessories.
2. If additional chlorination is required to all CCl_4 for example, the use of inert diluent in a non-isothermal, non-adiabatic reactor should be investigated. The program presented in this study can easily be amended to account for heat transfer through the reactor walls, which is necessary in a non-isothermal, non-adiabatic system.
3. While the recommended operating conditions discussed are reasonable based on the data generated, the true optimum reactor design can be determined only by reviewing the overall process economics.

Consideration must be given to equipment and operating costs of such factors as:

1) utilities
2) preparation of the reactant and inert feed streams
3) product separation and purification

before the optimum reactor can be designed.

NOMENCLATURE

C_i	Concentration of components, lb mole/ft^3.
cp	Specific heat, BTU/(lb mole)(^oK).
E	Activation energy, calories/mole.
F_i	Feed rate of components, lb mole/hr.
F_{TOT}	Total feed rate, lb mole/hr.
ΔF	Free energy of reaction, cal./(gm mole)(^oK).
ΔH_F	Heat of formation, BTU/lb mole.
ΔH_R	Heat of reaction, BTU/lb mole.
I	Diluent ratio, lb moles of inert per lb mole of CH_4.
k	Reaction rate constant, ft^3/(lb mole)(hr).
k_0	Frequency factor.
K_{eq}	Thermodynamic Equilibrium constant.
P_i	Partial pressure of key components, atm.
P_{TOT}	Total pressure, atm.
r_i	Reaction rate of key components, lb moles/(ft^3)(hr).
R	Ideal gas law constant 1.98 cal./(gm mole)(^oK) 0.73 (ft^3)(atm.)/(lb mole)(^oR).
t	Time, hrs.
T	Temperature, ^oK.
V_R	Reactor volume, ft^3.
X_A	Conversion of CH_4.
X_i	Conversion of key component.
y_i	Component mole fraction.

Subscripts

i	Refers to any key component.
F	Leaving, final, or outlet condition.
n	Refers to reaction number.
0	Entering, initial, or inlet condition.
1,2,3,4	Refers to the four key chlorination reactions.

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APPENDIX

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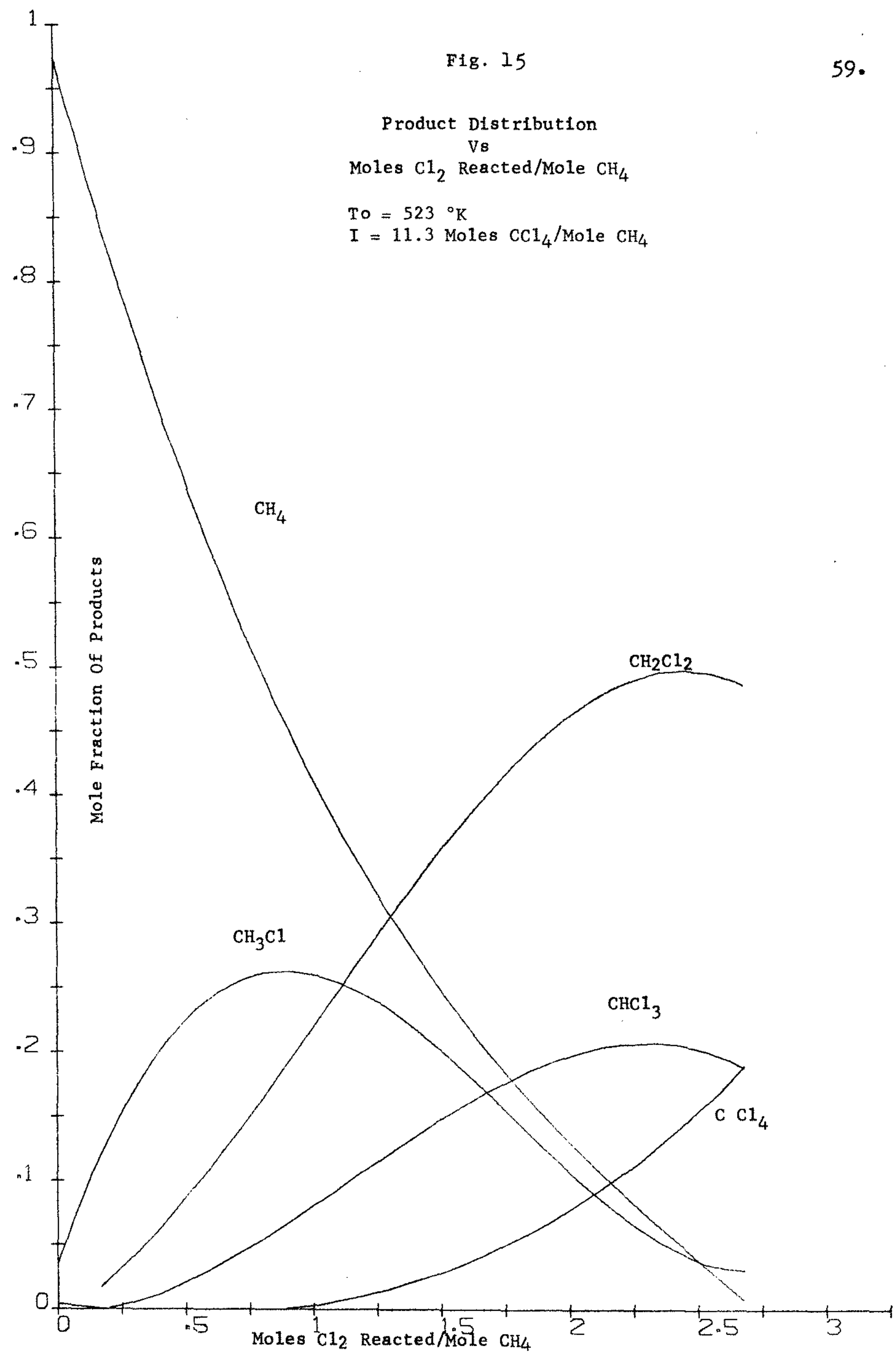

Fig. 15

Product Distribution
Vs
Moles Cl_2 Reacted/Mole CH_4

To = 523 °K
I = 11.3 Moles CCl_4/Mole CH_4

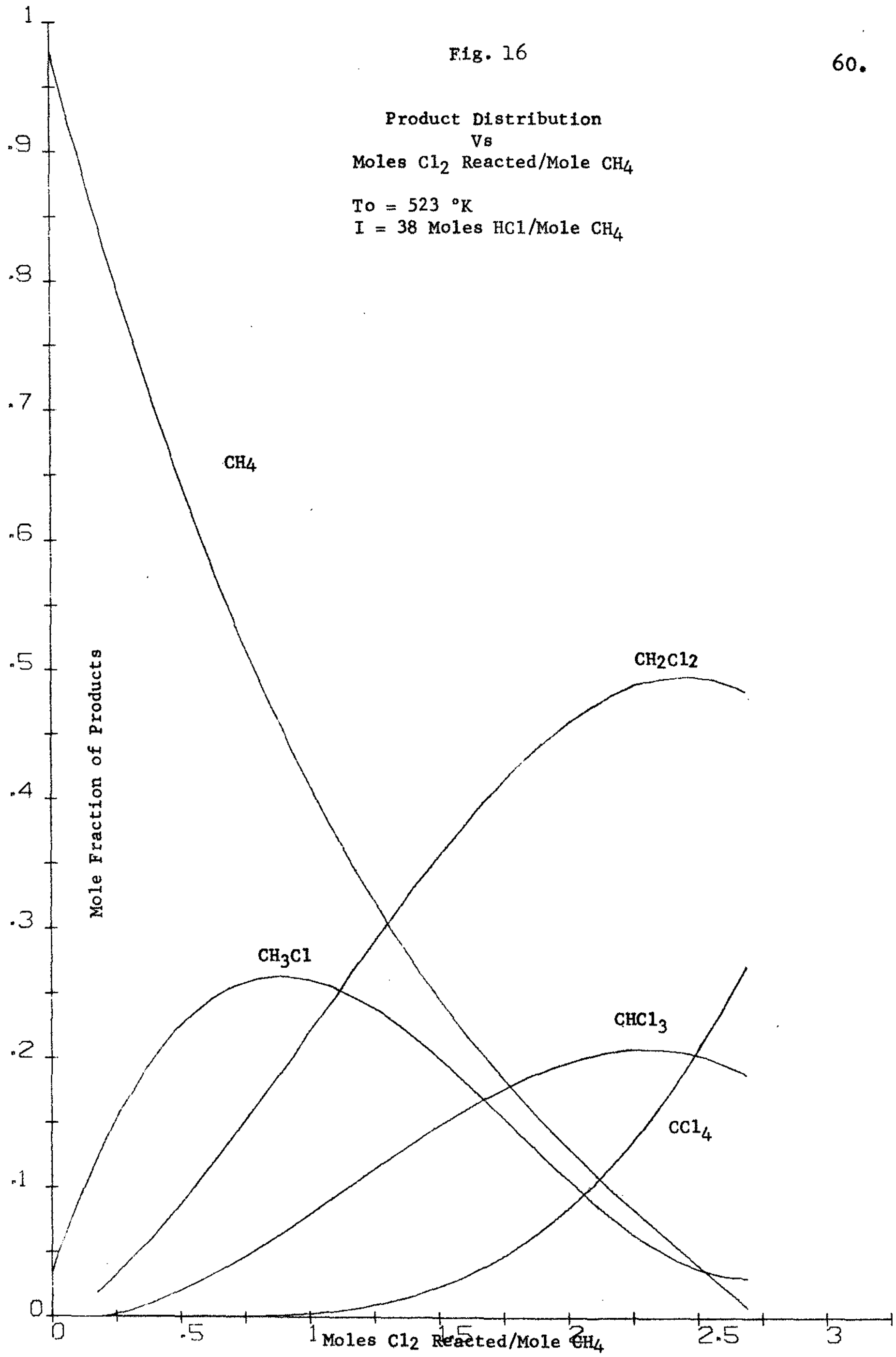
Fig. 16
Product Distribution
Vs
Moles Cl_2 Reacted/Mole CH_4
To = 523 °K
I = 38 Moles HCl/Mole CH_4
Mole Fraction of Products
Moles Cl_2 Reacted/Mole CH_4
CH_4
CH_2Cl_2
CH_3Cl
$CHCl_3$
CCl_4
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
.5
1
1.5
2
2.5
3

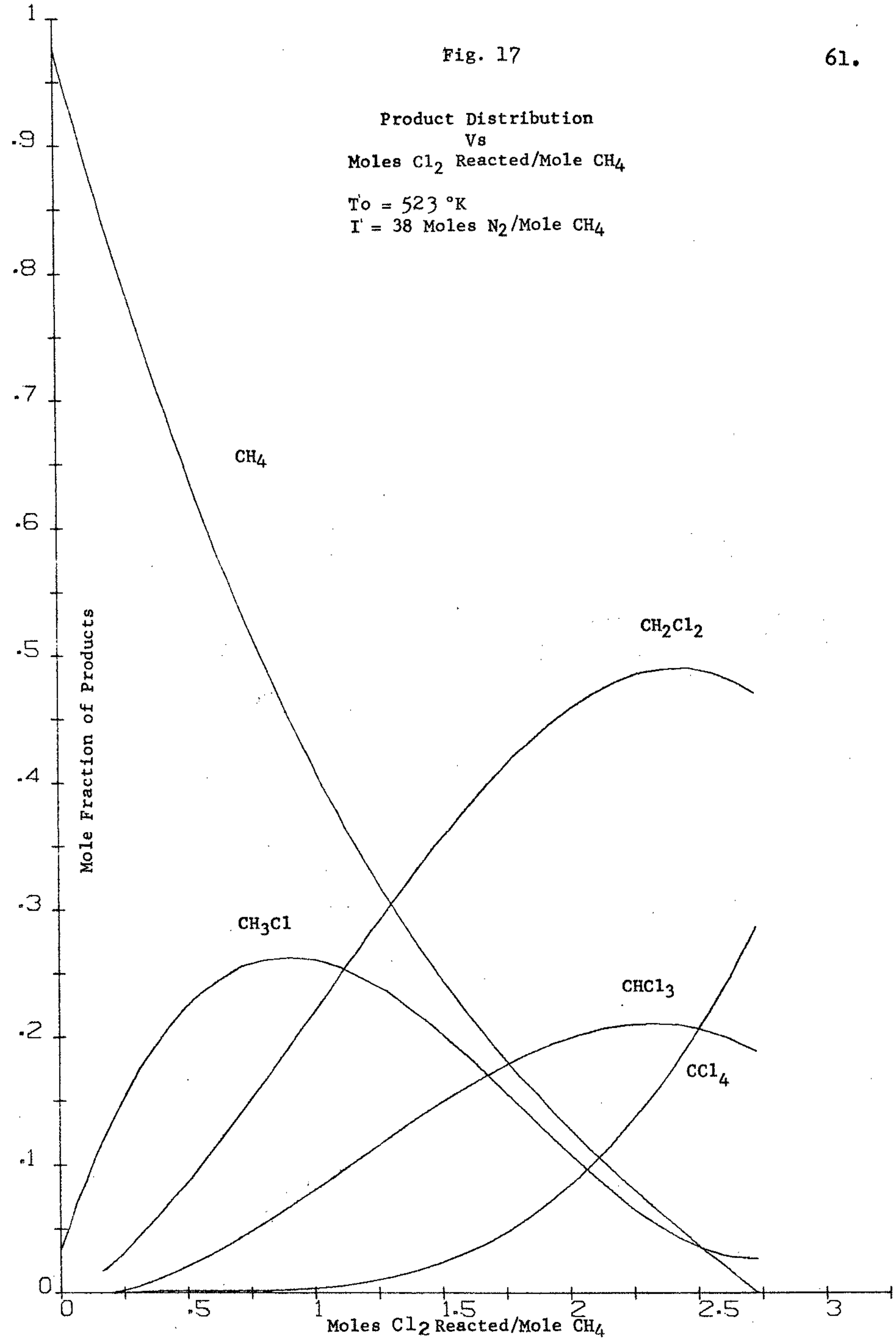
Fig. 17
Product Distribution
Vs
Moles Cl2 Reacted/Mole CH4
To = 523 °K
I' = 38 Moles N2/Mole CH4
CH4
CH2Cl2
CH3Cl
CHCl3
CCl4
Mole Fraction of Products
Moles Cl2 Reacted/Mole CH4
1
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
0
.5
1
1.5
2
2.5
3

```
C
C       SYMBOL    DESCRIPTION
C       ------    -----------
C       ACONV     CONVERSION OF METHANE
C       AT        ACTUAL TEMPERATURE,DEG K
C       A         METHANE
C       B         CHLORINE
C       C         METHYL CHLORIDE
C       D         METHYLENE CHLORIDE
C       E         CHLOROFORM
C       F         CARBON TETRACHLORIDE
C       N         NITROGEN
C       S         HYDROGEN CHLORIDE
C       CLOM      MOLES OF CHLORINE REACTED PER MOLE OF METHANE
C       CP        HEAT CAPACITY,BTU/LB.MOLE*DEG K
C       CPUSD      SPECIFIC HEAT EQUIVALENT TO CP
C       COEF       COEFFICIENTS OF RATE EQUATION TERMS
C       COEFU      COEFFICIENTS OF RATE EQUATION TERMS EQUIVALENT TO COEF
C       CON 1      FREQUENCY FACTOR
C       CON 2     CONVERSION FACTOR,1.8
C       CON 3      CONSTANT IN CP EQ.
C       CON 4      CONSTANT IN CP EQ.
C       CON 5      CONSTANT IN CP EQ.
C       CON 7      CONSTANT IN DHR EQ.
C       CON 8      CONSTANT IN DHR EQ.
C       CON 9      CONSTANT IN DHR EQ.
C       CON10      CONSTANT IN DHR EQ.
C       DHR       HEAT OF REACTION,BTU/LB.MOLE
C       DHRUD      HEAT OF INDIVIDUAL REACTIONS EQUIVALENT TO DHR
C       DL         CHANGE IN REACTOR VOLUME
C       DT        TEMPERATURE CHANGE
C       DY         CHANGE IN MOLE FRACTIONS OF COMPONENTS
C       E          ACTIVATION ENERGY
C       FAO        MOLAR FEED RATE OF METHANE,LB-MOLE/HR
C       FBO        MOLAR FEED RATE OF CHLORINE,LB-MOLE/HR
C       FFO        MOLAR FEED RATE OF CARBON TET,LB-MOLE/HR
C       FNO        MOLAR FEED RATE OF NITROGEN,LB-MOLE/HR
C       FSO       MOLAR FEED RATE OF HCL,LB-MOLE/HR
C       FTOT       TOTAL MOLAR FEED RATE,LB-MOLE/HR
C       GSCON      GAS CONSTANT,0.7302 ATM*CU-FT/ LB-MOLE*DEG R
C       HETRE     OVERALL ENTHALPY BALANCE
C       I          INDEX OF EQUATION
C       J          INDEX OF TERM OF EQUATION
C       L          REACTOR VOLUME
```



```
C       NERTN     RATIO OF NITROGEN TO METHANE IN FEED STREAM
C       NRHCL     RATIO OF HCL TO METHANE IN FEED STREAM
C       NRTCT     RATIO OF CARBON TET TO METHANE IN FEED STREAM
C       NMOLF     NORMALIZED MOLE FRACTION OF CHLORINATED COMPONENTS
C       P          PRESSURE,ATM
C       R          GAS CONSTANT,1.987BTU/LB-MOLE*DEG R
C       RAC       CORRECTED RATE CONSTANT
C       RTAVK      CORRECTED RATE CONSTANT EQUIVALENT TO RAC
C       REHET     OVERALL HEAT OF REACTION,BTU/LB-MOLE*DEG K
C       RERAT     REACTION RATE,LB.MOLE/CU.FT*HR
C       RRATE      REACTION RATE EQUIVALENT TO RERAT
C       RRATV      EQUIVALENT TO RRATE
C       RATPR      EQUIVALENT TO RRATV
C       RTCON     RATE CONSTANT,CU.FT./LB.MOLE*HR
C       T          INDEX OF TEMPERATURE ALONG THE TUBE
C       TERM      TERMS IN RATE EQUATION
C       TRM        TERM IN RATE EQUATION EQUIVALENT TO TERM
C       TO         INITIAL TEMPERATURE,DEG K
C       TMAX      MAXIMUM OUTLET TEMPERATURE,DEG K
C       XA        CONVERSION OF METHANE
C       XAMAX     MAXIMUM CONVERSION OF METHANE
C       YO        INITIAL MOLE FRACTION
C       YUSE2      EQUIVALENT TO Y
C       Y          MOLE FRACTIONS OF COMPONENTS
C
C
        A=2.
        CALL EXIT
        END
```

Function Statements

```
      FUNCTION CP   (CON2,CON3,CON4,CON5,T)
      CP   = CON2*(CON3+CON4*T-CON5*T*T)
      RETURN
      END
```

```
      FUNCTION DHR (CON2,CON7,CON8,CON9,CON10,T)
      DHR= CON2*(CON7+CON8*T+CON9*T*T+CON10*T*T*T)
      RETURN
      END
```

```
      FUNCTION HETRE (FTOT,Y,CP)
      DIMENSION Y(8),CP(8)
      HETRE=0.
      DO 35 J=1,8
   35 HETRE= HETRE+ FTOT*Y(J)*CP(J)
      RETURN
      END
```

```
      FUNCTION REHET (DHR,RERAT)
      DIMENSION DHR(4),RERAT(4)
      REHET=0.
      DO 30 J=1,4
   30 REHET= REHET+ DHR(J)*RERAT (J)
      RETURN
      END
```

```
      FUNCTION ACONV(YA,YAO)
      ACONV = 1-(YA/YAO)
      RETURN
      END
```

```
      FUNCTION CLOM ( YBO , YB , YAO )
C         CALCULATE MOLFS OF CHLORINE REACTED PER MOL OF METHANE.
      CLOM = ( YBO - YB ) / YAO
      RETURN
      END
```

```
      FUNCTION FTOT(F,M)
      DIMENSION F (2 )
      FTOT= 0.
      DO 29 I=1,M
29    FTOT= FTOT+ F(I)
      RETURN
      END
```

```
      FUNCTION YO    (FO, FTOT)
      YO =  FO/FTOT
      RETURN
      END
```

```
      FUNCTION RTCON (CON1,E,R,T)
      RTCON = CON1*EXP(-E/(R*T))
      RETURN
      END
```

```
      FUNCTION RAC (RTCON,P,GSCON,T)
      RAC=       (RTCON*P*P/(GSCON*GSCON*T*T))/3.24
      RETURN
      END
```

```
      FUNCTION TERM (COEF,RAC,YI,YJ)
      TERM= COEF*RAC*YI*YJ
      RETURN
      END
```

```
      FUNCTION RERAT  (TERM,M)
      DIMENSION TERM(2)
      RERAT  = 0.
      DO 25 J=1,M
25    RERAT  = RERAT  + TERM(J)
      RETURN
      END
```

```
      SUBROUTINE INPUT
      INTEGER T
      REAL L (51) , MOLFC (8)
      COMMON KIN,KOU,P,TO,R,GSCON,FTOTL,CON2,DL(51),L     ,FO(8),CON1(4),
     1       F(4),CON3(8),CON4(8),CON5(8),CON7(8),CON8(8),
     2       CON9(8),CON10(8),COEF(7,4),TMAX
      COMMON RATEK(4),RTAVK(4),TRM(4),CPUSD(8),DHRUD(4),
     1      Y(8, 51) , RRATE(8, 51) , DT, XA,    DY(8, 51) , T,     AT
     2 , XAMAX , MOLFC
      KOU=3
      KIN=2
C         READ INPUT FROM CARDS.
      READ (KIN,101)            ( FO ( I) , I = 1 , 8 )
 101  FORMAT (8F 9.2)
C        TEST IF ALL VALUES OF FO ARE 0.
      DO 95 I = 1 , 8
      IF ( FO ( I )  )   96 , 95 , 96
 95   CONTINUE
      CALL EXIT
C        IF SO , THEN EXIT.
 96   CONTINUE
      READ (KIN,102) ( CON1(I),E(I) ,I=1,4)
 102  FORMAT(4(E10.3,F8.0))
      READ (KIN,103)  CON2
 103  FORMAT (F4.2)
      READ (KIN,104)           ( CON3(I),CON4(I),CON5(I) ,I=1,8)
 104  FORMAT  (2(F8.4,2E10.3))
      READ (KIN,105)( CON7(I),CON8(I),CON9(I),CON10(I) ,I=1,4)
 105  FORMAT  (F8.0,F9.4, 2E13.3)
      READ (KIN,201) P,GSCON,R,TO,DT,TMAX,XAMAX
 201  FORMAT (F5.2,2F8.4,F9.1,F7.3,F9.2,F7.4)
      READ (KIN,202)  ((COEF(I,J),J=1,4),I=1,7)
 202  FORMAT (36F2.0)
C          PRINT INPUT.
      WRITE(KOU,301)             ( FO ( I) , I = 1 , 8 )
 301  FORMAT (1H1,'     FBO       FFO       FNO       FAO       FCO       FDO
     1     FEO       FSO'/(8F9.2))
      WRITE (KOU,302) ( CON1(I),E(I) ,I=1,4)
 302  FORMAT (1H0,'FREQ FACTOR      ACT ENERGY'/(E15.5,F13.0))
      WRITE (KOU,303) CON2
 303  FORMAT (1H0,'CONV FACTOR'/F5.2)
```

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```
      WRITE (KOU,304) ( CON3(I),CON4(I),CON5(I) ,I=1,8)
 304  FORMAT (1H0,'CONST    OF    CP'/(F10.4,2E15.4))
      WRITE (KOU,305) ( CON7(I),CON8(I),CON9(I),CON10(I) ,I=1,4)
 305  FORMAT (1H0,'CONST  OF  REACTION  HEAT'/(F10.0,F10.4,2E15.3))
      WRITE (KOU,401) P,GSCON,R,TO,DT,TMAX,XAMAX
 401  FORMAT (1H0,5X,'P           GSCON         R         TO         DT
     1  TMAX          XAMAX'/7F10.4)
      WRITE (KOU,402) ((COEF(I,J),J=1,4),I=1,7)
 402  FORMAT (1H0,'COEF'/(4F4.0))
      RETURN
      END

FEATURES SUPPORTED
 ONE WORD INTEGERS

CORE REQUIREMENTS FOR INPUT
 COMMON   2942  VARIABLES      4  PROGRAM    564

RELATIVE ENTRY POINT ADDRESS IS 00D2 (HEX)

END OF COMPILATION
```

```
      SUBROUTINE DERV
      INTEGER T
      REAL L (51) , MOLFC (8)
      DIMENSION YUSE2 (8) , RRATV (8)
      COMMON KIN,KOU,P,TO,R,GSCON,FTOTL,CON2,DL(51),L     ,FO(8),CON1(4),
     1       E(4),CON3(8),CON4(8),CON5(8),CON7(8),CON8(8),
     2       CON9(8),CON10(8),COEF(7,4),TMAX
      COMMON RATEK(4),RTAVK(4),TRM(4),CPUSD(8),DHRUD(4),
     1      Y(8, 51) , RRATE(8, 51) , DT, XA,    DY(8, 51) , T,     AT
     2 , XAMAX , MOLFC
C     EQUATION 1 TO CALCULATE RATE CONSTANT
      TUSED=AT
      DO 35 J=1,4
      CON= CON1(J)
      EUSED= E(J)
      RATEK(J)= RTCON (CON,EUSED,R,TUSED)
C     EQUATION 2 TO CALCULATE FOR CALCULATING CORRECTED RATE CONSTANT
      RKUSD= RATEK(J)
   35 RTAVK(J)= RAC (RKUSD,P,GSCON,TUSED)
C     EQUATION 3 TO CALCULATE INITIAL MOLE FRACTIONS
      IF ( T - 1 )   50 , 40 , 50
   40 CONTINUE
      DO 45 I=1,8
      FUSED= FO(I)
   45 Y(I,1)= YO(FUSED,FTOTL)
   50 CONTINUE
C     EQUATION 4 TO CALCULATE TERMS OF RATE EQUATION
      DO 65 I=1,7
      DO 55 J=1,4
      COEFU= COEF(I,J)
      RTAVU= RTAVK(J)
      YUSED= Y(J+3, T )
      YBU= Y(1, T )
   55 TRM(J)  = TERM(COEFU,RTAVU,YUSED,YBU)
C     EQUATION 5 TO CALCULATE REACTION RATE
      RRATE(I,T)= RERAT(TRM,4)
C     EQUATION 6 TO CALCULATE DY
      RRATV(I)= RRATE(I,T)
C     EQUATION 1' TO CALCULATE COMPONENT SPECIFIC HEAT
      TUSED=AT
      DO 75 J=1,8
```

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```
      CONU3= CON3(J)
      CONU4= CON4(J)
      CONU5= CON5(J)
   75 CPUSD(J)=  CP(CON2,CONU3,CONU4,CONU5,TUSED)
C     EQUATION 2' TO CALCULATE COMPONENT HEAT OF REACTION
      DO 85 J=1,4
      CONU7= CON7(J)
      CONU8= CON8(J)
      CONU9= CON9(J)
      COU10= CON10(J)
   85 DHRUD(J)= DHR(CON2,CONU7,CONU8,CONU9,COU10,TUSED)
      DO 95 J=1,8
   95 YUSE2(J)= Y(J, T )
C     EQUATION 5' TO CALCULATE HEAT BALANCE
   65 CONTINUE
      DL(T)=-DT*HETRE(FTOTL,YUSE2,CPUSD)/REHET(DHRUD,TRM)
      DO 98 I = 1 , 7
   98 DY(I,T)= RRATE(I,T)   *DL (T   ) / FTOTL
      DY ( 8 , T ) = 0.
C     EQUATION 7 TO CALCULATE CONVERSION OF COMPONENT A-(XA)
      YAU= Y(4,T)
      YAO= Y(4,1)
      XA= ACONV(YAU,YAO)
      CALL NMOLF
      RETURN
      END
```

```
      SUBROUTINE NMOLF
C     SUBROUTINE TO CALCULATE NORMALIZED MOL FRACTION.
      INTEGER T
      REAL L (51) , MOLFC (8) , NMOLS
      COMMON KIN,KOU,P,TO,R,GSCON,FTOTL,CON2,DL(51),L     ,FO(8),CON1(4),
     1       E(4),CON3(8),CON4(8),CON5(8),CON7(8),CON8(8),
     2       CON9(8),CON10(8),COEF(7,4),TMAX
      COMMON RATEK(4),RTAVK(4),TRM(4),CPUSD(8),DHRUD(4),
     1      Y(8, 51) , RRATE(8, 51) , DT, XA,     DY(8, 51) , T,      AT
     2 , XAMAX , MOLFC
      K = T
      YFS = Y(2,K) - Y (2,1)
      NMOLS     = YFS
      DO 31  J = 4 , 7
   31 NMOLS     = NMOLS     + Y (J , K )
      DO 34  J = 4 , 7
   34 MOLFC (J) = Y ( J , K)/ NMOLS
      MOLFC (2) =(Y ( 2 , K) - Y ( 2 , 1 ))/ NMOLS
      RETURN
      END
```

```
C      DV523 MAIN PROGRAM.
       INTEGER T
       REAL L (51) , MOLFC (8)
       REAL NERTN , NRTCT , NRHCL
       DIMENSION IV ( 8 )
       COMMON KIN,KOU,P,TO,R,GSCON,FTOTL,CON2,DL(51),L     ,FO(8),CON1(4),
      1        E(4),CON3(8),CON4(8),CON5(8),CON7(8),CON8(8),
      2        CON9(8),CON10(8),COEF(7,4),TMAX
       COMMON RATEK(4),RTAVK(4),TRM(4),CPUSD(8),DHRUD(4),
      1      Y(8, 51) , RRATE(8, 51) , DT, XA,     DY(8, 51) , T,      AT
      2 , XAMAX , MOLFC , CLRM
       DATA IV / 6 , 5 , 8 , 1 , 2 , 3 , 4 , 7 /
       NC = 8
 12    T=1
       CALL INPUT
       AT=TO
       FTOTL = FTOT(FO,NC)
       L(T)= 0.
C      CALCULATION OF INERT NITROGEN, CARBON TETRACHLORIDE AND
C          HYDROCHLORIC ACID
       NERTN = FO ( 3 ) / FO ( 4 )
       NRTCT = FO ( 2 ) / FO ( 4 )
       NRHCL = FO ( 8 ) / FO ( 4 )
       WRITE ( KOU , 310 ) NERTN , NRTCT , NRHCL , TO
 310   FORMAT ( 1 H1 , 25 X , 'INERT COMPONENTS' /
      1   5 X , 'NITROGEN =' , F 8.2 , 5 X , 'CARBON TET =' , F 8.2 ,
      2   5 X , 'HCL =' , F 8.2 //
      3   10 X , 'INLET TEMPERATURE =' , F 6.1 // )
C         PRINT NEW HEADINGS
       WRITE ( KOU , 311 )
 311   FORMAT ( 1 HO , 1 X , 'COUNTER' , 4 X , 'TEMPERATURE' , 4 X ,
      1   'VOLUME' , 6 X , 'XA' , 6 X , 'MOL FA' , 4 X , 'MOL FC' , 4 X ,
      2   'MOL FD' , 4 X , 'MOL FE' , 4 X , 'MOL FF'
      3   , 4 X , 'MOL CL2 REACT/ MOL CH4' )
       WRITE ( KOU , 313 )
 313   FORMAT ( 1 H  , 15 X , 'DEG. K' , 7 X , 'CU.FT.' )
       WRITE ( KOU , 312 )
 312   FORMAT ( 1 H  , 1 X , '-------' , 4 X , '-----------' , 4 X ,
      4   '------' , 6 X , '--' , 6 X , '------' , 4 X , '------' , 4 X ,
      5   '------' , 4 X , '------' , 4 X , '------'
```

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```
      6   , 4 X , '----------------------' )
 21    CONTINUE
       CALL DERV
       DO 35 I = 1 , NC
       IA = IV ( I )
 35    Y(I,T+1)= Y(I,T)+DY(IA,T)
C         ADD CALCULATION OF CHLOINE TO METHANE REACTION RATIO TO MAIN
       YBO = Y ( 1 , 1 )
       YAO = Y ( 4 , 1 )
       IF ( T - 1 )  43 , 43 , 45
 43    YB = Y ( 1 , 1 )
       GO TO 47
 45    YB = Y ( 1 , T )
 47    CONTINUE
       CLRM = CLOM ( YBO , YB , YAO )
       L(T+1)= L(T)+ DL(T)
       CALL OTPUT
       T=T+1
       AT= AT+DT
       IF (XA-XAMAX) 100,100,999
 100   IF (AT- TMAX) 21,21,999
 999   GO TO 12
       END
```

```
      SUBROUTINE OTPUT
      INTEGER T
      REAL L (51) , MOLFC (8)
      COMMON KIN,KOU,P,TO,R,GSCON,FTOTL,CON2,DL(51),L     ,FO(8),CON1(4),
     1       E(4),CON3(8),CON4(8),CON5(8),CON7(8),CON8(8),
     2       CON9(8),CON10(8),COEFF(7,4),TMAX
      COMMON RATEK(4),RTAVK(4),TRM(4),CPUSD(8),DHRUD(4),
     1      Y(8, 51) , RRATE(8, 51) , DT, XA,    DY(8, 51) , T,      AT
     2 , XAMAX , MOLFC , CLRM
C         PRINT OUTPUT.
C         BELOW IS FOR OTPUT ROUTINE
C        PAT   IS  PRINTED ACTUAL TEMPERATURE
      PAT = AT + .05
      WRITE ( KOU , 320 ) T ,PAT , L (T) , XA , ( MOLFC ( J ) , J=4,7 )
     1  , MOLFC ( 2) , CLRM
  320 FORMAT ( 1 H  , 4 X , I 2 , 8 X , F 8.1 , 4 X , F 9.2 , 4 X ,
     1 7 ( F 6 . 4 , 4 X ) )
      RETURN
      END
```

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	113.00	0.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF CP		
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT			
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	523.0001	4.0000	723.0001	99.0000

COEF			
-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

Run 1

Inlet Temp. - 523°K

11.3 Moles CCl_4/Mole CH_4

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 11.30 HCL = 0.00

INLET TEMPERATURE = 523.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	523.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	527.0	684.40	0.0500	0.9490	0.0500	0.0000	0.0000	0.0000	0.0500
3	531.0	1226.23	0.0955	0.9044	0.0908	0.0047	0.0000	0.0000	0.1003
4	535.0	1657.51	0.1372	0.8627	0.1242	0.0124	0.0006	0.0000	0.1505
5	539.0	2003.94	0.1757	0.8242	0.1517	0.0219	0.0020	0.0000	0.2017
6	543.0	2284.96	0.2115	0.7884	0.1745	0.0327	0.0042	0.0000	0.2528
7	547.0	2515.09	0.2450	0.7549	0.1933	0.0443	0.0072	0.0000	0.3040
8	551.0	2705.21	0.2766	0.7233	0.2090	0.0565	0.0108	0.0001	0.3554
9	555.0	2862.53	0.3066	0.6933	0.2219	0.0692	0.0151	0.0002	0.4070
10	559.0	2996.35	0.3351	0.6648	0.2325	0.0822	0.0199	0.0004	0.4587
11	563.0	3109.52	0.3625	0.6374	0.2410	0.0955	0.0251	0.0007	0.5106
12	567.0	3203.85	0.3887	0.6112	0.2477	0.1090	0.0308	0.0010	0.5626
13	571.0	3285.35	0.4140	0.5859	0.2529	0.1225	0.0367	0.0014	0.6147
14	575.0	3355.39	0.4384	0.5616	0.2566	0.1367	0.0430	0.0019	0.6670
15	579.0	3415.91	0.4619	0.5380	0.2591	0.1505	0.0494	0.0025	0.7194
16	583.0	3468.46	0.4849	0.5151	0.2604	0.1650	0.0561	0.0032	0.7719
17	587.0	3514.30	0.5070	0.4929	0.2606	0.1793	0.0629	0.0041	0.8246
18	591.0	3554.47	0.5286	0.4713	0.2599	0.1936	0.0698	0.0050	0.8773
19	595.0	3589.83	0.5495	0.4504	0.2583	0.2081	0.0769	0.0061	0.9302
20	599.0	3621.08	0.5700	0.4299	0.2558	0.2226	0.0840	0.0074	0.9831
21	603.0	3648.83	0.5899	0.4100	0.2526	0.2371	0.0911	0.0089	1.0362
22	607.0	3673.56	0.6093	0.3906	0.2487	0.2517	0.0983	0.0105	1.0894
23	611.0	3695.69	0.6283	0.3716	0.2442	0.2662	0.1055	0.0123	1.1428
24	615.0	3715.58	0.6468	0.3531	0.2390	0.2806	0.1126	0.0144	1.1962
25	619.0	3733.51	0.6648	0.3351	0.2333	0.2950	0.1197	0.0167	1.2497
26	623.0	3749.75	0.6825	0.3174	0.2270	0.3093	0.1267	0.0193	1.3034
27	627.0	3764.51	0.6997	0.3002	0.2203	0.3235	0.1336	0.0221	1.3571
28	631.0	3777.98	0.7165	0.2834	0.2132	0.3375	0.1404	0.0253	1.4110
29	635.0	3790.32	0.7329	0.2670	0.2057	0.3513	0.1471	0.0287	1.4649
30	639.0	3801.66	0.7489	0.2510	0.1979	0.3649	0.1536	0.0326	1.5190
31	643.0	3812.13	0.7645	0.2354	0.1896	0.3781	0.1599	0.0368	1.5732
32	647.0	3821.84	0.7797	0.2202	0.1811	0.3911	0.1660	0.0414	1.6275
33	651.0	3830.87	0.7945	0.2054	0.1723	0.4037	0.1719	0.0465	1.6819
34	655.0	3839.31	0.8089	0.1910	0.1634	0.4159	0.1775	0.0521	1.7364
35	659.0	3847.22	0.8229	0.1770	0.1542	0.4275	0.1828	0.0582	1.7910
36	663.0	3854.67	0.8365	0.1634	0.1450	0.4387	0.1878	0.0649	1.8458
37	667.0	3861.72	0.8496	0.1503	0.1356	0.4492	0.1924	0.0722	1.9006
38	671.0	3868.41	0.8623	0.1376	0.1262	0.4591	0.1966	0.0802	1.9556
39	675.0	3874.79	0.8745	0.1254	0.1168	0.4682	0.2003	0.0890	2.0107
40	679.0	3880.91	0.8863	0.1136	0.1075	0.4765	0.2036	0.0985	2.0659
41	683.0	3886.80	0.8976	0.1023	0.0982	0.4840	0.2064	0.1089	2.1213
42	687.0	3892.49	0.9083	0.0916	0.0891	0.4904	0.2085	0.1202	2.1768
43	691.0	3898.02	0.9186	0.0813	0.0802	0.4957	0.2100	0.1326	2.2324
44	695.0	3903.42	0.9283	0.0716	0.0715	0.4999	0.2108	0.1460	2.2881
45	699.0	3908.72	0.9374	0.0625	0.0631	0.5028	0.2108	0.1606	2.3440
46	703.0	3913.94	0.9460	0.0539	0.0551	0.5043	0.2100	0.1765	2.4000
47	707.0	3919.11	0.9539	0.0460	0.0475	0.5043	0.2083	0.1937	2.4562
48	711.0	3924.27	0.9612	0.0387	0.0403	0.5027	0.2057	0.2123	2.5126
49	715.0	3929.43	0.9678	0.0321	0.0337	0.4995	0.2020	0.2325	2.5691
50	719.0	3934.63	0.9738	0.0261	0.0277	0.4946	0.1972	0.2542	2.6257
51	723.0	3939.90	0.9790	0.0209	0.0223	0.4877	0.1913	0.2776	2.6825

Run 2

Inlet Temp. - 543°K

12.5 Moles CCl_4/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	125.00	0.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13510E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF CP		
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT			
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	543.0001	3.6000	723.0001	99.0000

COEF			
-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 12.50 HCL = 0.00

INLET TEMPERATURE = 543.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	543.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	546.6	289.43	0.0494	0.9505	0.0494	0.0000	0.0000	0.0000	0.0494
3	550.2	526.63	0.0945	0.9054	0.0899	0.0046	0.0000	0.0000	0.0991
4	553.8	722.56	0.1360	0.8639	0.1232	0.0123	0.0004	0.0000	0.1491
5	557.4	885.80	0.1744	0.8255	0.1509	0.0221	0.0013	0.0000	0.1993
6	561.0	1022.95	0.2103	0.7896	0.1738	0.0334	0.0029	0.0000	0.2498
7	564.6	1139.10	0.2440	0.7559	0.1930	0.0458	0.0051	0.0000	0.3003
8	568.2	1239.16	0.2759	0.7240	0.2098	0.0589	0.0079	0.0001	0.3511
9	571.8	1323.21	0.3061	0.6938	0.2220	0.0726	0.0112	0.0002	0.4020
10	575.4	1396.68	0.3350	0.6649	0.2327	0.0868	0.0150	0.0003	0.4530
11	579.0	1460.50	0.3626	0.6373	0.2414	0.1013	0.0192	0.0005	0.5042
12	582.6	1516.24	0.3891	0.6108	0.2482	0.1162	0.0237	0.0008	0.5555
13	586.2	1565.15	0.4146	0.5853	0.2534	0.1312	0.0287	0.0012	0.6069
14	589.8	1609.27	0.4392	0.5607	0.2572	0.1464	0.0339	0.0016	0.6584
15	593.4	1646.45	0.4630	0.5369	0.2597	0.1617	0.0394	0.0021	0.7101
16	597.0	1680.40	0.4861	0.5138	0.2610	0.1772	0.0451	0.0027	0.7618
17	600.6	1710.72	0.5084	0.4915	0.2612	0.1927	0.0510	0.0034	0.8137
18	604.2	1737.29	0.5301	0.4698	0.2604	0.2083	0.0570	0.0043	0.8656
19	607.8	1762.34	0.5512	0.4487	0.2587	0.2239	0.0633	0.0052	0.9177
20	611.4	1784.42	0.5717	0.4282	0.2561	0.2395	0.0696	0.0064	0.9699
21	615.0	1804.43	0.5917	0.4082	0.2529	0.2550	0.0760	0.0076	1.0221
22	618.6	1822.63	0.6112	0.3887	0.2489	0.2706	0.0825	0.0091	1.0745
23	622.2	1839.24	0.6302	0.3697	0.2442	0.2860	0.0891	0.0107	1.1269
24	625.8	1854.45	0.6487	0.3512	0.2390	0.3013	0.0957	0.0126	1.1795
25	629.4	1868.44	0.6668	0.3331	0.2332	0.3165	0.1023	0.0146	1.2322
26	633.0	1881.33	0.6844	0.3155	0.2269	0.3316	0.1089	0.0169	1.2849
27	636.6	1893.26	0.7016	0.2983	0.2201	0.3464	0.1154	0.0195	1.3377
28	640.2	1904.34	0.7184	0.2815	0.2129	0.3611	0.1219	0.0223	1.3907
29	643.8	1914.66	0.7347	0.2652	0.2053	0.3754	0.1284	0.0255	1.4437
30	647.4	1924.30	0.7507	0.2492	0.1973	0.3895	0.1347	0.0290	1.4969
31	651.0	1933.35	0.7662	0.2337	0.1891	0.4032	0.1410	0.0328	1.5501
32	654.6	1941.87	0.7813	0.2186	0.1805	0.4165	0.1470	0.0370	1.6034
33	658.2	1949.91	0.7960	0.2039	0.1718	0.4294	0.1530	0.0417	1.6568
34	661.8	1957.54	0.8103	0.1896	0.1628	0.4419	0.1587	0.0468	1.7104
35	665.4	1964.80	0.8242	0.1757	0.1537	0.4538	0.1642	0.0524	1.7640
36	669.0	1971.73	0.8377	0.1622	0.1444	0.4651	0.1695	0.0586	1.8177
37	672.6	1978.37	0.8507	0.1492	0.1351	0.4757	0.1744	0.0653	1.8715
38	676.2	1984.76	0.8633	0.1366	0.1257	0.4856	0.1791	0.0727	1.9255
39	679.8	1990.94	0.8754	0.1245	0.1164	0.4947	0.1834	0.0808	1.9795
40	683.4	1996.93	0.8870	0.1129	0.1071	0.5029	0.1872	0.0896	2.0337
41	687.0	2002.76	0.8982	0.1017	0.0979	0.5102	0.1907	0.0993	2.0879
42	690.6	2008.46	0.9088	0.0911	0.0888	0.5165	0.1936	0.1098	2.1423
43	694.2	2014.06	0.9190	0.0809	0.0800	0.5216	0.1959	0.1214	2.1968
44	697.8	2019.59	0.9285	0.0714	0.0714	0.5254	0.1977	0.1339	2.2515
45	701.4	2025.06	0.9376	0.0623	0.0631	0.5280	0.1987	0.1476	2.3062
46	705.0	2030.50	0.9460	0.0539	0.0551	0.5291	0.1990	0.1625	2.3611
47	708.6	2035.94	0.9536	0.0461	0.0476	0.5288	0.1985	0.1787	2.4162
48	712.2	2041.40	0.9610	0.0389	0.0406	0.5268	0.1972	0.1963	2.4713
49	715.8	2046.91	0.9675	0.0324	0.0341	0.5231	0.1948	0.2153	2.5267
50	719.4	2057.49	0.9734	0.0265	0.0281	0.5177	0.1915	0.2359	2.5822
51	723.0	2058.16	0.9786	0.0213	0.0227	0.5106	0.1872	0.2580	2.6378

Run 3

Inlet Temp. - 553°K

13.3 Moles CCl_4/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	133.00	0.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13010E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF	CP	
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.1350E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
8.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	553.0001	3.4000	723.0001	99.0000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 13.30 HCL = 0.00

INLET TEMPERATURE = 553.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	553.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	556.4	198.24	0.0494	0.9505	0.0494	0.0000	0.0000	0.0000	0.0494
3	559.8	363.24	0.0945	0.9054	0.0899	0.0046	0.0000	0.0000	0.0991
4	563.2	501.77	0.1360	0.8639	0.1233	0.0123	0.0003	0.0000	0.1491
5	566.6	619.08	0.1746	0.8253	0.1510	0.0223	0.0011	0.0000	0.1993
6	570.0	719.21	0.2106	0.7893	0.1741	0.0339	0.0025	0.0000	0.2497
7	573.4	805.31	0.2445	0.7554	0.1934	0.0466	0.0044	0.0000	0.3003
8	576.8	879.84	0.2766	0.7233	0.2093	0.0602	0.0068	0.0001	0.3510
9	580.2	944.74	0.3071	0.6928	0.2225	0.0745	0.0098	0.0002	0.4019
10	583.6	1001.58	0.3361	0.6638	0.2333	0.0892	0.0132	0.0003	0.4529
11	587.0	1051.62	0.3639	0.6360	0.2420	0.1043	0.0170	0.0005	0.5040
12	590.4	1095.88	0.3906	0.6093	0.2488	0.1198	0.0211	0.0007	0.5552
13	593.8	1135.20	0.4163	0.5836	0.2540	0.1355	0.0256	0.0011	0.6066
14	597.2	1170.30	0.4411	0.5588	0.2577	0.1513	0.0304	0.0015	0.6581
15	600.6	1201.75	0.4651	0.5348	0.2601	0.1674	0.0355	0.0019	0.7096
16	604.0	1230.03	0.4883	0.5116	0.2613	0.1835	0.0408	0.0025	0.7613
17	607.4	1255.57	0.5108	0.4891	0.2614	0.1996	0.0464	0.0032	0.8131
18	610.8	1278.72	0.5326	0.4673	0.2605	0.2158	0.0521	0.0040	0.8650
19	614.2	1299.77	0.5538	0.4461	0.2587	0.2320	0.0580	0.0049	0.9169
20	617.6	1318.97	0.5744	0.4255	0.2561	0.2482	0.0640	0.0060	0.9690
21	621.0	1336.56	0.5945	0.4054	0.2526	0.2643	0.0702	0.0072	1.0212
22	624.4	1352.71	0.6141	0.3858	0.2485	0.2804	0.0764	0.0086	1.0734
23	627.8	1367.60	0.6331	0.3668	0.2437	0.2963	0.0827	0.0102	1.1258
24	631.2	1381.37	0.6517	0.3482	0.2384	0.3121	0.0891	0.0120	1.1782
25	634.6	1394.14	0.6698	0.3301	0.2324	0.3277	0.0955	0.0139	1.2308
26	638.0	1406.02	0.6874	0.3125	0.2260	0.3432	0.1020	0.0162	1.2834
27	641.4	1417.12	0.7047	0.2952	0.2191	0.3584	0.1084	0.0186	1.3361
28	644.8	1427.51	0.7214	0.2785	0.2117	0.3733	0.1148	0.0214	1.3889
29	648.2	1437.28	0.7378	0.2621	0.2040	0.3880	0.1212	0.0244	1.4418
30	651.6	1446.48	0.7537	0.2462	0.1960	0.4023	0.1275	0.0278	1.4948
31	655.0	1455.19	0.7692	0.2307	0.1876	0.4162	0.1337	0.0315	1.5479
32	658.4	1463.45	0.7843	0.2156	0.1790	0.4297	0.1398	0.0357	1.6010
33	661.8	1471.32	0.7990	0.2009	0.1701	0.4423	0.1458	0.0402	1.6543
34	665.2	1478.83	0.8133	0.1866	0.1611	0.4553	0.1516	0.0452	1.7077
35	668.6	1486.04	0.8271	0.1728	0.1519	0.4672	0.1572	0.0507	1.7611
36	672.0	1492.97	0.8405	0.1594	0.1426	0.4785	0.1626	0.0567	1.8147
37	675.4	1499.66	0.8535	0.1465	0.1332	0.4890	0.1677	0.0633	1.8683
38	678.8	1506.15	0.8659	0.1340	0.1238	0.4988	0.1725	0.0706	1.9221
39	682.2	1512.46	0.8780	0.1219	0.1144	0.5078	0.1771	0.0786	1.9759
40	685.6	1518.62	0.8895	0.1104	0.1051	0.5158	0.1812	0.0873	2.0299
41	689.0	1524.66	0.9006	0.0993	0.0959	0.5228	0.1849	0.0968	2.0840
42	692.4	1530.60	0.9111	0.0888	0.0869	0.5287	0.1881	0.1073	2.1382
43	695.8	1536.47	0.9211	0.0788	0.0781	0.5334	0.1908	0.1187	2.1925
44	699.2	1542.30	0.9306	0.0693	0.0696	0.5369	0.1928	0.1311	2.2469
45	702.6	1548.11	0.9394	0.0605	0.0614	0.5389	0.1943	0.1447	2.3014
46	706.0	1553.91	0.9477	0.0522	0.0535	0.5395	0.1950	0.1595	2.3561
47	709.4	1559.75	0.9553	0.0446	0.0461	0.5386	0.1949	0.1756	2.4109
48	712.8	1565.63	0.9624	0.0375	0.0392	0.5359	0.1939	0.1931	2.4659
49	716.2	1571.59	0.9687	0.0312	0.0328	0.5316	0.1920	0.2121	2.5210
50	719.6	1577.65	0.9744	0.0255	0.0270	0.5256	0.1892	0.2329	2.5763
51	723.0	1583.84	0.9795	0.0204	0.0218	0.5177	0.1853	0.2545	2.6317

Run 4

Inlet Temp. - 563^oK

14.1 Moles CCl_4/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	141.00	0.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58540E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF CP		
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT			
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	563.0001	3.2000	723.0001	99.0000

COEF			
-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS
NITROGEN = 0.00 CARBON TET = 14.10 HCL = 0.00

INLET TEMPERATURE = 563.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	563.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	566.2	136.73	0.0491	0.9508	0.0491	0.0000	0.0000	0.0000	0.0491
3	569.4	252.27	0.0939	0.9060	0.0894	0.0045	0.0000	0.0000	0.0985
4	572.6	350.73	0.1353	0.8646	0.1229	0.0122	0.0002	0.0000	0.1482
5	575.8	435.38	0.1738	0.8261	0.1505	0.0222	0.0009	0.0000	0.1980
6	579.0	500.71	0.2090	0.7901	0.1736	0.0339	0.0021	0.0000	0.2481
7	582.2	572.66	0.2437	0.7562	0.1930	0.0468	0.0037	0.0000	0.2983
8	585.4	628.79	0.2759	0.7241	0.2090	0.0607	0.0059	0.0001	0.3487
9	588.6	678.32	0.3063	0.6936	0.2223	0.0753	0.0084	0.0001	0.3992
10	591.8	722.26	0.3355	0.6644	0.2332	0.0905	0.0114	0.0003	0.4498
11	595.0	761.43	0.3634	0.6365	0.2420	0.1060	0.0148	0.0004	0.5006
12	598.2	796.49	0.3902	0.6097	0.2489	0.1220	0.0185	0.0007	0.5515
13	601.4	828.01	0.4160	0.5839	0.2541	0.1382	0.0226	0.0010	0.6025
14	604.6	856.47	0.4408	0.5591	0.2579	0.1545	0.0269	0.0013	0.6535
15	607.8	882.24	0.4649	0.5350	0.2603	0.1711	0.0316	0.0018	0.7047
16	611.0	905.69	0.4892	0.5119	0.2615	0.1877	0.0365	0.0023	0.7560
17	614.2	927.06	0.5107	0.4892	0.2617	0.2044	0.0416	0.0029	0.8074
18	617.4	946.64	0.5326	0.4673	0.2608	0.2211	0.0469	0.0037	0.8589
19	620.6	964.62	0.5539	0.4460	0.2590	0.2379	0.0524	0.0045	0.9104
20	623.8	981.19	0.5746	0.4254	0.2563	0.2546	0.0580	0.0055	0.9621
21	627.0	996.50	0.5947	0.4052	0.2529	0.2712	0.0638	0.0067	1.0138
22	630.2	1010.70	0.6143	0.3856	0.2457	0.2877	0.0697	0.0080	1.0656
23	633.4	1023.91	0.6334	0.3566	0.2439	0.3041	0.0757	0.0094	1.1175
24	636.6	1036.23	0.6520	0.3480	0.2385	0.3204	0.0818	0.0111	1.1695
25	639.8	1047.75	0.6701	0.3298	0.2326	0.3364	0.0880	0.0130	1.2216
26	643.0	1056.57	0.6877	0.3122	0.2261	0.3523	0.0941	0.0150	1.2738
27	646.2	1068.75	0.7050	0.2949	0.2192	0.3679	0.1004	0.0174	1.3261
28	649.4	1078.36	0.7217	0.2782	0.2118	0.3832	0.1066	0.0200	1.3784
29	652.6	1087.47	0.7381	0.2618	0.2041	0.3982	0.1128	0.0229	1.4308
30	655.8	1096.12	0.7540	0.2459	0.1960	0.4128	0.1190	0.0261	1.4833
31	659.0	1104.36	0.7695	0.2304	0.1877	0.4270	0.1251	0.0296	1.5359
32	662.2	1112.24	0.7846	0.2153	0.1790	0.4408	0.1312	0.0335	1.5886
33	665.4	1119.79	0.7993	0.2006	0.1701	0.4540	0.1371	0.0378	1.6414
34	668.6	1127.06	0.8135	0.1864	0.1611	0.4667	0.1429	0.0426	1.6942
35	671.8	1134.07	0.8273	0.1726	0.1519	0.4788	0.1486	0.0478	1.7472
36	675.0	1140.87	0.8407	0.1592	0.1426	0.4903	0.1540	0.0536	1.8002
37	678.2	1147.47	0.8536	0.1463	0.1332	0.5010	0.1593	0.0599	1.8533
38	681.4	1153.91	0.8661	0.1339	0.1238	0.5109	0.1643	0.0669	1.9066
39	684.6	1160.20	0.8780	0.1219	0.1143	0.5199	0.1690	0.0745	1.9599
40	687.8	1166.39	0.8896	0.1103	0.1052	0.5279	0.1734	0.0829	2.0133
41	691.0	1172.49	0.9006	0.0993	0.0962	0.5350	0.1774	0.0921	2.0669
42	694.2	1178.52	0.9111	0.0888	0.0870	0.5409	0.1809	0.1021	2.1205
43	697.4	1184.52	0.9210	0.0789	0.0782	0.5456	0.1840	0.1131	2.1743
44	700.6	1190.49	0.9304	0.0695	0.0697	0.5490	0.1865	0.1251	2.2281
45	703.8	1196.47	0.9393	0.0606	0.0615	0.5507	0.1884	0.1383	2.2821
46	707.0	1202.48	0.9475	0.0524	0.0537	0.5514	0.1895	0.1526	2.3362
47	710.2	1208.55	0.9551	0.0448	0.0464	0.5504	0.1901	0.1682	2.3905
48	713.4	1214.68	0.9621	0.0378	0.0395	0.5477	0.1897	0.1851	2.4449
49	716.6	1220.92	0.9684	0.0315	0.0331	0.5432	0.1885	0.2035	2.4994
50	719.8	1227.27	0.9741	0.0258	0.0274	0.5370	0.1862	0.2233	2.5540
51	723.0	1233.80	0.9792	0.0207	0.0222	0.5290	0.1831	0.2447	2.6088

Run 5

Inlet Temp. - 573°K

15.0 Moles CCl_4/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	150.00	0.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF	CP	
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	9.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	573.0001	3.0000	723.0001	99.0000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 15.00 HCL = 0.00

INLET TEMPERATURE 573.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	573.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	576.0	75.46	0.0487	0.9512	0.0487	0.0000	0.0000	0.0000	0.0487
3	579.0	172.07	0.0933	0.9066	0.0889	0.0044	0.0000	0.0000	0.0978
4	582.0	250.48	0.1345	0.8654	0.1221	0.0121	0.0002	0.0000	0.1471
5	585.0	312.74	0.1728	0.8271	0.1499	0.0221	0.0008	0.0000	0.1967
6	588.0	367.42	0.2088	0.7911	0.1731	0.0338	0.0018	0.0000	0.2464
7	591.0	415.76	0.2427	0.7572	0.1925	0.0469	0.0032	0.0000	0.2962
8	594.0	458.73	0.2748	0.7251	0.2086	0.0610	0.0050	0.0000	0.3462
9	597.0	497.13	0.3053	0.6946	0.2220	0.0758	0.0072	0.0001	0.3963
10	600.0	531.61	0.3345	0.6654	0.2330	0.0913	0.0099	0.0002	0.4466
11	603.0	562.70	0.3625	0.6374	0.2418	0.1072	0.0129	0.0004	0.4969
12	606.0	[illegible]	0.3893	0.6106	0.2468	0.1236	0.0162	0.0006	0.5474
13	609.0	616.47	0.4152	0.5847	0.2542	0.1402	0.0199	0.0009	0.5980
14	612.0	639.82	0.4402	0.5598	0.2580	0.1570	0.0238	0.0012	0.6487
15	615.0	661.21	0.4643	0.5356	0.2605	0.1740	0.0280	0.0016	0.6994
16	618.0	680.85	0.4876	0.5123	0.2617	0.1911	0.0325	0.0021	0.7503
17	621.0	698.96	0.5102	0.4897	0.2619	0.2083	0.0372	0.0027	0.8012
18	624.0	715.70	0.5322	0.4677	0.2610	0.2256	0.0421	0.0033	0.8523
19	627.0	731.23	0.5535	0.4464	0.2592	0.2428	0.0472	0.0041	0.9034
20	630.0	745.66	0.5742	0.4257	0.2566	0.2599	0.0525	0.0051	0.9546
21	633.0	759.13	0.5944	0.4055	0.2532	0.2770	0.0579	0.0061	1.0059
22	636.0	771.72	0.6140	0.3859	0.2490	0.2940	0.0634	0.0073	1.0573
23	639.0	783.54	0.6331	0.3668	0.2442	0.3109	0.0691	0.0087	1.1087
24	642.0	794.66	0.6517	0.3482	0.2388	0.3276	0.0749	0.0102	1.1603
25	645.0	805.15	0.6699	0.3300	0.2329	0.3441	0.0808	0.0120	1.2119
26	648.0	815.08	0.6876	0.3123	0.2264	0.3603	0.0867	0.0140	1.2636
27	651.0	824.49	0.7048	0.2951	0.2195	0.3763	0.0927	0.0161	1.3153
28	654.0	833.45	0.7216	0.2783	0.2121	0.3920	0.0987	0.0186	1.3672
29	657.0	842.00	0.7380	0.2620	0.2044	0.4073	0.1048	0.0213	1.4191
30	660.0	850.19	0.7539	0.2460	0.1963	0.4223	0.1108	0.0243	1.4711
31	663.0	858.04	0.7694	0.2305	0.1879	0.4368	0.1168	0.0277	1.5232
32	666.0	865.60	0.7845	0.2155	0.1793	0.4508	0.1228	0.0314	1.5754
33	669.0	872.90	0.7991	0.2008	0.1704	0.4644	0.1287	0.0355	1.6276
34	672.0	879.97	0.8133	0.1866	0.1614	0.4773	0.1345	0.0400	1.6800
35	675.0	886.84	0.8271	0.1728	0.1522	0.4896	0.1402	0.0450	1.7324
36	678.0	893.54	0.8405	0.1594	0.1429	0.5013	0.1457	0.0505	1.7849
37	681.0	900.08	0.8534	0.1465	0.1335	0.5121	0.1510	0.0565	1.8375
38	684.0	906.51	0.8658	0.1341	0.1242	0.5222	0.1562	0.0631	1.8902
39	687.0	912.83	0.8778	0.1221	0.1148	0.5313	0.1611	0.0704	1.9429
40	690.0	919.07	0.8893	0.1106	0.1055	0.5395	0.1657	0.0785	1.9958
41	693.0	925.26	0.9003	0.0996	0.0964	0.5466	0.1699	0.0872	2.0488
42	696.0	931.42	0.9107	0.0892	0.0874	0.5525	0.1738	0.0969	2.1018
43	699.0	937.56	0.9207	0.0792	0.0786	0.5573	0.1772	0.1074	2.1550
44	702.0	943.72	0.9301	0.0698	0.0701	0.5607	0.1801	0.1190	2.2083
45	705.0	949.91	0.9389	0.0610	0.0620	0.5627	0.1824	0.1316	2.2617
46	708.0	956.16	0.9471	0.0528	0.0542	0.5632	0.1842	0.1454	2.3152
47	711.0	962.48	0.9547	0.0452	0.0468	0.5621	0.1852	0.1605	2.3689
48	714.0	968.91	0.9617	0.0382	0.0400	0.5593	0.1854	0.1768	2.4227
49	717.0	975.46	0.9680	0.0319	0.0336	0.5548	0.1846	0.1946	2.4766
50	720.0	982.17	0.9737	0.0262	0.0278	0.5486	0.1833	0.2138	2.5306
51	723.0	989.05	0.9787	0.0212	0.0226	0.5406	0.1808	0.2345	2.5848

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	380.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF CP		
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT			
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	523.0001	4.0000	723.0001	99.5000

COEF			
-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

Run 6
Inlet Temp. - 523°K
38 Moles HCl/Mole CH_4

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 0.00 HCL = 38.00

INLET TEMPERATURE - 523.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	523.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	527.0	4176.46	0.0509	0.9490	0.0509	0.0000	0.0000	0.0000	0.0509
3	531.0	8552.41	0.0971	0.9028	0.0922	0.0049	0.0000	0.0000	0.1021
4	535.0	11553.99	0.1394	0.8605	0.1259	0.0128	0.0006	0.0000	0.1535
5	539.0	13962.44	0.1783	0.8216	0.1536	0.0226	0.0021	0.0000	0.2051
6	543.0	15914.52	0.2144	0.7855	0.1763	0.0336	0.0044	0.0000	0.2569
7	547.0	17512.07	0.2482	0.7517	0.1951	0.0454	0.0075	0.0000	0.3089
8	551.0	18831.15	0.2800	0.7199	0.2107	0.0578	0.0113	0.0001	0.3610
9	555.0	19920.17	0.3101	0.6898	0.2234	0.0706	0.0157	0.0003	0.4132
10	559.0	20849.99	0.3388	0.6611	0.2338	0.0838	0.0206	0.0005	0.4655
11	563.0	21627.46	0.3662	0.6337	0.2422	0.0972	0.0260	0.0007	0.5179
12	567.0	22286.04	0.3926	0.6073	0.2487	0.1109	0.0318	0.0011	0.5704
13	571.0	22852.60	0.4179	0.5820	0.2537	0.1247	0.0379	0.0015	0.6231
14	575.0	23337.76	0.4423	0.5576	0.2572	0.1387	0.0442	0.0020	0.6758
15	579.0	23756.87	0.4659	0.5340	0.2595	0.1528	0.0508	0.0026	0.7286
16	583.0	24120.70	0.4888	0.5111	0.2606	0.1670	0.0576	0.0034	0.7815
17	587.0	24438.05	0.5109	0.4890	0.2606	0.1814	0.0646	0.0042	0.8344
18	591.0	24716.12	0.5325	0.4674	0.2597	0.1957	0.0716	0.0052	0.8875
19	595.0	24960.85	0.5534	0.4465	0.2579	0.2102	0.0788	0.0064	0.9406
20	599.0	25177.16	0.5738	0.4261	0.2553	0.2247	0.0860	0.0077	0.9939
21	603.0	25369.15	0.5937	0.4062	0.2520	0.2392	0.0932	0.0092	1.0472
22	607.0	25540.25	0.6130	0.3869	0.2479	0.2536	0.1005	0.0109	1.1005
23	611.0	25693.35	0.6319	0.3680	0.2432	0.2681	0.1077	0.0128	1.1540
24	615.0	25830.89	0.6503	0.3496	0.2379	0.2825	0.1149	0.0149	1.2076
25	619.0	25954.93	0.6683	0.3316	0.2321	0.2968	0.1220	0.0173	1.2612
26	623.0	26067.24	0.6859	0.3140	0.2258	0.3110	0.1291	0.0199	1.3149
27	627.0	26169.31	0.7030	0.2969	0.2190	0.3250	0.1360	0.0228	1.3687
28	631.0	26262.44	0.7197	0.2802	0.2118	0.3389	0.1428	0.0260	1.4226
29	635.0	26347.73	0.7360	0.2639	0.2042	0.3525	0.1495	0.0296	1.4765
30	639.0	26426.16	0.7519	0.2480	0.1963	0.3659	0.1560	0.0335	1.5306
31	643.0	26498.55	0.7673	0.2326	0.1880	0.3791	0.1623	0.0378	1.5847
32	647.0	26565.64	0.7824	0.2175	0.1795	0.3918	0.1684	0.0425	1.6390
33	651.0	26628.04	0.7971	0.2028	0.1707	0.4043	0.1742	0.0477	1.6933
34	655.0	26686.33	0.8114	0.1885	0.1618	0.4162	0.1798	0.0534	1.7477
35	659.0	26740.99	0.8252	0.1747	0.1527	0.4277	0.1851	0.0596	1.8022
36	663.0	26792.46	0.8386	0.1613	0.1434	0.4387	0.1900	0.0664	1.8568
37	667.0	26841.13	0.8516	0.1483	0.1341	0.4490	0.1945	0.0738	1.9114
38	671.0	26887.35	0.8642	0.1357	0.1248	0.4587	0.1986	0.0819	1.9662
39	675.0	26931.42	0.8763	0.1236	0.1154	0.4676	0.2023	0.0908	2.0211
40	679.0	26973.65	0.8879	0.1120	0.1062	0.4757	0.2055	0.1004	2.0761
41	683.0	27014.28	0.8990	0.1009	0.0970	0.4829	0.2081	0.1109	2.1313
42	687.0	27053.55	0.9097	0.0902	0.0879	0.4891	0.2101	0.1224	2.1865
43	691.0	27091.70	0.9198	0.0801	0.0791	0.4942	0.2115	0.1348	2.2418
44	695.0	27128.93	0.9294	0.0705	0.0705	0.4982	0.2122	0.1484	2.2973
45	699.0	27163.44	0.938[illegible]	0.0615	0.0622	0.5000	0.2120	0.1631	2.3529
46	703.0	27201.43	0.9468	0.0531	0.0543	0.5022	0.2111	0.1791	2.4087
47	707.0	27237.08	0.9546	0.0453	0.0468	0.5021	0.2092	0.1964	2.4645
48	711.0	27272.59	0.9618	0.0381	0.0398	0.5003	0.2064	0.2151	2.5206
49	715.0	27306.14	0.9683	0.0316	0.0322	0.4970	0.2026	0.2353	2.5767
50	719.0	27340.92	0.9742	0.0257	0.0273	0.4919	0.1977	0.2571	2.6331
51	723.0	27380.12	0.9793	0.0206	0.0220	0.4851	0.1917	0.2803	2.6896

Run 7

Inlet Temp. - 543°K

43 Moles HCl/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	430.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF	CP	
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	543.0001	3.6000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 0.00 HCL = 43.00

INLET TEMPERATURE = 543.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	543.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	546.6	2219.21	0.0511	0.9488	0.0511	0.0000	0.0000	0.0000	0.0511
3	550.2	4034.75	0.0975	0.9024	0.0926	0.0049	0.0000	0.0000	0.1025
4	553.8	5532.39	0.1401	0.8598	0.1265	0.0131	0.0004	0.0000	0.1541
5	557.4	6779.01	0.1794	0.8205	0.1545	0.0234	0.0015	0.0000	0.2059
6	561.0	7825.80	0.2161	0.7838	0.1776	0.0352	0.0032	0.0000	0.2579
7	564.6	8711.97	0.2505	0.7495	0.1966	0.0481	0.0056	0.0000	0.3100
8	568.2	9467.73	0.2829	0.7170	0.2123	0.0617	0.0086	0.0001	0.3623
9	571.8	10116.68	0.3136	0.6863	0.2252	0.0759	0.0121	0.0002	0.4147
10	575.4	10677.38	0.3429	0.6570	0.2356	0.0906	0.0161	0.0004	0.4672
11	579.0	11164.62	0.3709	0.6290	0.2439	0.1055	0.0206	0.0006	0.5198
12	582.6	11590.30	0.3977	0.6022	0.2504	0.1207	0.0255	0.0009	0.5725
13	586.2	11964.04	0.4235	0.5764	0.2552	0.1361	0.0307	0.0013	0.6253
14	589.8	12293.74	0.4484	0.5515	0.2585	0.1517	0.0363	0.0018	0.6781
15	593.4	12585.88	0.4724	0.5275	0.2605	0.1673	0.0421	0.0023	0.7311
16	597.0	12845.86	0.4956	0.5043	0.2614	0.1830	0.0481	0.0030	0.7841
17	600.6	13078.16	0.5181	0.4818	0.2611	0.1988	0.0543	0.0038	0.8373
18	604.2	13286.55	0.5400	0.4599	0.2599	0.2145	0.0607	0.0047	0.8905
19	607.8	13474.22	0.5612	0.4387	0.2577	0.2303	0.0673	0.0058	0.9437
20	611.4	13643.85	0.5818	0.4181	0.2547	0.2460	0.0740	0.0070	0.9971
21	615.0	13797.74	0.6019	0.3980	0.2510	0.2617	0.0807	0.0084	1.0505
22	618.6	13937.86	0.6215	0.3784	0.2466	0.2772	0.0875	0.0100	1.1040
23	622.2	14065.89	0.6405	0.3594	0.2415	0.2927	0.0944	0.0118	1.1576
24	625.8	14183.28	0.6590	0.3409	0.2358	0.3080	0.1012	0.0138	1.2112
25	629.4	14291.30	0.6771	0.3228	0.2296	0.3232	0.1081	0.0160	1.2650
26	633.0	14391.04	0.6947	0.3052	0.2229	0.3381	0.1150	0.0186	1.3188
27	636.6	14483.45	0.7119	0.2880	0.2156	0.3526	0.1218	0.0213	1.3727
28	640.2	14569.37	0.7286	0.2713	0.2082	0.3673	0.1285	0.0244	1.4266
29	643.8	14649.53	0.7449	0.2550	0.2003	0.3814	0.1352	0.0279	1.4807
30	647.4	14724.58	0.7608	0.2391	0.1920	0.3952	0.1417	0.0317	1.5348
31	651.0	14795.09	0.7762	0.2237	0.1835	0.4086	0.1481	0.0359	1.5890
32	654.6	14861.58	0.7912	0.2087	0.1747	0.4216	0.1544	0.0405	1.6432
33	658.2	14924.49	0.8058	0.1941	0.1657	0.4340	0.1604	0.0455	1.6976
34	661.8	14984.25	0.8200	0.1799	0.1565	0.4460	0.1662	0.0511	1.7521
35	665.4	15041.21	0.8337	0.1662	0.1472	0.4573	0.1716	0.0572	1.8066
36	669.0	15095.73	0.8470	0.1530	0.1378	0.4680	0.1771	0.0639	1.8612
37	672.6	15148.09	0.8598	0.1401	0.1284	0.4779	0.1820	0.0713	1.9159
38	676.2	15198.59	0.8721	0.1278	0.1189	0.4871	0.1866	0.0793	1.9707
39	679.8	15247.48	0.8840	0.1159	0.1095	0.4954	0.1908	0.0882	2.0257
40	683.4	15295.02	0.8953	0.1046	0.1002	0.5027	0.1945	0.0978	2.0807
41	687.0	15341.42	0.9062	0.0937	0.0911	0.5090	0.1977	0.1083	2.1358
42	690.6	15386.92	0.9165	0.0834	0.0821	0.5141	0.2003	0.1198	2.1910
43	694.2	15431.72	0.9263	0.0736	0.0734	0.5181	0.2023	0.1324	2.2464
44	697.8	15476.02	0.9355	0.0644	0.0650	0.5207	0.2036	0.1461	2.3019
45	701.4	15520.03	0.9441	0.0558	0.0569	0.5219	0.2041	0.1610	2.3575
46	705.0	15563.94	0.9521	0.0478	0.0493	0.5216	0.2036	0.1772	2.4132
47	708.6	15607.95	0.9594	0.0405	0.0421	0.5197	0.2027	0.1948	2.4691
48	712.2	15652.27	0.9661	0.0338	0.0355	0.5162	0.2005	0.2138	2.5251
49	715.8	15697.1[illegible]	0.9721	0.0279	0.0294	0.510[illegible]	0.1973	0.2344	2.5812
50	719.4	15742.64	0.9775	0.0224	0.0239	0.5038	0.1931	0.2566	2.6376
51	723.0	15789.12	0.9822	0.0177	0.0190	0.4950	0.1877	0.2804	2.6940

Run 8

Inlet Temp. - 553°K

45 Moles HCl/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	450.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST	OF	CP
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	553.0001	3.4000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 0.00 HCL = 45.00

INLET TEMPERATURE = 553.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	553.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	556.4	1485.06	0.0502	0.9498	0.0502	0.0000	0.0000	0.0000	0.0502
3	559.8	2719.61	0.0960	0.9040	0.0913	0.0047	0.0000	0.0000	0.1008
4	563.2	3755.17	0.1381	0.8619	0.1253	0.0127	0.0003	0.0000	0.1516
5	566.6	4631.47	0.1771	0.8229	0.1529	0.0230	0.0012	0.0000	0.2026
6	570.0	5379.08	0.2135	0.7864	0.1760	0.0348	0.0026	0.0000	0.2537
7	573.4	6021.65	0.2477	0.7522	0.1952	0.0478	0.0046	0.0000	0.3050
8	576.8	6577.68	0.2800	0.7199	0.2110	0.0616	0.0071	0.0001	0.3564
9	580.2	7061.31	0.3107	0.6892	0.2241	0.0761	0.0102	0.0002	0.4080
10	583.6	7485.72	0.3399	0.6600	0.2347	0.0911	0.0137	0.0003	0.4596
11	587.0	7856.85	0.3679	0.6320	0.2432	0.1064	0.0176	0.0005	0.5113
12	590.4	8188.88	0.3947	0.6052	0.2498	0.1221	0.0219	0.0008	0.5632
13	593.8	8482.13	0.4205	0.5794	0.2546	0.1379	0.0265	0.0011	0.6151
14	597.2	8743.82	0.4454	0.5545	0.2583	0.1539	0.0314	0.0015	0.6671
15	600.6	8976.31	0.4694	0.5305	0.2605	0.1701	0.0367	0.0020	0.7192
16	604.0	9189.24	0.4926	0.5073	0.2615	0.1862	0.0421	0.0026	0.7713
17	607.4	9379.71	0.5151	0.4848	0.2614	0.2025	0.0476	0.0034	0.8235
18	610.8	9552.32	0.5370	0.4629	0.2603	0.2187	0.0536	0.0042	0.8758
19	614.2	9709.31	0.5582	0.4417	0.2583	0.2350	0.0596	0.0052	0.9282
20	617.6	9852.58	0.5788	0.4211	0.2554	0.2512	0.0658	0.0063	0.9807
21	621.0	9983.77	0.5989	0.4010	0.2518	0.2673	0.0720	0.0075	1.0332
22	624.4	10104.31	0.6184	0.3815	0.2475	0.2833	0.0784	0.0090	1.0858
23	627.8	10215.42	0.6374	0.3625	0.2426	0.2993	0.0848	0.0106	1.1385
24	631.2	10318.18	0.6560	0.3439	0.2371	0.3150	0.0913	0.0124	1.1912
25	634.6	10413.52	0.6740	0.3259	0.2310	0.3306	0.0978	0.0145	1.2440
26	638.0	10502.26	0.6916	0.3083	0.2244	0.3460	0.1043	0.0168	1.2969
27	641.4	10585.13	0.7088	0.2912	0.2174	0.3611	0.1108	0.0193	1.3498
28	644.8	10662.76	0.7255	0.2744	0.2099	0.3759	0.1173	0.0222	1.4028
29	648.2	10735.72	0.7417	0.2582	0.2021	0.3904	0.1237	0.0253	1.4559
30	651.6	10804.52	0.7576	0.2423	0.1939	0.4046	0.1301	0.0288	1.5091
31	655.0	10869.60	0.7730	0.2269	0.1855	0.4183	0.1363	0.0327	1.5623
32	658.4	10931.38	0.7880	0.2119	0.1768	0.4317	0.1425	0.0369	1.6157
33	661.8	10990.22	0.8026	0.1973	0.1679	0.4445	0.1485	0.0416	1.6691
34	665.2	11046.45	0.8167	0.1832	0.1588	0.4568	0.1543	0.0467	1.7225
35	668.6	11100.36	0.8304	0.1695	0.1496	0.4684	0.1599	0.0524	1.7761
36	672.0	11152.27	0.8437	0.1562	0.1403	0.4795	0.1653	0.0586	1.8297
37	675.4	11202.40	0.8565	0.1434	0.1309	0.4898	0.1704	0.0654	1.8835
38	678.8	11250.99	0.8689	0.1310	0.1215	0.4992	0.1752	0.0728	1.9373
39	682.2	11298.27	0.8808	0.1191	0.1122	0.5079	0.1796	0.0810	1.9912
40	685.6	11344.46	0.8922	0.1077	0.1029	0.5156	0.1836	0.0900	2.0452
41	689.0	11389.75	0.9031	0.0968	0.0939	0.5222	0.1872	0.0997	2.0993
42	692.4	11434.34	0.9135	0.0864	0.0848	0.5273	0.1903	0.1104	2.1535
43	695.8	11478.41	0.9233	0.0766	0.0761	0.5321	0.1929	0.1221	2.2079
44	699.2	11522.15	0.9326	0.0673	0.0677	0.5351	0.1948	0.1349	2.2623
45	702.6	11565.75	0.9413	0.0586	0.0599	0.5368	0.1961	0.1488	2.3168
46	706.0	11609.37	0.9494	0.0505	0.0518	0.5370	0.1966	0.1639	2.3715
47	709.4	11653.21	0.9569	0.0430	0.0446	0.5356	0.1963	0.1803	2.4263
48	712.8	11697.45	0.9638	0.0361	0.0377	0.5326	0.1951	0.1981	2.4813
49	716.2	11742.27	0.9700	0.0299	0.0315	0.5279	0.1930	0.2174	2.5364
50	719.6	11787.87	0.9755	0.0244	0.0259	0.5214	0.1898	0.2382	2.5916
51	723.0	11834.45	0.9804	0.0195	0.0209	0.5131	0.1857	0.2606	2.6469

Run 2

Inlet Temp. - 563°K

48 Moles HCl/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	480.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF	CP	
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	563.0001	3.2000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN 0.00 CARBON TET 6.00 HCL 48.00

INLET TEMPERATURE = 563.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XT	MOL FA	MOL FC	MOL FD	MOL FC	MOL FF	MOL CL2 REACT/ MOL CH4
1	563.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	566.2	1060.96	[illegible]	0.9493	0.0502	[illegible]	[illegible]	[illegible]	0.0501
3	569.4	[illegible]	[illegible]	[illegible]	0.0911	0.0047	0.0000	0.0000	0.1005
4	572.6	2719.21	[illegible]	[illegible]	0.1249	0.0127	[illegible]	0.0000	0.1512
5	575.8	3373.12	0.1765	0.8230	0.1527	0.0231	[illegible]	0.0000	0.2020
6	579.0	3940.20	0.2133	0.7666	0.1759	0.0351	0.0022	0.0000	0.2530
7	582.2	4434.67	0.2477	0.7522	0.1952	0.0463	0.0039	0.0000	0.3042
8	585.4	4867.55	0.2901	0.7198	0.2112	0.0625	0.0062	0.0001	0.3554
9	588.6	5251.43	0.3109	0.6890	0.2243	0.0775	0.0088	0.0002	0.4066
10	591.8	5591.08	0.3405	0.6596	0.2350	0.0929	0.0120	0.0003	0.4583
11	595.0	5892.54	0.3684	0.6315	0.2435	0.1088	0.0155	0.0005	0.5099
12	598.2	6164.93	0.3954	0.6045	0.2502	0.1250	0.0194	0.0007	0.5615
13	601.4	6408.69	0.4214	0.5785	0.2552	0.1414	0.0236	0.0010	0.6133
14	604.6	6628.75	0.4464	0.5535	0.2587	0.1580	0.0281	0.0014	0.6651
15	607.8	6828.17	0.4705	0.5294	0.2605	0.1747	0.0329	0.0019	0.7170
16	611.0	7009.54	0.4939	0.5062	0.2613	0.1914	0.0380	0.0024	0.7690
17	614.2	7175.08	0.5165	0.4834	0.2616	0.2084	0.0432	0.0031	0.8211
18	617.4	7326.05	0.5383	0.4614	0.2609	0.2253	0.0487	0.0039	0.8732
19	620.6	7465.07	0.5598	0.4401	0.2594	0.2421	0.0544	0.0048	0.9254
20	623.8	7594.37	0.5805	0.4194	0.2559	0.2589	0.0602	0.0059	0.9777
21	627.0	7713.11	0.6007	0.3992	0.2518	0.2756	0.0661	0.0071	1.0300
22	630.2	7823.04	0.6203	0.3796	0.2474	0.2921	0.0722	0.0084	1.0824
23	633.4	7925.72	0.6394	0.3605	0.2423	0.3085	0.0784	0.0100	1.1349
24	636.6	8021.37	0.6580	0.3419	0.2367	0.3248	0.0846	0.0117	1.1874
25	639.8	8110.91	0.6761	0.3238	0.2305	0.3408	0.0909	0.0137	1.2400
26	643.0	8194.99	0.6937	0.3062	0.2238	0.3566	0.0972	0.0159	1.2927
27	646.2	8274.13	0.7109	0.2890	0.2167	0.3721	0.1036	0.0183	1.3455
28	649.4	8349.00	0.7276	0.2723	0.2092	0.3873	0.1099	0.0211	1.3983
29	652.6	8419.90	0.7439	0.2560	0.2012	0.4021	0.1163	0.0241	1.4512
30	655.8	8487.29	0.7598	0.2401	0.1930	0.4166	0.1226	0.0275	1.5041
31	659.0	8551.57	0.7752	0.2247	0.1845	0.4306	0.1288	0.0312	1.5571
32	662.2	8613.05	0.7902	0.2097	0.1757	0.4441	0.1349	0.0353	1.6102
33	665.4	8672.05	0.8047	0.1952	0.1667	0.4571	0.1409	0.0398	1.6634
34	668.6	8728.96	0.8188	0.1811	0.1576	0.4695	0.1468	0.0448	1.7167
35	671.8	8783.74	0.8325	0.1674	0.1483	0.4813	0.1525	0.0503	1.7700
36	675.0	8836.94	0.8458	0.1541	0.1389	0.4924	0.1580	0.0563	1.8234
37	678.2	8885.68	0.8585	[illegible]	0.1295	0.5027	[illegible]	[illegible]	[illegible]
38	681.4	[illegible]	[illegible]	0.1291	[illegible]	0.5121	[illegible]	[illegible]	[illegible]
39	684.6	[illegible]	[illegible]	0.1172	[illegible]	0.5206	0.1729	[illegible]	[illegible]
40	687.8	9027.30	0.8940	0.1059	0.1015	0.5282	0.1772	[illegible]	[illegible]
41	691.0	[illegible]	0.9049	0.0951	[illegible]	0.5346	[illegible]	[illegible]	[illegible]
42	694.2	9132.03	0.9151	0.0848	[illegible]	0.5393	[illegible]	[illegible]	[illegible]
43	697.4	[illegible]	0.9249	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	0.9341	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
46	707.0	[illegible]	[illegible]	[illegible]	[illegible]	0.5477	[illegible]	[illegible]	[illegible]
[illegible]	710.2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	0.9647	0.0352	[illegible]	0.5423	[illegible]	[illegible]	[illegible]
49	716.6	9460.36	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	719.8	[illegible]	0.9762	[illegible]	0.0252	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	0.9810	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Run 10

Inlet Temp. - 573°K

51 Moles HCl/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	510.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF	CP	
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-04
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	573.0001	3.0000	723.0001	99.0000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 0.00 HCL = 51.00

INLET TEMPERATURE = 573.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	573.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	576.0	760.26	0.0496	0.9503	0.0496	0.0000	0.0000	0.0000	0.0496
3	579.0	1410.55	0.0949	0.9050	0.0903	0.0046	0.0000	0.0000	0.0996
4	582.0	1972.37	0.1367	0.8632	0.1239	0.0125	0.0002	0.0000	0.1497
5	585.0	2461.93	0.1755	0.8244	0.1518	0.0228	0.0008	0.0000	0.2001
6	588.0	2891.72	0.2118	0.7881	0.1750	0.0348	0.0018	0.0000	0.2506
7	591.0	3271.53	0.2461	0.7538	0.1944	0.0482	0.0033	0.0000	0.3012
8	594.0	3609.14	0.2785	0.7214	0.2105	0.0626	0.0052	0.0000	0.3520
9	597.0	3910.83	0.3093	0.6906	0.2237	0.0777	0.0076	0.0001	0.4028
10	600.0	4181.73	0.3387	0.6612	0.2345	0.0935	0.0103	0.0003	0.4538
11	603.0	4426.07	0.3669	0.6330	0.2432	0.1097	0.0134	0.0004	0.5049
12	606.0	4647.36	0.3939	0.6060	0.2500	0.1263	0.0168	0.0006	0.5560
13	609.0	4848.55	0.4199	0.5800	0.2551	0.1431	0.0206	0.0009	0.6072
14	612.0	5032.16	0.4449	0.5550	0.2587	0.1601	0.0247	0.0013	0.6585
15	615.0	5200.30	0.4692	0.5307	0.2609	0.1773	0.0290	0.0017	0.7099
16	618.0	5354.79	0.4926	0.5073	0.2620	0.1946	0.0336	0.0022	0.7614
17	621.0	5497.21	0.5153	0.4846	0.2619	0.2120	0.0385	0.0028	0.8129
18	624.0	5628.91	0.5373	0.4626	0.2608	0.2293	0.0435	0.0035	0.8645
19	627.0	5751.08	0.5586	0.4413	0.2587	0.2466	0.0488	0.0044	0.9162
20	630.0	5864.73	0.5794	0.4205	0.2559	0.2639	0.0542	0.0053	0.9679
21	633.0	5970.78	0.5996	0.4003	0.2522	0.2810	0.0597	0.0064	1.0197
22	636.0	6070.03	0.6192	0.3807	0.2479	0.2981	0.0654	0.0077	1.0715
23	639.0	6163.17	0.6383	0.3616	0.2429	0.3149	0.0712	0.0091	1.1234
24	642.0	6250.83	0.6569	0.3430	0.2373	0.3316	0.0771	0.0108	1.1754
25	645.0	6333.58	0.6751	0.3248	0.2311	0.3481	0.0831	0.0126	1.2275
26	648.0	6411.90	0.6927	0.3072	0.2245	0.3643	0.0892	0.0146	1.2796
27	651.0	6486.25	0.7099	0.2900	0.2173	0.3802	0.0953	0.0169	1.3318
28	654.0	6557.04	0.7266	0.2733	0.2098	0.3958	0.1014	0.0195	1.3840
29	657.0	6624.62	0.7429	0.2570	0.2019	0.4110	0.1076	0.0223	1.4363
30	660.0	6689.33	0.7588	0.2411	0.1937	0.4258	0.1137	0.0255	1.4887
31	663.0	6751.48	0.7742	0.2257	0.1852	0.4401	0.1198	0.0290	1.5411
32	666.0	6811.35	0.7892	0.2107	0.1765	0.4540	0.1258	0.0328	1.5936
33	669.0	6869.19	0.8038	0.1961	0.1675	0.4673	0.1318	0.0371	1.6462
34	672.0	6925.25	0.8179	0.1820	0.1584	0.4800	0.1376	0.0418	1.6989
35	675.0	6979.75	0.8316	0.1683	0.1491	0.4920	0.1434	0.0470	1.7516
36	678.0	7032.91	0.8448	0.1551	0.1397	0.5033	0.1489	0.0527	1.8044
37	681.0	7084.93	0.8576	0.1423	0.1304	0.5138	0.1543	0.0590	1.8573
38	684.0	7136.01	0.8699	0.1300	0.1210	0.5235	0.1594	0.0659	1.9102
39	687.0	7186.32	0.8817	0.1182	0.1116	0.5322	0.1643	0.0735	1.9633
40	690.0	7236.05	0.8931	0.1068	0.1024	0.5399	0.1688	0.0818	2.0164
41	693.0	7285.39	0.9039	0.0960	0.0932	0.5466	0.1730	0.0910	2.0696
42	696.0	7334.50	0.9142	0.0857	0.0843	0.5520	0.1767	0.1010	2.1229
43	699.0	7383.57	0.9240	0.0759	0.0756	0.5562	0.1800	0.1119	2.1764
44	702.0	7432.77	0.9332	0.0667	0.0673	0.5590	0.1828	0.1239	2.2299
45	705.0	7482.29	0.9418	0.0581	0.0592	0.5604	0.1850	0.1371	2.2835
46	708.0	7532.29	0.9498	0.0501	0.0516	0.5602	0.1864	0.1514	2.3373
47	711.0	7582.97	0.9572	0.0427	0.0444	0.5585	0.1872	0.1669	2.3911
48	714.0	7634.52	0.9639	0.0360	0.0377	0.5550	0.1872	0.1839	2.4451
49	717.0	7687.13	0.9700	0.0299	0.0316	0.5498	0.1862	0.2022	2.4993
50	720.0	7741.00	0.9755	0.0244	0.0260	0.5429	0.1844	0.2220	2.5535
51	723.0	7796.34	0.9803	0.0196	0.0210	0.5342	0.1815	0.2434	2.6079

Run 11

Inlet Temp. - 523°K

38 Moles N_2/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	380.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF	CP	
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	523.0001	4.0000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 38.00 CARBON TET = 0.00 HCL = 0.00

INLET TEMPERATURE = 523.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	523.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	527.0	4825.27	0.0514	0.9485	0.0514	0.0000	0.0000	0.0000	0.0514
3	531.0	8639.53	0.0981	0.9018	0.0931	0.0050	0.0000	0.0000	0.1031
4	535.0	11671.44	0.1407	0.8592	0.1270	0.0130	0.0006	0.0000	0.1551
5	539.0	14104.43	0.1799	0.8200	0.1547	0.0230	0.0021	0.0000	0.2073
6	543.0	16076.84	0.2163	0.7836	0.1776	0.0341	0.0045	0.0000	0.2597
7	547.0	17591.55	0.2504	0.7495	0.1964	0.0461	0.0077	0.0000	0.3123
8	551.0	19025.35	0.2824	0.7175	0.2119	0.0587	0.0116	0.0001	0.3649
9	555.0	20136.16	0.3128	0.6871	0.2246	0.0717	0.0161	0.0003	0.4178
10	559.0	21068.21	0.3417	0.6582	0.2349	0.0850	0.0212	0.0005	0.4707
11	563.0	21855.64	0.3693	0.6306	0.2431	0.0986	0.0267	0.0008	0.5238
12	567.0	22525.12	0.3958	0.6041	0.2495	0.1124	0.0326	0.0011	0.5770
13	571.0	23097.68	0.4213	0.5786	0.2543	0.1264	0.0389	0.0015	0.6303
14	575.0	23590.07	0.4459	0.5540	0.2577	0.1405	0.0454	0.0021	0.6837
15	579.0	24015.75	0.4696	0.5303	0.2598	0.1548	0.0522	0.0027	0.7372
16	583.0	24385.58	0.4926	0.5073	0.2607	0.1691	0.0591	0.0035	0.7908
17	587.0	24708.44	0.5150	0.4849	0.2606	0.1836	0.0662	0.0044	0.8445
18	591.0	24991.59	0.5367	0.4632	0.2595	0.1981	0.0735	0.0054	0.8984
19	595.0	25241.02	0.5578	0.4421	0.2575	0.2126	0.0808	0.0066	0.9523
20	599.0	25461.70	0.5783	0.4216	0.2547	0.2272	0.0882	0.0080	1.0063
21	603.0	25657.77	0.5983	0.4016	0.2511	0.2418	0.0956	0.0096	1.0604
22	607.0	25832.69	0.6178	0.3821	0.2469	0.2564	0.1030	0.0113	1.1146
23	611.0	25989.39	0.6368	0.3631	0.2420	0.2709	0.1105	0.0133	1.1688
24	615.0	26130.32	0.6553	0.3446	0.2364	0.2853	0.1178	0.0155	1.2232
25	619.0	26257.57	0.6734	0.3265	0.2304	0.2997	0.1252	0.0180	1.2777
26	623.0	26372.93	0.6910	0.3089	0.2238	0.3139	0.1324	0.0208	1.3323
27	627.0	26477.92	0.7082	0.2917	0.2168	0.3279	0.1395	0.0238	1.3870
28	631.0	26573.85	0.7250	0.2749	0.2094	0.3418	0.1465	0.0272	1.4417
29	635.0	26661.85	0.7414	0.2585	0.2016	0.3554	0.1533	0.0309	1.4966
30	639.0	26742.88	0.7574	0.2425	0.1934	0.3688	0.1600	0.0351	1.5516
31	643.0	26817.79	0.7729	0.2270	0.1849	0.3818	0.1664	0.0396	1.6066
32	647.0	26887.33	0.7880	0.2119	0.1762	0.3945	0.1726	0.0446	1.6618
33	651.0	26952.14	0.8027	0.1972	0.1672	0.4067	0.1786	0.0500	1.7171
34	655.0	27012.79	0.8170	0.1829	0.1581	0.4185	0.1843	0.0560	1.7725
35	659.0	27069.78	0.8309	0.1690	0.1488	0.4297	0.1896	0.0626	1.8280
36	663.0	27123.55	0.8443	0.1556	0.1394	0.4404	0.1945	0.0698	1.8836
37	667.0	27174.51	0.8573	0.1426	0.1299	0.4504	0.1991	0.0777	1.9393
38	671.0	27223.02	0.8698	0.1301	0.1205	0.4597	0.2032	0.0863	1.9951
39	675.0	27269.40	0.8819	0.1180	0.1110	0.4681	0.2069	0.0957	2.0511
40	679.0	27313.94	0.8934	0.1065	0.1016	0.4757	0.2099	0.1060	2.1072
41	683.0	27356.91	0.9045	0.0954	0.0924	0.4823	0.2124	0.1171	2.1634
42	687.0	27398.58	0.9150	0.0849	0.0833	0.4879	0.2143	0.1293	2.2198
43	691.0	27439.17	0.9249	0.0750	0.0745	0.4922	0.2154	0.1426	2.2762
44	695.0	27478.91	0.9343	0.0656	0.0659	0.4953	0.2158	0.1571	2.3329
45	699.0	27518.01	0.9431	0.0568	0.0577	0.4971	0.2153	0.1728	2.3897
46	703.0	27556.69	0.9513	0.0486	0.0500	0.4973	0.2139	0.1899	2.4466
47	707.0	27595.15	0.9588	0.0411	0.0426	0.4961	0.2116	0.2084	2.5037
48	711.0	27633.59	0.9657	0.0342	0.0358	0.4931	0.2082	0.2285	2.5609
49	715.0	27672.23	0.9719	0.0280	0.0296	0.4884	0.2037	0.2501	2.6184
50	719.0	27711.27	0.9774	0.0225	0.0239	0.4820	0.1980	0.2734	2.6760
51	723.0	27750.94	0.9823	0.0176	0.0189	0.4737	0.1912	0.2984	2.7338

Run 12

Inlet Temp. - $543^{o}K$

41 Moles N_2/Mole CH_4

FBO	FFO	FNO	FAC	FCO	FDC	FEO	FSO
42.00	0.00	410.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF	CP	
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	543.0001	3.6000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	0.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 41.00 CARBON TET = 0.00 HCL = 0.00

INLET TEMPERATURE = 543.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	543.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	546.6	1979.57	0.0496	0.9503	0.0496	0.0000	0.0000	0.0000	0.0496
3	550.2	3600.85	0.0948	0.9051	0.0902	0.0046	0.0000	0.0000	0.0995
4	553.8	4939.28	0.1364	0.8635	0.1236	0.0124	0.0004	0.0000	0.1496
5	557.4	6053.85	0.1749	0.8250	0.1512	0.0222	0.0013	0.0000	0.2000
6	561.0	6989.87	0.2108	0.7891	0.1742	0.0336	0.0029	0.0000	0.2505
7	564.6	7782.18	0.2445	0.7554	0.1933	0.0459	0.0052	0.0000	0.3011
8	568.2	8457.68	0.2764	0.7235	0.2091	0.0591	0.0079	0.0001	0.3519
9	571.8	9037.44	0.3066	0.6933	0.2222	0.0728	0.0113	0.0002	0.4029
10	575.4	9538.06	0.3355	0.6644	0.2329	0.0870	0.0150	0.0003	0.4539
11	579.0	9972.79	0.3630	0.6369	0.2415	0.1016	0.0192	0.0006	0.5051
12	582.6	10352.29	0.3895	0.6104	0.2483	0.1164	0.0238	0.0008	0.5563
13	586.2	10685.20	0.4150	0.5849	0.2535	0.1314	0.0287	0.0012	0.6077
14	589.8	10978.60	0.4395	0.5604	0.2573	0.1466	0.0340	0.0016	0.6591
15	593.4	11238.32	0.4633	0.5366	0.2597	0.1619	0.0394	0.0021	0.7107
16	597.0	11469.19	0.4863	0.5136	0.2610	0.1773	0.0451	0.0027	0.7623
17	600.6	11675.26	0.5086	0.4913	0.2611	0.1928	0.0510	0.0034	0.8140
18	604.2	11859.89	0.5302	0.4697	0.2604	0.2083	0.0571	0.0043	0.8658
19	607.8	12025.96	0.5512	0.4487	0.2587	0.2239	0.0633	0.0053	0.9177
20	611.4	12175.87	0.5717	0.4282	0.2562	0.2394	0.0696	0.0064	0.9697
21	615.0	12311.69	0.5916	0.4083	0.2529	0.2549	0.0760	0.0077	1.0218
22	618.6	12435.17	0.6110	0.3889	0.2489	0.2704	0.0825	0.0091	1.0740
23	622.2	12547.84	0.6299	0.3700	0.2443	0.2858	0.0890	0.0107	1.1262
24	625.8	12650.98	0.6484	0.3515	0.2391	0.3010	0.0956	0.0126	1.1785
25	629.4	12745.74	0.6664	0.3335	0.2333	0.3162	0.1021	0.0146	1.2309
26	633.0	12833.08	0.6839	0.3160	0.2270	0.3312	0.1087	0.0169	1.2834
27	636.6	12913.86	0.7010	0.2989	0.2203	0.3460	0.1152	0.0194	1.3360
28	640.2	12988.83	0.7177	0.2822	0.2131	0.3605	0.1217	0.0223	1.3887
29	643.8	13058.63	0.7340	0.2659	0.2056	0.3748	0.1280	0.0254	1.4414
30	647.4	13123.86	0.7499	0.2500	0.1977	0.3889	0.1343	0.0288	1.4942
31	651.0	13185.02	0.7654	0.2345	0.1895	0.4026	0.1405	0.0326	1.5472
32	654.6	13242.55	0.7804	0.2195	0.1810	0.4159	0.1466	0.0368	1.6002
33	658.2	13296.88	0.7951	0.2048	0.1723	0.4287	0.1524	0.0414	1.6533
34	661.8	13348.35	0.8093	0.1906	0.1634	0.4412	0.1581	0.0465	1.7065
35	665.4	13397.30	0.8232	0.1767	0.1544	0.4531	0.1636	0.0520	1.7598
36	669.0	13444.01	0.8366	0.1633	0.1452	0.4644	0.1688	0.0581	1.8132
37	672.6	13488.76	0.8496	0.1503	0.1359	0.4750	0.1737	0.0647	1.8666
38	676.2	13531.80	0.8621	0.1378	0.1266	0.4850	0.1784	0.0720	1.9202
39	679.8	13573.35	0.8742	0.1257	0.1173	0.4942	0.1826	0.0800	1.9739
40	683.4	13613.61	0.8858	0.1141	0.1080	0.5025	0.1865	0.0887	2.0277
41	687.0	13652.80	0.8970	0.1029	0.0989	0.5099	0.1899	0.0982	2.0816
42	690.6	13691.09	0.9076	0.0923	0.0898	0.5163	0.1928	0.1086	2.1357
43	694.2	13728.66	0.9178	0.0821	0.0810	0.5215	0.1952	0.1200	2.1898
44	697.8	13765.69	0.9274	0.0725	0.0724	0.5256	0.1969	0.1323	2.2441
45	701.4	13802.35	0.9364	0.0635	0.0641	0.5283	0.1980	0.1458	2.2985
46	705.0	13838.78	0.9449	0.0550	0.0562	0.5297	0.1984	0.1604	2.3530
47	708.6	13875.17	0.9527	0.0472	0.0486	0.5296	0.1980	0.1764	2.4077
48	712.2	13911.67	0.9600	0.0399	0.0416	0.5280	0.1967	0.1936	2.4625
49	715.8	13948.45	0.9666	0.0333	0.0350	0.5246	0.1945	0.2123	2.5175
50	719.4	13985.67	0.9725	0.0274	0.0290	0.5196	0.1913	0.2325	2.5726
51	723.0	14023.51	0.9778	0.0221	0.0235	0.5128	0.1871	0.2543	2.6279

Run 13

Inlet Temp. - 553°K

44 Moles N_2/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF	CP	
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF	REACTION	HEAT	
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	553.0001	3.4000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 44.00 CARBON TET = 0.00 HCL = 0.00

INLET TEMPERATURE = 553.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	553.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	556.4	1416.11	0.0499	0.9500	0.0499	0.0000	0.0000	0.0000	0.0499
3	559.8	2593.84	0.0954	0.9045	0.0907	0.0047	0.0000	0.0000	0.1001
4	563.2	3582.06	0.1372	0.8627	0.1243	0.0126	0.0003	0.0000	0.1505
5	566.6	4418.49	0.1760	0.8239	0.1521	0.0227	0.0011	0.0000	0.2012
6	570.0	5132.20	0.2123	0.7876	0.1752	0.0344	0.0026	0.0000	0.2520
7	573.4	5745.70	0.2463	0.7536	0.1944	0.0473	0.0045	0.0000	0.3030
8	576.8	6276.63	0.2785	0.7214	0.2103	0.0610	0.0070	0.0001	0.3541
9	580.2	6738.91	0.3091	0.6908	0.2234	0.0754	0.0100	0.0002	0.4053
10	583.6	7143.70	0.3382	0.6617	0.2341	0.0903	0.0134	0.0003	0.4566
11	587.0	7500.00	0.3661	0.6338	0.2427	0.1055	0.0173	0.0005	0.5081
12	590.4	7815.14	0.3929	0.6070	0.2494	0.1210	0.0215	0.0008	0.5596
13	593.8	8095.15	0.4186	0.5813	0.2545	0.1368	0.0261	0.0011	0.6113
14	597.2	8345.01	0.4435	0.5564	0.2581	0.1527	0.0310	0.0015	0.6630
15	600.6	8568.89	0.4674	0.5325	0.2603	0.1688	0.0361	0.0020	0.7148
16	604.0	8770.28	0.4907	0.5093	0.2614	0.1850	0.0415	0.0026	0.7668
17	607.4	8952.11	0.5131	0.4868	0.2614	0.2012	0.0471	0.0033	0.8188
18	610.8	9116.89	0.5350	0.4649	0.2604	0.2174	0.0529	0.0041	0.8709
19	614.2	9266.74	0.5562	0.4437	0.2585	0.2336	0.0589	0.0051	0.9230
20	617.6	9403.49	0.5768	0.4231	0.2557	0.2498	0.0650	0.0062	0.9753
21	621.0	9528.70	0.5969	0.4030	0.2522	0.2659	0.0712	0.0074	1.0276
22	624.4	9643.74	0.6164	0.3835	0.2480	0.2820	0.0775	0.0088	1.0800
23	627.8	9749.77	0.6354	0.3645	0.2431	0.2979	0.0839	0.0104	1.1326
24	631.2	9847.82	0.6540	0.3459	0.2377	0.3136	0.0903	0.0122	1.1851
25	634.6	9938.78	0.6720	0.3279	0.2317	0.3292	0.0967	0.0142	1.2378
26	638.0	10023.44	0.6897	0.3102	0.2251	0.3446	0.1032	0.0165	1.2905
27	641.4	10102.50	0.7068	0.2931	0.2182	0.3598	0.1097	0.0190	1.3434
28	644.8	10176.55	0.7236	0.2763	0.2108	0.3747	0.1161	0.0218	1.3963
29	648.2	10246.14	0.7399	0.2600	0.2030	0.3893	0.1225	0.0249	1.4493
30	651.6	10311.75	0.7558	0.2441	0.1949	0.4035	0.1289	0.0284	1.5024
31	655.0	10373.82	0.7712	0.2287	0.1865	0.4173	0.1351	0.0321	1.5555
32	658.4	10432.73	0.7863	0.2136	0.1778	0.4307	0.1412	0.0363	1.6088
33	661.8	10488.83	0.8009	0.1990	0.1689	0.4437	0.1472	0.0409	1.6621
34	665.2	10542.44	0.8151	0.1848	0.1599	0.4561	0.1530	0.0460	1.7155
35	668.6	10593.85	0.8289	0.1710	0.1507	0.4679	0.1586	0.0516	1.7690
36	672.0	10643.33	0.8422	0.1577	0.1413	0.4790	0.1640	0.0577	1.8227
37	675.4	10691.11	0.8551	0.1448	0.1320	0.4894	0.1691	0.0644	1.8764
38	678.8	10737.43	0.8675	0.1324	0.1226	0.4991	0.1739	0.0718	1.9302
39	682.2	10782.50	0.8795	0.1204	0.1132	0.5078	0.1784	0.0799	1.9841
40	685.6	10826.52	0.8910	0.1089	0.1039	0.5157	0.1825	0.0887	2.0381
41	689.0	10869.68	0.9020	0.0980	0.0948	0.5225	0.1861	0.0984	2.0922
42	692.4	10912.18	0.9124	0.0875	0.0858	0.5282	0.1893	0.1090	2.1465
43	695.8	10954.18	0.9223	0.0776	0.0770	0.5327	0.1919	0.1206	2.2009
44	699.2	10995.88	0.9317	0.0682	0.0685	0.5360	0.1939	0.1332	2.2553
45	702.6	11037.43	0.9405	0.0594	0.0603	0.5376	0.1952	0.1470	2.3100
46	706.0	11079.01	0.9487	0.0512	0.0526	0.5382	0.1958	0.1620	2.3647
47	709.4	11120.81	0.9563	0.0436	0.0452	0.5370	0.1956	0.1783	2.4196
48	712.8	11162.99	0.9632	0.0367	0.0384	0.5341	0.1946	0.1960	2.4746
49	716.2	11205.73	0.9695	0.0304	0.0321	0.5296	0.1925	0.2151	2.5298
50	719.6	11249.23	0.9751	0.0248	0.0264	0.5232	0.1895	0.2358	2.5851
51	723.0	11293.66	0.9800	0.0199	0.0212	0.5151	0.1855	0.2581	2.6406

Run 14

Inlet Temp. - 563°K

47 Moles N_2/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	470.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF CP		
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT			
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	563.0001	3.2000	723.0001	99.5000

COEF			
-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 47.00 CARBON TET = 0.00 HCL = 0.00

INLET TEMPERATURE = 563.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	563.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	566.2	1015.84	0.0498	0.9501	0.0498	0.0000	0.0000	0.0000	0.0498
3	569.4	1873.07	0.0953	0.9046	0.0906	0.0046	0.0000	0.0000	0.1000
4	572.6	2603.38	0.1372	0.8627	0.1243	0.0126	0.0002	0.0000	0.1504
5	575.8	3230.95	0.1761	0.8239	0.1521	0.0228	0.0010	0.0000	0.2010
6	579.0	3774.45	0.2124	0.7875	0.1753	0.0348	0.0022	0.0000	0.2517
7	582.2	4248.41	0.2466	0.7533	0.1946	0.0479	0.0039	0.0000	0.3026
8	585.4	4664.33	0.2790	0.7209	0.2106	0.0621	0.0061	0.0001	0.3537
9	588.6	5031.39	0.3097	0.6902	0.2238	0.0769	0.0087	0.0002	0.4048
10	591.8	5357.03	0.3391	0.6608	0.2345	0.0923	0.0118	0.0003	0.4561
11	595.0	5647.30	0.3671	0.6328	0.2431	0.1081	0.0153	0.0005	0.5075
12	598.2	5907.23	0.3941	0.6058	0.2499	0.1242	0.0191	0.0007	0.5590
13	601.4	6140.95	0.4200	0.5799	0.2549	0.1406	0.0233	0.0010	0.6106
14	604.6	6351.95	0.4450	0.5549	0.2585	0.1571	0.0278	0.0014	0.6622
15	607.8	6543.17	0.4691	0.5308	0.2607	0.1738	0.0326	0.0019	0.7140
16	611.0	6717.09	0.4925	0.5074	0.2617	0.1906	0.0376	0.0024	0.7658
17	614.2	6875.82	0.5151	0.4848	0.2616	0.2074	0.0428	0.0031	0.8177
18	617.4	7021.19	0.5371	0.4628	0.2605	0.2243	0.0483	0.0038	0.8697
19	620.6	7154.76	0.5584	0.4415	0.2585	0.2411	0.0539	0.0047	0.9218
20	623.8	7277.89	0.5791	0.4208	0.2557	0.2579	0.0597	0.0058	0.9740
21	627.0	7391.75	0.5993	0.4006	0.2520	0.2745	0.0656	0.0070	1.0262
22	630.2	7497.37	0.6189	0.3810	0.2477	0.2911	0.0716	0.0083	1.0785
23	633.4	7595.64	0.6380	0.3619	0.2427	0.3075	0.0778	0.0099	1.1309
24	636.6	7687.37	0.6566	0.3433	0.2371	0.3238	0.0840	0.0116	1.1834
25	639.8	7773.24	0.6747	0.3252	0.2310	0.3399	0.0902	0.0135	1.2359
26	643.0	7853.87	0.6924	0.3075	0.2243	0.3557	0.0965	0.0157	1.2886
27	646.2	7929.82	0.7096	0.2903	0.2172	0.3712	0.1029	0.0181	1.3413
28	649.4	8001.58	0.7264	0.2735	0.2097	0.3865	0.1092	0.0208	1.3941
29	652.6	8069.59	0.7427	0.2572	0.2018	0.4014	0.1155	0.0238	1.4469
30	655.8	8134.24	0.7586	0.2413	0.1936	0.4159	0.1218	0.0272	1.4999
31	659.0	8195.89	0.7741	0.2258	0.1851	0.4299	0.1280	0.0309	1.5529
32	662.2	8254.87	0.7891	0.2108	0.1763	0.4435	0.1341	0.0349	1.6060
33	665.4	8311.47	0.8037	0.1962	0.1674	0.4566	0.1402	0.0394	1.6592
34	668.6	3365.98	0.8179	0.1820	0.1582	0.4691	0.1460	0.0444	1.7125
35	671.8	8418.64	0.8316	0.1683	0.1489	0.4810	0.1517	0.0498	1.7658
36	675.0	8469.69	0.8449	0.1550	0.1396	0.4921	0.1572	0.0558	1.8193
37	678.2	8519.35	0.8577	0.1422	0.1301	0.5025	0.1625	0.0624	1.8728
38	681.4	8567.82	0.8701	0.1298	0.1207	0.5120	0.1675	0.0697	1.9265
39	684.6	8615.32	0.8820	0.1179	0.1113	0.5207	0.1722	0.0776	1.9802
40	687.8	8662.01	0.8934	0.1065	0.1020	0.5283	0.1765	0.0864	2.0341
41	691.0	8708.11	0.9042	0.0957	0.0929	0.5349	0.1804	0.0959	2.0880
42	694.2	8753.77	0.9146	0.0853	0.0839	0.5403	0.1839	0.1064	2.1421
43	697.4	8799.18	0.9244	0.0755	0.0752	0.5444	0.1868	0.1178	2.1963
44	700.6	8844.53	0.9336	0.0663	0.0668	0.5472	0.1892	0.1304	2.2506
45	703.8	8890.97	0.9423	0.0576	0.0587	0.5485	0.1909	0.1440	2.3050
46	707.0	8935.70	0.9503	0.0496	0.0510	0.5484	0.1919	0.1589	2.3596
47	710.2	8981.90	0.9578	0.0421	0.0438	0.5466	0.1921	0.1752	2.4143
48	713.4	9028.74	0.9645	0.0354	0.0371	0.5431	0.1914	0.1928	2.4691
49	716.6	9076.42	0.9706	0.0293	0.0309	0.5379	0.1898	0.2119	2.5241
50	719.8	9125.13	0.9761	0.0238	0.0253	0.5309	0.1872	0.2325	2.5792
51	723.0	9175.08	0.9809	0.0192	0.0204	0.5221	0.1836	0.2547	2.6345

Run 15

Inlet Temp. - 573°K

50 Moles N_2/Mole CH_4

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	500.00	10.00	0.00	0.00	0.00	0.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR

1.80

CONST OF CP		
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT			
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
1.0000	0.7300	1.9870	573.0001	3.0000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 50.00 CARBON TET = 0.00 HCL = 0.00

INLET TEMPERATURE = 573.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	573.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	576.0	730.64	0.0494	0.9505	0.0494	0.0000	0.0000	0.0000	0.0494
3	579.0	1355.78	0.0946	0.9053	0.0900	0.0046	0.0000	0.0000	0.0992
4	582.0	1895.98	0.1362	0.8637	0.1235	0.0124	0.0002	0.0000	0.1492
5	585.0	2366.80	0.1750	0.8249	0.1514	0.0227	0.0008	0.0000	0.1994
6	588.0	2780.20	0.2112	0.7887	0.1746	0.0345	0.0018	0.0000	0.2497
7	591.0	3145.57	0.2454	0.7545	0.1940	0.0479	0.0033	0.0000	0.3002
8	594.0	3470.38	0.2777	0.7222	0.2101	0.0623	0.0052	0.0000	0.3508
9	597.0	3760.67	0.3085	0.6914	0.2234	0.0773	0.0075	0.0001	0.4015
10	600.0	4021.34	0.3379	0.6620	0.2342	0.0930	0.0102	0.0002	0.4524
11	603.0	4256.48	0.3660	0.6339	0.2430	0.1092	0.0133	0.0004	0.5033
12	606.0	4469.45	0.3930	0.6069	0.2498	0.1257	0.0167	0.0006	0.5544
13	609.0	4663.10	0.4190	0.5809	0.2549	0.1426	0.0205	0.0009	0.6055
14	612.0	4839.83	0.4441	0.5558	0.2586	0.1596	0.0245	0.0012	0.6567
15	615.0	5001.69	0.4683	0.5316	0.2609	0.1767	0.0289	0.0017	0.7080
16	618.0	5150.43	0.4917	0.5082	0.2619	0.1940	0.0334	0.0022	0.7594
17	621.0	5287.55	0.5144	0.4855	0.2619	0.2113	0.0383	0.0028	0.8109
18	624.0	5414.37	0.5364	0.4635	0.2608	0.2287	0.0433	0.0035	0.8624
19	627.0	5532.00	0.5578	0.4421	0.2589	0.2460	0.0485	0.0043	0.9140
20	630.0	5641.46	0.5786	0.4213	0.2560	0.2632	0.0539	0.0053	0.9657
21	633.0	5743.60	0.5988	0.4011	0.2524	0.2804	0.0594	0.0064	1.0175
22	636.0	5839.20	0.6184	0.3815	0.2481	0.2975	0.0651	0.0076	1.0694
23	639.0	5928.92	0.6376	0.3623	0.2431	0.3144	0.0709	0.0091	1.1213
24	642.0	6013.39	0.6562	0.3437	0.2375	0.3311	0.0768	0.0107	1.1733
25	645.0	6093.12	0.6744	0.3255	0.2314	0.3475	0.0828	0.0125	1.2253
26	648.0	6168.60	0.6920	0.3079	0.2247	0.3638	0.0888	0.0145	1.2775
27	651.0	6240.26	0.7093	0.2906	0.2176	0.3797	0.0949	0.0168	1.3297
28	654.0	6308.49	0.7260	0.2739	0.2101	0.3954	0.1011	0.0194	1.3819
29	657.0	6373.65	0.7424	0.2575	0.2022	0.4106	0.1072	0.0222	1.4343
30	660.0	6436.05	0.7583	0.2416	0.1940	0.4255	0.1133	0.0253	1.4867
31	663.0	6495.99	0.7738	0.2261	0.1855	0.4399	0.1194	0.0288	1.5393
32	666.0	6553.74	0.7888	0.2111	0.1767	0.4538	0.1255	0.0327	1.5918
33	669.0	6609.54	0.8034	0.1965	0.1677	0.4671	0.1315	0.0369	1.6445
34	672.0	6663.64	0.8176	0.1823	0.1586	0.4798	0.1373	0.0416	1.6973
35	675.0	6716.25	0.8313	0.1686	0.1493	0.4919	0.1431	0.0468	1.7501
36	678.0	6767.58	0.8446	0.1553	0.1399	0.5033	0.1486	0.0525	1.8030
37	681.0	6817.82	0.8574	0.1425	0.1305	0.5139	0.1540	0.0588	1.8560
38	684.0	6867.16	0.8697	0.1302	0.1211	0.5236	0.1592	0.0657	1.9091
39	687.0	6915.78	0.8816	0.1183	0.1117	0.5323	0.1641	0.0733	1.9623
40	690.0	6963.85	0.8930	0.1069	0.1024	0.5401	0.1686	0.0817	2.0156
41	693.0	7011.56	0.9038	0.0961	0.0933	0.5468	0.1728	0.0908	2.0690
42	696.0	7059.08	0.9142	0.0857	0.0843	0.5522	0.1766	0.1009	2.1225
43	699.0	7106.57	0.9240	0.0759	0.0756	0.5564	0.1799	0.1119	2.1761
44	702.0	7154.20	0.9332	0.0667	0.0672	0.5592	0.1827	0.1239	2.2298
45	705.0	7202.17	0.9418	0.0581	0.0592	0.5606	0.1849	0.1371	2.2837
46	708.0	7250.63	0.9499	0.0500	0.0515	0.5604	0.1864	0.1514	2.3376
47	711.0	7299.78	0.9573	0.0426	0.0443	0.5586	0.1872	0.1671	2.3917
48	714.0	7349.80	0.9640	0.0359	0.0376	0.5551	0.1871	0.1841	2.4460
49	717.0	7400.87	0.9702	0.0297	0.0314	0.5498	0.1862	0.2025	2.5003
50	720.0	7453.20	0.9756	0.0243	0.0258	0.5428	0.1844	0.2225	2.5548
51	723.0	7507.00	0.9804	0.0195	0.0209	0.5340	0.1815	0.2439	2.6095

Run 16

Inlet Temp. - 553°K

45 Moles HCl/Mole CH_4, P - 2.8 atm

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	450.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF CP

8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT

-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
2.8000	0.7300	1.9870	553.0001	3.4000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 0.00 HCL = 45.00

INLET TEMPERATURE = 553.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	553.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	556.4	189.42	0.0502	0.9497	0.0502	0.0000	0.0000	0.0000	0.0502
3	559.8	346.89	0.0960	0.9039	0.0913	0.0047	0.0000	0.0000	0.1008
4	563.2	478.97	0.1381	0.8618	0.1250	0.0127	0.0003	0.0000	0.1516
5	566.6	590.74	0.1771	0.8228	0.1529	0.0230	0.0012	0.0000	0.2026
6	570.0	686.10	0.2135	0.7864	0.1760	0.0348	0.0026	0.0000	0.2537
7	573.4	768.06	0.2477	0.7522	0.1952	0.0478	0.0046	0.0000	0.3050
8	576.8	838.99	0.2800	0.7199	0.2110	0.0616	0.0071	0.0001	0.3564
9	580.2	900.74	0.3107	0.6892	0.2241	0.0761	0.0102	0.0002	0.4080
10	583.6	954.81	0.3399	0.6600	0.2347	0.0911	0.0137	0.0003	0.4596
11	587.0	1002.40	0.3679	0.6320	0.2432	0.1064	0.0176	0.0005	0.5113
12	590.4	1044.50	0.3947	0.6052	0.2498	0.1221	0.0219	0.0008	0.5632
13	593.8	1081.90	0.4205	0.5794	0.2548	0.1379	0.0265	0.0011	0.6151
14	597.2	1115.28	0.4454	0.5545	0.2583	0.1539	0.0314	0.0015	0.6671
15	600.6	1145.19	0.4694	0.5305	0.2605	0.1700	0.0367	0.0020	0.7192
16	604.0	1172.09	0.4926	0.5073	0.2615	0.1862	0.0421	0.0026	0.7713
17	607.4	1196.39	0.5151	0.4848	0.2614	0.2025	0.0478	0.0034	0.8235
18	610.8	1218.40	0.5370	0.4629	0.2603	0.2187	0.0536	0.0042	0.8758
19	614.2	1238.43	0.5582	0.4417	0.2583	0.2350	0.0596	0.0052	0.9282
20	617.6	1256.70	0.5788	0.4211	0.2554	0.2512	0.0658	0.0063	0.9807
21	621.0	1273.44	0.5989	0.4010	0.2518	0.2673	0.0720	0.0075	1.0332
22	624.4	1288.81	0.6184	0.3815	0.2475	0.2833	0.0784	0.0090	1.0858
23	627.8	1302.98	0.6374	0.3625	0.2426	0.2993	0.0848	0.0106	1.1385
24	631.2	1316.09	0.6560	0.3439	0.2371	0.3150	0.0913	0.0124	1.1912
25	634.6	1328.25	0.6740	0.3259	0.2310	0.3306	0.0978	0.0145	1.2440
26	638.0	1339.57	0.6916	0.3083	0.2244	0.3460	0.1043	0.0168	1.2969
27	641.4	1350.14	0.7088	0.2912	0.2174	0.3611	0.1108	0.0193	1.3498
28	644.8	1360.04	0.7255	0.2744	0.2099	0.3759	0.1173	0.0222	1.4028
29	648.2	1369.35	0.7417	0.2582	0.2021	0.3904	0.1237	0.0253	1.4559
30	651.6	1378.12	0.7576	0.2423	0.1939	0.4046	0.1301	0.0288	1.5091
31	655.0	1386.43	0.7730	0.2269	0.1855	0.4183	0.1363	0.0327	1.5623
32	658.4	1394.31	0.7880	0.2119	0.1768	0.4317	0.1425	0.0369	1.6157
33	661.8	1401.81	0.8026	0.1973	0.1679	0.4445	0.1485	0.0416	1.6691
34	665.2	1408.98	0.8167	0.1832	0.1588	0.4568	0.1543	0.0467	1.7225
35	668.6	1415.86	0.8304	0.1695	0.1496	0.4684	0.1599	0.0524	1.7761
36	672.0	1422.48	0.8437	0.1562	0.1403	0.4795	0.1653	0.0586	1.8297
37	675.4	1428.87	0.8565	0.1434	0.1309	0.4898	0.1704	0.0654	1.8835
38	678.8	1435.07	0.8689	0.1310	0.1215	0.4992	0.1752	0.0728	1.9373
39	682.2	1441.10	0.8808	0.1191	0.1122	0.5079	0.1796	0.0810	1.9912
40	685.6	1446.99	0.8922	0.1077	0.1029	0.5156	0.1836	0.0900	2.0452
41	689.0	1452.77	0.9031	0.0968	0.0938	0.5222	0.1872	0.0997	2.0993
42	692.4	1458.46	0.9135	0.0864	0.0848	0.5278	0.1903	0.1104	2.1535
43	695.8	1464.08	0.9233	0.0766	0.0761	0.5321	0.1929	0.1221	2.2079
44	699.2	1469.66	0.9326	0.0673	0.0677	0.5351	0.1948	0.1349	2.2623
45	702.6	1475.22	0.9413	0.0586	0.0595	0.5368	0.1961	0.1488	2.3168
46	706.0	1480.78	0.9494	0.0505	0.0518	0.5370	0.1966	0.1639	2.3715
47	709.4	1486.38	0.9569	0.0430	0.0446	0.5356	0.1963	0.1803	2.4263
48	712.8	1492.02	0.9638	0.0361	0.0378	0.5326	0.1951	0.1981	2.4813
49	716.2	1497.74	0.9700	0.0299	0.0316	0.5279	0.1930	0.2174	2.5364
50	719.6	1503.55	0.9755	0.0244	0.0259	0.5214	0.1898	0.2382	2.5916
51	723.0	1509.49	0.9804	0.0195	0.0209	0.5131	0.1857	0.2606	2.6469

Run 17

Inlet Temp. - 563°K

48 Moles HCl/Mole CH_4, P - 2.8 atm

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	480.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF CP		
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT			
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
2.8000	0.7300	1.9870	563.0001	3.2000	723.0001	99.5000

COEF			
-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 0.00 HCL = 48.00

INLET TEMPERATURE = 563.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	563.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	566.2	135.32	0.0501	0.9498	0.0501	0.0000	0.0000	0.0000	0.0501
3	569.4	249.48	0.0958	0.9041	0.0911	0.0047	0.0000	0.0000	0.1005
4	572.6	346.71	0.1378	0.8621	0.1248	0.0127	0.0002	0.0000	0.1512
5	575.8	430.24	0.1769	0.8230	0.1527	0.0230	0.0010	0.0000	0.2020
6	579.0	502.57	0.2133	0.7866	0.1759	0.0351	0.0022	0.0000	0.2530
7	582.2	565.64	0.2477	0.7522	0.1952	0.0483	0.0039	0.0000	0.3042
8	585.4	620.98	0.2801	0.7198	0.2112	0.0625	0.0062	0.0001	0.3554
9	588.6	669.82	0.3109	0.6890	0.2243	0.0775	0.0088	0.0002	0.4068
10	591.8	713.14	0.3403	0.6596	0.2350	0.0929	0.0120	0.0003	0.4583
11	595.0	751.76	0.3684	0.6315	0.2435	0.1088	0.0155	0.0005	0.5099
12	598.2	786.34	0.3954	0.6045	0.2502	0.1250	0.0194	0.0007	0.5615
13	601.4	817.43	0.4214	0.5785	0.2552	0.1414	0.0236	0.0010	0.6133
14	604.6	845.50	0.4464	0.5535	0.2587	0.1580	0.0281	0.0014	0.6651
15	607.8	870.94	0.4705	0.5294	0.2608	0.1748	0.0329	0.0019	0.7170
16	611.0	894.07	0.4939	0.5060	0.2618	0.1916	0.0380	0.0024	0.7690
17	614.2	915.18	0.5165	0.4834	0.2616	0.2084	0.0432	0.0031	0.8211
18	617.4	934.52	0.5385	0.4614	0.2605	0.2253	0.0487	0.0039	0.8732
19	620.6	952.29	0.5598	0.4401	0.2584	0.2421	0.0544	0.0048	0.9254
20	623.8	968.67	0.5805	0.4194	0.2555	0.2589	0.0602	0.0059	0.9777
21	627.0	983.81	0.6007	0.3992	0.2518	0.2756	0.0661	0.0071	1.0300
22	630.2	997.86	0.6203	0.3796	0.2474	0.2921	0.0722	0.0084	1.0824
23	633.4	1010.93	0.6394	0.3605	0.2423	0.3085	0.0784	0.0100	1.1349
24	636.6	1023.13	0.6580	0.3419	0.2367	0.3248	0.0846	0.0117	1.1874
25	639.8	1034.55	0.6761	0.3238	0.2305	0.3408	0.0909	0.0137	1.2400
26	643.0	1045.28	0.6937	0.3062	0.2238	0.3566	0.0972	0.0159	1.2927
27	646.2	1055.38	0.7109	0.2890	0.2167	0.3721	0.1036	0.0183	1.3455
28	649.4	1064.92	0.7276	0.2723	0.2092	0.3873	0.1099	0.0211	1.3983
29	652.6	1073.96	0.7439	0.2560	0.2012	0.4021	0.1163	0.0241	1.4512
30	655.8	1082.56	0.7598	0.2401	0.1930	0.4166	0.1226	0.0275	1.5041
31	659.0	1090.76	0.7752	0.2247	0.1845	0.4306	0.1288	0.0312	1.5571
32	662.2	1098.60	0.7902	0.2097	0.1757	0.4441	0.1349	0.0353	1.6102
33	665.4	1106.13	0.8047	0.1952	0.1667	0.4571	0.1409	0.0398	1.6634
34	668.6	1113.37	0.8188	0.1811	0.1576	0.4695	0.1468	0.0448	1.7167
35	671.8	1120.37	0.8325	0.1674	0.1483	0.4813	0.1525	0.0503	1.7700
36	675.0	1127.16	0.8458	0.1541	0.1389	0.4924	0.1580	0.0563	1.8234
37	678.2	1133.76	0.8585	0.1414	0.1295	0.5027	0.1632	0.0630	1.8769
38	681.4	1140.20	0.8708	0.1291	0.1201	0.5121	0.1682	0.0703	1.9305
39	684.6	1146.51	0.8827	0.1172	0.1108	0.5206	0.1729	0.0783	1.9841
40	687.8	1152.71	0.8940	0.1059	0.1015	0.5282	0.1772	0.0870	2.0379
41	691.0	1158.84	0.9048	0.0951	0.0924	0.5346	0.1811	0.0966	2.0918
42	694.2	1164.90	0.9151	0.0848	0.0834	0.5399	0.1845	0.1071	2.1457
43	697.4	1170.93	0.9249	0.0750	0.0748	0.5440	0.1874	0.1186	2.1998
44	700.6	1176.95	0.9341	0.0658	0.0664	0.5467	0.1897	0.1312	2.2540
45	703.8	1182.98	0.9427	0.0572	0.0583	0.5480	0.1913	0.1449	2.3082
46	707.0	1189.04	0.9506	0.0493	0.0507	0.5477	0.1922	0.1598	2.3627
47	710.2	1195.17	0.9580	0.0419	0.0435	0.5458	0.1924	0.1761	2.4172
48	713.4	1201.38	0.9647	0.0352	0.0369	0.5423	0.1917	0.1937	2.4719
49	716.6	1207.70	0.9708	0.0291	0.0307	0.5371	0.1900	0.2128	2.5267
50	719.8	1214.15	0.9762	0.0237	0.0252	0.5300	0.1874	0.2334	2.5816
51	723.0	1220.76	0.9810	0.0189	0.0203	0.5212	0.1838	0.2555	2.6367

Run 18

Inlet Temp. - 573°K

.51 Moles HCl/Mole CH_4, P - 2.8 atm

FBO	FFO	FNO	FAO	FCO	FDO	FEO	FSO
42.00	0.00	0.00	10.00	0.00	0.00	0.00	510.00

FREQ FACTOR	ACT ENERGY
0.79800E 17	30036.
0.13910E 18	29902.
0.58940E 13	18930.
0.45770E 18	33290.

CONV FACTOR
1.80

CONST OF CP		
8.0520	0.1080E-02	0.0000E 00
14.7871	0.2320E-01	0.1371E-04
6.4320	0.1320E-02	0.0000E 00
4.3478	0.1350E-01	0.0000E 00
2.9846	0.2500E-01	0.9357E-05
5.0794	0.2840E-01	0.1314E-04
9.2951	0.2710E-01	0.1421E-04
6.6140	0.8100E-03	0.0000E 00

CONST OF REACTION HEAT			
-24833.	-0.3912	0.147E-02	-0.833E-06
-24280.	1.6770	-0.206E-03	-0.333E-06
-25631.	4.0260	-0.292E-02	0.833E-06
-24209.	5.1360	-0.402E-02	0.125E-05

P	GSCON	R	TO	DT	TMAX	XAMAX
2.8000	0.7300	1.9870	573.0001	3.0000	723.0001	99.5000

COEF

-1.	0.	0.	0.
1.	-1.	0.	0.
0.	1.	-1.	0.
0.	0.	1.	-1.
0.	0.	0.	1.
-1.	-1.	-1.	-1.
1.	1.	1.	1.

INERT COMPONENTS

NITROGEN = 0.00 CARBON TET = 0.00 HCL = 51.00

INLET TEMPERATURE = 573.0

COUNTER	TEMPERATURE DEG. K	VOLUME CU.FT.	XA	MOL FA	MOL FC	MOL FD	MOL FE	MOL FF	MOL CL2 REACT/ MOL CH4
1	573.0	0.00	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	576.0	96.97	0.0496	0.9503	0.0496	0.0000	0.0000	0.0000	0.0496
3	579.0	179.91	0.0949	0.9050	0.0903	0.0046	0.0000	0.0000	0.0996
4	582.0	251.57	0.1367	0.8632	0.1239	0.0125	0.0002	0.0000	0.1497
5	585.0	314.02	0.1755	0.8244	0.1518	0.0228	0.0008	0.0000	0.2001
6	588.0	368.84	0.2118	0.7881	0.1750	0.0348	0.0018	0.0000	0.2506
7	591.0	417.28	0.2461	0.7538	0.1944	0.0482	0.0033	0.0000	0.3012
8	594.0	460.35	0.2785	0.7214	0.2105	0.0626	0.0052	0.0000	0.3520
9	597.0	498.83	0.3093	0.6906	0.2237	0.0777	0.0076	0.0001	0.4028
10	600.0	533.38	0.3387	0.6612	0.2345	0.0935	0.0103	0.0003	0.4538
11	603.0	564.55	0.3669	0.6330	0.2432	0.1097	0.0134	0.0004	0.5049
12	606.0	592.77	0.3939	0.6060	0.2500	0.1263	0.0168	0.0006	0.5560
13	609.0	618.43	0.4199	0.5800	0.2551	0.1431	0.0206	0.0009	0.6072
14	612.0	641.85	0.4449	0.5550	0.2587	0.1601	0.0247	0.0013	0.6585
15	615.0	663.30	0.4692	0.5307	0.2609	0.1773	0.0290	0.0017	0.7099
16	618.0	683.01	0.4926	0.5073	0.2620	0.1946	0.0336	0.0022	0.7614
17	621.0	701.17	0.5153	0.4846	0.2619	0.2120	0.0385	0.0028	0.8129
18	624.0	717.97	0.5373	0.4626	0.2608	0.2293	0.0435	0.0035	0.8645
19	627.0	733.55	0.5586	0.4413	0.2587	0.2466	0.0488	0.0044	0.9162
20	630.0	748.05	0.5794	0.4205	0.2559	0.2639	0.0542	0.0053	0.9679
21	633.0	761.58	0.5996	0.4003	0.2522	0.2810	0.0597	0.0064	1.0197
22	636.0	774.23	0.6192	0.3807	0.2479	0.2981	0.0654	0.0077	1.0715
23	639.0	786.11	0.6383	0.3616	0.2429	0.3149	0.0712	0.0091	1.1234
24	642.0	797.30	0.6569	0.3430	0.2373	0.3316	0.0771	0.0108	1.1754
25	645.0	807.85	0.6751	0.3248	0.2311	0.3481	0.0831	0.0126	1.2275
26	648.0	817.84	0.6927	0.3072	0.2245	0.3643	0.0892	0.0146	1.2796
27	651.0	827.32	0.7099	0.2900	0.2173	0.3802	0.0953	0.0169	1.3318
28	654.0	836.35	0.7266	0.2733	0.2098	0.3958	0.1014	0.0195	1.3840
29	657.0	844.97	0.7429	0.2570	0.2019	0.4110	0.1076	0.0223	1.4363
30	660.0	853.23	0.7588	0.2411	0.1937	0.4258	0.1137	0.0255	1.4887
31	663.0	861.15	0.7742	0.2257	0.1852	0.4401	0.1198	0.0290	1.5411
32	666.0	868.79	0.7892	0.2107	0.1765	0.4540	0.1258	0.0328	1.5936
33	669.0	876.17	0.8038	0.1961	0.1675	0.4673	0.1318	0.0371	1.6462
34	672.0	883.32	0.8179	0.1820	0.1584	0.4800	0.1376	0.0418	1.6989
35	675.0	890.27	0.8316	0.1683	0.1491	0.4920	0.1434	0.0470	1.7516
36	678.0	897.05	0.8448	0.1551	0.1397	0.5033	0.1489	0.0527	1.8044
37	681.0	903.69	0.8576	0.1423	0.1304	0.5138	0.1543	0.0590	1.8573
38	684.0	910.20	0.8699	0.1300	0.1210	0.5235	0.1594	0.0659	1.9102
39	687.0	916.62	0.8817	0.1182	0.1116	0.5322	0.1643	0.0735	1.9633
40	690.0	922.96	0.8931	0.1068	0.1024	0.5399	0.1688	0.0818	2.0164
41	693.0	929.25	0.9039	0.0960	0.0932	0.5466	0.1730	0.0910	2.0696
42	696.0	935.52	0.9142	0.0857	0.0843	0.5520	0.1767	0.1010	2.1229
43	699.0	941.78	0.9240	0.0759	0.0756	0.5562	0.1800	0.1119	2.1764
44	702.0	948.05	0.9332	0.0667	0.0673	0.5590	0.1828	0.1239	2.2299
45	705.0	954.37	0.9418	0.0581	0.0592	0.5604	0.1850	0.1371	2.2835
46	708.0	960.75	0.9498	0.0501	0.0516	0.5602	0.1864	0.1514	2.3373
47	711.0	967.21	0.9572	0.0427	0.0444	0.5585	0.1872	0.1669	2.3911
48	714.0	973.79	0.9639	0.0360	0.0377	0.5550	0.1872	0.1839	2.4451
49	717.0	980.50	0.9700	0.0299	0.0316	0.5498	0.1862	0.2022	2.4993
50	720.0	987.37	0.9755	0.0244	0.0260	0.5429	0.1844	0.2220	2.5535
51	723.0	994.43	0.9803	0.0196	0.0210	0.5342	0.1815	0.2434	2.6079