FINAL PROGRESS REPORT

STUDY OF CATALYTIC REACTORS
FOR HYDROGEN-OXYGEN IGNITION

by

Arthur S. Kesten

prepared for
NATIONAL AERONAUTICS
AND SPACE ADMINISTRATION

JULY, 1969

CONTRACT NASW-1795

United Aircraft Research Laboratories

UNITED AIRCRAFT CORPORATION

EAST HARTFORD, CONNECTICUT
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Report H910721

Study of Catalytic Reactors for Hydrogen-Oxygen Ignition

Final Progress Report

August 28, 1968 - May 28, 1969

Contract NASW-1795

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ABSTRACT

An analytical study of a catalytic ignition system to promote hydrogen-oxygen combustion was performed in order to establish procedures capable of predicting the steady-state behavior of the system. The study included the development of a computer program which is used to calculate the steady-state axial temperature and reactant concentration profiles in typical reaction chamber configurations. The computer program is based upon a mathematical model of the reactor system which considers both thermal and catalytic reaction of hydrogen and oxygen, along with simultaneous heat and mass transfer between the free-gas phase and the gas within the pores of the catalyst pellets. The computer program has been used to evaluate the effects of chamber pressure, feed temperature, stoichiometry, helium dilution, mass flow rate and catalyst bed configuration on the steady-state behavior of the reactor system.
FOREWORD

This work was performed by United Aircraft Research Laboratories for the National Aeronautics and Space Administration under Contract NASW-1795 initiated August 28, 1968.

Included among those who cooperated in performance of the work under Contract NASW-1795 were Dr. A. S. Kesten, Program Manager, Dr. W. G. Burwell, Chief, Kinetics and Thermal Sciences Section, Mrs. E. Smith, and Mr. D. B. Smith of UARL.

This work was conducted under program management of the NASA Lewis Research Center and the Technical Manager was Mr. P. N. Herr, NASA Lewis Research Center, Cleveland, Ohio.
SUMMARY

The Research Laboratories of United Aircraft Corporation under contract with the National Aeronautics and Space Administration are performing an analytical study of a catalytic ignition system to promote hydrogen-oxygen combustion. This final technical report summarizes the first phase of this work which was performed under Contract NASW-1795 from August 28, 1968 to May 28, 1969. Work during this period has included the development of a computer program which is used to calculate the steady-state axial temperature and reactant concentration profiles in typical reaction chamber configurations. The computer program is based upon a mathematical model of the reactor system which considers both thermal and catalytic reaction of hydrogen and oxygen, along with simultaneous heat and mass transfer between the free-gas phase and the gas within the pores of the catalyst pellets. The possibility that water vapor produced by catalytic reaction within hot catalyst particles might condense or freeze in the colder bulk gas phase has been taken into account in the model. The computer program has been used to evaluate the effects of chamber pressure, feed temperature, stoichiometry, helium dilution, mass flow rate and catalyst bed configuration on the steady-state behavior of the reactor system.
INTRODUCTION

Effective design of a catalytic ignition system to promote hydrogen-oxygen combustion requires the capability for predicting the effects of the design and operating characteristics of the reactor system on the transient and steady-state performance of the system. This general capability did not exist although the feasibility of using catalysts to promote hydrogen-oxygen combustion had been demonstrated in a number of experimental investigations (Refs. 1, 2 and 3). These investigations did not adequately assess the effects on reactor performance of such parameters as chamber pressure, feed temperature, stoichiometry, mass flow rate, and catalyst size distribution. Nor did these investigations adequately specify ignition limits or ignition delay times. To achieve this information, a comprehensive theoretical analysis is required which considers the simultaneous processes of heat transfer, diffusion, and chemical reaction in the catalytic reactor. Such an analysis had already been performed at UARL for catalytic reactors which promote hydrazine decomposition (Refs. 4, 5 and 6). Computer programs had been developed to predict both steady-state and transient performance of these reactors. Preliminary investigations at UARL indicated that these computer programs could be extended to predict the steady-state and transient performance of the hydrogen-oxygen system.

Based upon the above investigations, a comprehensive analytical program directed initially at the steady-state analysis was formulated with the objectives of (a) extending the analysis for predicting the steady-state temperature and concentration distributions in monopropellant hydrazine catalytic reactors to the bipropellant hydrogen-oxygen system, (b) developing a computer program based on this extended analysis, (c) performing calculations using this computer program to demonstrate the effects of various system parameters on the steady-state performance of the reactor, and thus to define the regimes in which ignition is possible, and (d) defining the processes controlling the overall reaction rate in different regions of the reaction system in order to facilitate adaptation of the transient analysis of hydrazine catalytic reactor to the hydrogen-oxygen system. This effort is described in detail in succeeding sections of this report.
Steady-State Model of Hydrogen-Oxygen Catalytic Ignition System

The analysis of a catalytic ignition system to promote hydrogen-oxygen combustion pertains to a reaction chamber of arbitrary cross section packed with catalyst particles into which hydrogen and oxygen are injected with and without an inert carrier gas. Catalyst particles are represented as "equivalent" spheres with a diameter taken as a function of the particle size and shape. Both thermal and catalytic reaction of hydrogen and oxygen are considered in developing equations describing the concentration distributions of these reactants. Diffusion of reactants from the interstitial (free-gas) phase to the outside surface of the catalyst pellets is taken into account. Since the catalyst material is impregnated on the interior and exterior surfaces of porous particles, the diffusion of reactants into the porous structure must also be considered. In addition, the conduction of heat within the porous particles must be considered since the hydrogen-oxygen reaction is accompanied by the evolution of heat. The possibility that water vapor produced by catalytic reaction within hot catalyst particles might condense or freeze in the colder bulk gas is also taken into account in the model.

The general equations describing the rates of change with axial distance of the weight-fractions of each of the chemical species in the interstitial phase are

\[
\frac{d w_i^{H_2}}{d z} = - \frac{1}{G} \left\{ r_{\text{hom}} \delta + k_c H_2 A_p \left[ c_i^{H_2} - (c_p)_s^{H_2} \right] \right\}, \quad (1)
\]

\[
\frac{d w_i^{O_2}}{d z} = - \frac{1}{G} \left\{ r_{\text{hom}} \delta \frac{M^{O_2}}{2 M^{H_2}} + k_c O_2 A_p \left[ c_i^{O_2} - (c_p)_s^{O_2} \right] \right\}, \quad (2)
\]

\[
\frac{d w_i^{H_2O}}{d z} = \frac{1}{G} \left\{ r_{\text{hom}} \delta \frac{M^{H_2O}}{M^{H_2}} - k_c H_2O(v) A_p \left[ c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)} \right] \right\}, \quad (3)
\]
The rates of change of species concentrations with axial distance are then given by

\[
\frac{dc_{i,j}}{dz} = \rho_i \frac{dw_{i,j}}{dz} + w_{i,j} \frac{dp_i}{dz}
\]

(5)

where

\[
\frac{1}{\rho_i} \frac{dp_i}{dz} \left[ 1 - w_{i,H_2O(s)} - w_{i,H_2O(l)} \right] = \frac{dw_{i,H_2O(s)}}{dz} + \frac{dw_{i,H_2O(l)}}{dz}
\]

\[
+ \frac{\rho_i^{(v)}}{\rho_i} \left[ \frac{1}{\rho} \frac{dP}{dz} + \frac{1}{\bar{M}^{(v)}} \frac{d\bar{M}^{(v)}}{dz} - \frac{1}{T_i} \frac{dT_i}{dz} \right]
\]

and

\[
\frac{1}{\bar{M}^{(v)}} \frac{d\bar{M}^{(v)}}{dz} = - \left[ \sum_{(vapor)} \frac{dW_{i,j}}{dz} \right] \sum_{(vapor)} \frac{w_{i,j}}{M_j^{(vapor)}}
\]

Heat and mass transfer coefficients may be estimated from (Ref. 7)

\[
J_{tc} = 0.74 \bar{c}_{f}^{(v)} G \left( \frac{G}{A_D \mu} \right)^{-0.41}
\]

(8)

\[
k_{tc}^{(v)} = \frac{61G}{\rho_i^{(v)D_i,j}} \left( \frac{\mu}{\rho_i^{(v)D_i,j}} \right)^{-0.667} \left( \frac{G}{A_D \mu} \right)^{-0.41}
\]

(9)

In the entrance region of the reactor, where the temperature in the interstitial phase is low enough to cause freezing of the water vapor diffusing out of the catalyst particles, the change in enthalpy of the interstitial phase with axial distance is
given by

\[
\frac{d h_i}{dz} = - \frac{1}{G} \left\{ Hr_{\text{hom}} \delta + \lambda_c A_p \left[ T_i - (T_p)_g \right] + k_c H_2O(v) A_p \left[ c_i H_2O(v) - (c_p)_s H_2O(v) \right] \left[ \Delta h^f + \Delta h^c \right] \right\} \tag{10}
\]

In this "ice region"

\[
\frac{d w_i^{H_2O}}{dz} = \frac{d w_i^{H_2O(s)}}{dz} \tag{11}
\]

In the higher temperature, "ice-liquid region" of the reactor, the change in enthalpy of the interstitial phase with distance is given by

\[
\frac{d h_i}{dz} = - \frac{1}{G} \left\{ Hr_{\text{hom}} \delta + \lambda_c A_p \left[ T_i - (T_p)_g \right] + k_c H_2O(v) A_p \left[ c_i H_2O(v) - (c_p)_s H_2O(v) \right] \left[ \Delta h^c + \frac{h_i - h_i^{(s)}}{h_i^{(s-l)} - h_i^{(s)}} \right] \right\} \tag{12}
\]

and the rates of change of ice and liquid weight-fractions are given by

\[
\frac{d w_i^{H_2O(s)}}{dz} = \frac{d w_i^{H_2O}}{dz} \left[ \frac{h_i^{(s-l)} - h_i}{h_i^{(s-l)} - h_i^{(s)}} \right] - \frac{1}{(h_i^{(s-l)} - h_i^{(s)})} \frac{d h_i}{dz} \tag{13}
\]

\[
\frac{d w_i^{H_2O(l)}}{dz} = \frac{d w_i^{H_2O}}{dz} \left[ \frac{h_i - h_i^{(s)}}{h_i^{(s-l)} - h_i^{(s)}} \right] + \frac{1}{(h_i^{(s-l)} - h_i^{(s)})} \frac{d h_i}{dz} \tag{14}
\]
where, at a fixed axial position, \( z \), in the ice-liquid region, the enthalpy required for melting the ice existing at that position may be calculated from

\[
h_i^{(s\rightarrow l)} = h_i(z) + \Delta H^f_{W_i}^{H_2O(s)}(z)
\]

(15)

At still higher temperatures, where water exists in liquid form in the interstitial phase, the change in enthalpy with distance is given by

\[
\frac{d \Delta h_i}{dz} = \frac{1}{G} \left\{ H_{r hom} S + \Delta h_c A_p \left[ T_i - (T_p)_s \right] + k_c^{H_2O(v)} A_p \left[ C_i^{H_2O(v)} - (C_p)_s^{H_2O(v)} \right] \left[ \Delta H^C \right]\right\}
\]

(16)

In this "liquid region"

\[
\frac{d w_i^{H_2O}}{dz} = \frac{d w_i^{H_2O(w)}}{dz}
\]

(17)

In the "liquid-vapor region" of the reactor, the change in enthalpy with axial distance is given by

\[
\frac{d \Delta h_i}{dz} = \frac{1}{G} \left\{ H_{r hom} S + \Delta h_c A_p \left[ T_i - (T_p)_s \right] + k_c^{H_2O(v)} A_p \left[ C_i^{H_2O(v)} - (C_p)_s^{H_2O(v)} \right] \left[ \Delta H^C \left( \frac{h_i - h_i^{(l)}}{h_i^{(l-v)} - h_i^{(l)}} \right) \right]\right\}
\]

(18)

and the rates of change of liquid and water vapor weight-fractions are given by

\[
\frac{d w_i^{H_2O(l)}}{dz} = \frac{d w_i^{H_2O}}{dz} \left[ \frac{h_i^{(l-v)} - h_i}{h_i^{(l-v)} - h_i^{(l)}} \right] - \frac{1}{(h_i^{(l-v)} - h_i^{(l)})} \frac{d \Delta h_i}{dz}
\]

(19)
\[
\frac{d\omega_i^{H_2O(v)}}{dz} = \frac{d\omega_i^{H_2O}}{dz} \left[ \frac{\dot{h}_i - h_i^{(L)}}{h_i(L-v) - h_i^{(L)}} \right] + \frac{1}{(h_i(L-v) - h_i^{(L)})} \frac{d\dot{h}_i}{dz}
\]

where, at a fixed axial position in this region, the enthalpy required for vaporizing the liquid existing at that position may be calculated from

\[h_i^{(L-v)} = h_i(z) + \Delta H_{w_i}^{H_2O}(z)\]

In the high temperature, all vapor, region of the reactor, the change in enthalpy with distance is given by

\[\frac{d\dot{h}_i}{dz} = -\frac{1}{G} \left\{ \Delta H_{\text{hom}}^S + \dot{\lambda}_c \Delta \rho \left[ T_i - (T_p)_s \right] \right\}\]

and

\[\frac{d\omega_i^{H_2O}}{dz} = \frac{d\omega_i^{H_2O(v)}}{dz}\]

Species concentrations and temperatures at the outside surfaces of the catalyst particles can be determined, together with the concentration and temperature profiles throughout the particles, using an integral equation method described in Appendix I. It should be noted that under steady-state conditions, successful operation of the hydrogen-oxygen catalytic ignition system requires that water produced by catalytic reaction remain as vapor within the catalyst particles. Should the partial pressure of water vapor exceed the vapor pressure at any point within a catalyst pellet, condensation (or freezing) of water vapor within the porous structure would "poison" the catalyst and prevent further reaction.

Finite difference methods have been used to program for digital computation the differential equations describing the changes with axial distance of enthalpy and species concentrations in the interstitial phase. These equations are solved
simultaneously with the integral equations describing the diffusional processes within the pores of the catalyst particles at each of a number of axial positions in the reaction chamber. The number and sizes of axial increments into which the reactor is divided are determined relative to the local rates of change of enthalpy of the interstitial phase with axial distance. A listing of the computer program is contained in Appendix II.

**Kinetics Information**

A number of investigators have assembled kinetics information for the gas phase reaction of hydrogen and oxygen (Refs. 8, 9 and 10). While the reported reaction rates are all quite low for even the highest temperatures of interest here, the activation energies and orders of reaction reported in these studies are in serious disagreement. A rate expression which agrees fairly well with the data reported in Ref. 10 and with the overall order of the reaction reported in Ref. 8 was chosen for use in this work, since the results given in Ref. 10 were obtained in a reactor similar to the one of interest here. The expression is

\[ r_{\text{hom}} = 0.16 \times 10^{14} c_1^2 c_2 c_1^0_2 e^{-35,800/T_1} \text{ lbs H}_2 \text{ reacted/ft}^3\text{-sec} \]

\[ (= 0.10 \times 10^{13} c_1^2 c_2 c_1^0_2 e^{-19,889/T_1} \text{ kg H}_2 \text{ reacted/m}^3\text{-sec}) \]  

(24)

where the concentrations are in lb/ft\(^3\) (kg/m\(^3\)) and \(T_1\) is in deg R (deg K).

Estimating the chemical kinetic rate law and constants appropriate to the catalytic reaction of hydrogen and oxygen is quite difficult. Although a substantial number of experimental investigations have been conducted with this objective, the results of various investigators differ considerably for diverse conditions of concentration, temperature and catalyst. These results indicate that, even for low temperature reaction on platinum family metals, the reaction mechanism changes with gas composition. Reaction of chemisorbed oxygen with hydrogen molecules in the gas phase appears to be the rate-controlling step in systems where excess oxygen is present, while this relatively slow reaction does not seem to influence the overall reaction rate in systems containing excess hydrogen. For low temperature, hydrogen rich systems, Miller and Deans (Ref. 11) and Maymo and Smith (Ref. 12) report an activation energy of approximately 5.5 kcal and an order of reaction with respect to oxygen of 0.8. In the latter study, the rate of reaction was found to be uninfluenced by the presence of water in the vapor phase. No work was done in these studies to estimate the order of reaction with respect to hydrogen. In the present work the results of Refs. 11 and 12 were used together with an assumed first order dependence of reaction rate on hydrogen concentration to get a reaction rate expression of the form*:

*The assumption of first order kinetics with respect to hydrogen should not introduce any great error in the rate expression so long as the expression is applied to a system where hydrogen is present in large excess.
The rate constant, \( \alpha \), is specific to the type and structure of the platinum family metal employed.

It was originally intended to estimate \( \alpha \) for a particular catalyst by using the steady-state program to find the value of \( \alpha \) for which calculated axial temperature profiles exhibited the best agreement with temperatures measured in engine tests being performed by TRW. Although these temperature measurements are not yet available, preliminary test results (Ref. 13) indicate that, under steady-state conditions, reaction on Shell 405 catalyst may be so fast that the hydrogen-oxygen reaction may be diffusion-controlled throughout the reactor. That is, the value of \( \alpha \) for the Shell catalyst may be so high that reaction occurs essentially instantaneously upon contact of the reactants with the catalyst surface.

**Results of Calculations**

Sample calculations have been made using the computer program to test the effectiveness of the steady-state model as well as to predict temperature and concentration profiles in typical catalytic ignition systems. Calculations have been made using a value of the catalytic reaction rate constant, \( \alpha \), high enough to insure that the hydrogen-oxygen reaction was diffusion-controlled throughout the reactor. The results of one computer run are plotted in Figs. 1 through 3 for a reactor packed with 14-18 mesh catalyst particles and for a nominal chamber pressure of 10 psia (6.89 \( \times \) \( 10^5 \) N/m\(^2\)), a mixture ratio of 1.0 lb O\(_2\)/lb H\(_2\), an inlet temperature of 210 deg R (117 deg K), and no helium dilution. The calculations were made for a reaction chamber 0.5 in. (0.013 m) long and 0.87 in. (0.022 m) in diameter, with a total propellant flow of 0.0053 lb/sec (0.0024 kg/sec); this corresponds to a mass flow rate of 1.28 lb/ft\(^2\)-sec (6.25 kg/m\(^2\)-sec). In order to accommodate this rather high flow rate in this low pressure system, the upstream chamber pressure was taken as 30 psia (2.07 \( \times \) \( 10^5 \) N/m\(^2\)) (in subsequent calculations at lower flow rates the upstream chamber pressure was lowered correspondingly). The calculated axial temperature and chamber pressure profiles for this reference case are shown in Fig. 1. The axial concentration profiles for hydrogen, oxygen, and water (solid, liquid and vapor) are shown in Fig. 2 and the associated mole-fraction profiles are illustrated in Fig. 3.

The effect of feed temperature on the axial temperature profile associated with the reference case cited above is depicted in Fig. 4. Also illustrated in Fig. 4 is the effect of feed temperature for a reaction chamber packed with 1/16 in. (0.16 \( \times \) \( 10^{-2} \) m) diameter spheres; all other conditions were taken as those of the reference case. It should be noted that the temperature profiles associated with
the smaller (14-18) mesh particles are steeper because heat and mass transfer rates vary inversely with particle size.

The effect of stoichiometry on temperature profiles is illustrated in Fig. 5 for both the reference case and for the bed configuration consisting of 1/16 in. (0.16 x 10^-2 m) spheres. In each of the curves illustrated here the inlet oxygen concentration was fixed at the same value used in the reference case and mixture ratios above 1.0 were achieved by replacing the appropriate amount of hydrogen with helium. Under these conditions, the higher mixture ratios result in higher gas temperatures because helium has a lower heat capacity than hydrogen.

The effect of helium dilution on temperature distributions is shown in Fig. 6 for the two bed configurations. Here the mixture ratio was fixed at 1.0 and various amounts of diluent gas were added to the inlet mixture. Here temperatures decrease with increasing helium concentration simply because there is less oxygen to react.

The effects of mass flow rate on axial temperature profiles are illustrated in Figs. 7 through 9 for both bed configurations and for three different inlet helium concentrations. In Fig. 7 the effect of varying the mass flow rate from 0.26 lb/ft^2-sec (1.27 kg/m^2-sec) to 1.28 lb/ft^2-sec (6.25 kg/m^2-sec) is illustrated for a system with no helium dilution. Axial temperature profiles are plotted for various mass flow rates in Fig. 8 for an inlet helium weight-fraction of 0.25 and in Fig. 9 for an inlet helium weight-fraction of 0.50.

In order to evaluate the effects of higher chamber pressure and higher mass flow rates on the steady-state behavior of these reactors, calculations were made for a reactor 0.43 in. (0.011 m) in diameter, with the total propellant flow remaining at 0.0053 lb/sec (0.0024 kg/sec); this corresponds to a mass flow rate of 5.24 lb/ft^2-sec (25.6 kg/m^2-sec). The nominal chamber pressure was taken as 100 psia (6.89 x 10^5 N/m^2) while the other reactor design and operating conditions were chosen as those of the reference case cited previously. The calculated axial temperature and chamber pressure profiles for this case are shown in Fig. 10. The axial concentration profiles for hydrogen, oxygen and water are shown in Fig. 11 and the associated mole-fraction profiles are illustrated in Fig. 12.

For this higher pressure reactor, the effects of mass flow rate on axial temperature profiles are illustrated for a reactor packed with 14-18 mesh particles and for a reactor packed with 1/16 in. (0.16 x 10^-2 m) spheres in Figs. 13 through 15. Calculations were made for a mixture ratio of 1.0 and for mass flow rates varying between 1.05 lb/ft^2-sec (5.12 kg/m^2-sec) and 5.25 lb/ft^2-sec (25.6 kg/m^2-sec). The results of these calculations are plotted in Fig. 13 for a system with no helium dilution, in Fig. 14 for an inlet helium weight-fraction of 0.25, and in Fig. 15 for an inlet helium weight-fraction of 0.50.
Definition of Rate-Controlling Processes

As noted previously, preliminary indications (Ref. 13) are that, under steady-state conditions, diffusion of reactants from the free-gas phase to the surface of the catalyst particles may control the rate of the hydrogen-oxygen reaction throughout the reactor. Although the calculated results described in the preceding section were based on this assumption, further validation is required using detailed engine test data. If the assumption is valid, it implies that at steady-state, catalyst particle temperatures at an axial position near the inlet of the reactor are considerably higher than the bulk fluid temperature at the same axial position. It is apparent that this same condition cannot exist in the early stages of transient operation if the catalyst bed is initially at a temperature close to the inlet propellant temperature. In the latter case the reaction rate may well be controlled by diffusion and reaction within the porous catalyst particles. A transient model of a hydrogen-oxygen catalytic ignition system should therefore consider both film and pore diffusion of heat and mass as well as the chemical kinetics of catalytic reaction of hydrogen and oxygen. In addition, consideration should be given to the effects on transient reactor behavior of the temporary reduction in catalyst activity caused by capillary condensation or freezing of water in cold catalyst particles.
REFERENCES


REFERENCES (cont'd)


LIST OF SYMBOLS

a
Radius of spherical catalyst particle, ft (m)

$A_p$
Total external surface of catalyst particle per unit volume of bed, $\text{ft}^{-1} (\text{m}^{-1})$

c$_i$
Reactant concentration in interstitial fluid, $\text{lb/ft}^3$ ($\text{kg/m}^3$)

c$_p$
Reactant concentration in gas phase within the porous catalyst particle, $\text{lb/ft}^3$ ($\text{kg/m}^3$)

$C_f$
Specific heat of fluid in the interstitial phase, $\text{Btu/lb-deg R (Cal/kg-deg K)}$

$\overline{C_f}$
Average specific heat of fluid in the interstitial phase, $\text{Btu/lb-deg R (Cal/kg-deg K)}$

$D_i$
Diffusion coefficient of reactant gas in the interstitial phase, $\text{ft}^2/\text{sec (m}^2/\text{sec)}$

$D_p$
Diffusion coefficient of reactant gas in the porous particle, $\text{ft}^2/\text{sec (m}^2/\text{sec)}$

G
Mass flow rate, $\text{lb/ft}^2$-$\text{sec (kg/m}^2$-$\text{sec)}$

$h_i$
Enthalpy, $\text{Btu/lb (Cal/kg)}$

$h_i(s)$
Enthalpy at the Ice/Ice-Liquid interface, $\text{Btu/lb (Cal/kg)}$

$h_i(s-l)$
Enthalpy at the Ice-Liquid/Liquid interface, $\text{Btu/lb (Cal/kg)}$

$h_i(l)$
Enthalpy at the Liquid/Liquid-Vapor interface, $\text{Btu/lb (Cal/kg)}$

$h_i(l-v)$
Enthalpy at the Liquid-Vapor/Vapor interface, $\text{Btu/lb (Cal/kg)}$

$\overline{h}_c$
Heat transfer coefficient, $\text{Btu/ft}^2$-$\text{sec-deg R (Cal/m}^2$-$\text{sec-deg K)}$

H
Heat of reaction, $\text{Btu/lb (Cal/kg)}$

$\Delta H^c$
Heat of condensation, $\text{Btu/lb (Cal/kg)}$

$\Delta H^f$
Heat of fusion, $\text{Btu/lb (Cal/kg)}$

$K_c$
Mass transfer coefficient, $\text{ft/\text{sec (m/sec)}}$

$K_p$
Thermal conductivity of the porous catalyst particle, $\text{Btu/ft}$-$\text{sec-deg R (Cal/m}$-$\text{sec-deg K)}$
Molecular weight, lb/lb mole (kg/kg mole)

Average molecular weight, lb/lb mole (kg/kg mole)

Chamber pressure, psia (N/m²)

Rate of (heterogeneous) chemical reaction on the catalyst surfaces, lb/ft³-sec (kg/m³-sec)

Rate of (homogeneous) chemical reaction in the interstitial phase, lb/ft³-sec (kg/m³-sec)

Temperature, deg R (deg K)

Weight fraction of reactant in interstitial phase

Radial distance from the spherical catalyst particle, ft (m)

Axial distance, ft (m)

Catalytic reaction rate constant

Interparticle void fraction

Viscosity of interstitial fluid, lb/ft·sec (kg/m·sec)

Density of interstitial fluid, lb/ft³ (kg/m³)

Subscripts

F Refers to feed

i Refers to interstitial phase

p Refers to gas within the porous catalyst particle

s Refers to surface of catalyst particle

Superscripts

\( \text{H}_2\text{O}(s) \) Refers to water in the solid phase

\( \text{H}_2\text{O}(l) \) Refers to water in the liquid phase

\( \text{H}_2\text{O}(v) \) Refers to water in the vapor phase

J Refers to chemical species (e.g. \( \text{H}_2, \text{O}_2, \text{H}_2\text{O}, \text{He} \))

(v) Refers to vapor phase
The system under consideration is a spherical porous catalyst pellet which is surrounded by a stagnant film of fluid. Reactant molecules must diffuse through this film and into the interstices of the porous particle before reacting on the catalytic surfaces. In describing the diffusion of mass within a porous pellet, it is assumed that Fick's law applies and that changes in the mass density of fluid within the particle are negligible relative to changes in concentrations of the reacting species. Fourier's law is used to describe heat conduction within the catalyst pellet. Pressure changes within the particle resulting from non-equimolar diffusion are neglected as is heat transported by pore diffusion of mass. Heat and mass transfer coefficients are used to describe film diffusion of heat and mass. Assuming constant diffusion coefficients, $D_p$, and thermal conductivities, $K_p$, within the porous structure, the equations describing heat and mass transfer of a single reactant in a catalyst particle may be written as

\[
D_p \nabla^2 c_p - r_{\text{het}} = 0
\]

\[
K_p \nabla^2 T_p - H r_{\text{het}} = 0
\]

where the concentration, $c_p$, and rate of reaction, $r_{\text{het}}$, are expressed in mass units. The boundary conditions which consider diffusion of heat and mass through a film surrounding a spherical particle are

\[
D_p \left( \frac{dc_p}{dx} \right)_s = k_c \left[ c_i - (c_p)_s \right]
\]

\[
H D_p \left( \frac{dc_p}{dx} \right)_s = k_c \left[ T_i - (T_p)_s \right]
\]
Using Eqs. (I-1) and (I-2), Prater (Ref. 14) has pointed out that temperature and concentration are related quite simply by

\[ T_p - (T_p)_s = -\frac{H D_p}{K_p} [(c_p)_s - c_p]. \]  

(I-5)

The use of this relationship enables the reaction rate, \( r_{\text{net}} \), to be written, for given surface conditions, as a function of concentration alone instead of concentration and temperature. It is only necessary, then, to solve Eq. (I-1) with \( r_{\text{net}} = r_{\text{net}} (c_p) \), subject to boundary conditions (I-3) and (I-4). The solution is derived in Refs. 5 and 15 as an implicit integral equation given by

\[ c_p(x) = c_i - \left[ \frac{1}{x} - \frac{a k_c - D_p}{a^2 k_c} \right] \int_0^x \frac{r_{\text{net}} (c_p)}{D_p} \, d\xi \]

- \[ \int_x^a \left[ \frac{1}{\xi} - \frac{a k_c - D_p}{a^2 k_c} \right] \xi^2 \frac{r_{\text{net}} (c_p)}{D_p} \, d\xi \]  

(I-6)

Equation (I-6) can be solved numerically to determine the concentration at any point in a porous particle in terms of \( c_i \), the concentration in the bulk fluid. Because of the dependence of the reaction rate, \( r_{\text{net}} \), on particle surface temperature, \( (T_p)_s \), and reactant concentration, \( (c_p)_s \), it is necessary to solve Eq. (I-6) simultaneously with Eqs. (I-3) and (I-4) to determine the concentration profile within the particle. Numerical methods have been developed to accomplish this and these have been programmed for digital computation.

An important generalization of the integral method presented above involves a description of multiple reaction systems. Consider a reacting system where

\[ aA + bB + \ldots \rightarrow tT + \ldots \]

It is apparent that the rate of the reaction can be expressed in terms of any of the reactants or products; however, the rate may be a function of the concentration of any or all of those species. The concentration profile of any species within a porous catalyst particle must then be determined by simultaneous solution of

\[ D_p^A \nabla^2 c_p^A - r_{\text{net}}^A (c_p^A, c_p^B, \ldots, c_p^T, \ldots, T_p) = 0 \]  

(I-7)
\[ D_p^B \nabla^2 c_p^B - \frac{b}{a} \frac{M^B}{M^A} r_{het}^A (c_p^A, c_p^B, \ldots, c_p^T, \ldots, T_p) = \frac{H}{a} \]  
(I-8)

\[ D_p^T \nabla^2 c_p^T + \frac{f}{a} \frac{M^T}{M^A} r_{het}^A (c_p^A, c_p^B, \ldots, c_p^T, \ldots, T_p) = 0 \]  
(I-9)

and

\[ K_p \nabla^2 T_p - H^A r_{het}^A (c_p^A, c_p^B, \ldots, c_p^T, \ldots, T_p) = 0 \]  
(I-10)

where the diffusion coefficients and thermal conductivities are again taken as constant, and the heat of reaction, \( H^A \), is expressed in terms of heat absorbed per unit mass of species A. The boundary conditions which consider film diffusion of mass and heat are

\[ D_p^A \frac{\partial c_p}{\partial x} \bigg|_{S} = k_c^A \left[ c_i^A - (c_p)_s^A \right] \]  
(I-11)

\[ D_p^B \frac{\partial c_p}{\partial x} \bigg|_{S} = \frac{b M^B}{a M^A} D_p^A \frac{\partial c_p}{\partial x} \bigg|_{S} = k_c^B \left[ c_i^B - (c_p)_s^B \right] \]  
(I-12)

\[ D_p^T \frac{\partial c_p}{\partial x} \bigg|_{S} = -\frac{M^T}{a M^A} D_p^A \frac{\partial c_p}{\partial x} \bigg|_{S} = k_c^T \left[ c_i^T - (c_p)_s^T \right] \]  
(I-13)

and

\[ H^A D_p^A \frac{\partial T}{\partial x} \bigg|_{S} = \mathcal{J}_c \left[ T_i - (T_p)_s \right] \]  
(I-14)

As noted previously, Prater (Ref. 14) has pointed out that temperature and reactant concentration are related by Eq. (5), where the concentrations, \( c_p \) and \( (c_p)_s \), refer
in this case to species A. The same procedure used in Ref. 14 can be employed to relate all reactant and product concentrations at any point within the porous catalyst particle to the concentration of reactant A at the same point. Thus

\[
\begin{align*}
    c_p^B - (c_p)_s^B &= \frac{bM^B}{\alpha M^A} \frac{D_p^A}{D_p^B} \left[ c_p^A - (c_p)_s^A \right] \\
    \vdots \\
    (I-15)
\end{align*}
\]

\[
\begin{align*}
    c_p^T - (c_p)_s^T &= \frac{1M^T}{\alpha M^A} \frac{D_p^A}{D_p^T} \left[ (c_p)_s^A - c_p^A \right] \\
    \vdots \\
    (I-16)
\end{align*}
\]

Surface concentrations, \((c_p)_s\), of all reactants and products can be written in terms of the surface concentration of reactant A and the known concentrations in the bulk fluid by combining Eqs. (I-11) and (I-12) and then Eqs. (I-11) and (I-13) to get

\[
\begin{align*}
    c_i^B - (c_p)_s^B &= \frac{bM^B}{\alpha M^A} \frac{k_c^A}{k_c^B} \left[ c_i^A - (c_p)_s^A \right] \\
    \vdots \\
    (I-17)
\end{align*}
\]

\[
\begin{align*}
    c_i^T - (c_p)_s^T &= \frac{1M^T}{\alpha M^A} \frac{k_c^A}{k_c^T} \left[ (c_p)_s^A - c_i^A \right] \\
    \vdots \\
    (I-18)
\end{align*}
\]

With particle temperature and reactant and product concentration distributions all expressed in terms of the concentration profile of one reactant, the reaction rate at any point in the particle, \(r_{\text{het}}\), can be expressed, for given surface conditions, as a function of the local concentration of one reactant only. Thus, as in the case of a single reactant, integral Eq. (I-6) (with concentrations referring to reactant A) may be solved simultaneously with boundary conditions (I-11) and (I-14) to fully determine the concentration and temperature profiles within the porous catalyst particle.
APPENDIX II

LISTING OF STEADY-STATE COMPUTER PROGRAM
READ (5,2) (MPVSL(1), I=1:4)
READ (5,1) (APVSL(1), I=5:10, OFZ4)
READ (5,2) (APVSL(1), I=5:10, OFZ5, NZTBL)
READ (5,2) (ULPSL(1), I=1:4)
READ (5,2) (ULPSL(1), I=5:10, OFZ4)
READ (5,2) (ULPSL(1), I=5:10, OFZ5, NZTBL)
WRITE (0,999)

999 FORMAT (//55X,"A VS Z TABLE")
      WRITE (0,22) (AVSZ(1), I=1:4)
22 FORMAT (4X,15.5)
      WRITE (0,23) (AVSZ(1), I=5:10, OFZ4)
23 FORMAT (1X,15.5)
      WRITE (0,25) (AVSZ(1), I=5:10, OFZ5, NZTBL)
      WRITE (0,24)
24 FORMAT (//)
      WRITE (0,997)
997 FORMAT (54X,"14H AP VS Z TABLE")
      WRITE (0,22) (APVSL(1), I=1:4)
      WRITE (0,23) (APVSL(1), I=5:10, OFZ4)
      WRITE (0,25) (APVSL(1), I=5:10, OFZ5, NZTBL)
      WRITE (0,24)
      WRITE (0,995)
995 FORMAT (52X,"17H ULPZ VS Z TABLE")
      WRITE (0,22) (ULPSL(1), I=1:4)
      WRITE (0,23) (ULPSL(1), I=5:10, OFZ4)
      WRITE (0,25) (ULPSL(1), I=5:10, OFZ5, NZTBL)
      WRITE (0,24)
P1N = T
      T1N = T
      H1N = T
      C1IN = C1
      C2IN = C2
      C3IN = C3
      C4IN = C4
GO TO 111

11 PCHECK = 0.
POLD = P1N
       P = P1N + 5
       WRITE (0,12) P
12 FORMAT (11, ////////////////////////////////// 22A 1 PRESSURE HAS GONE NEGATIVE ---- RAISE X INPUT PRESSURE TO P = **110.4** PSIA AND START OVER*)
       P1N = T
       C1 = C1IN*P/POLD
       C2 = C2IN*P/POLD
       C3 = C3IN*P/POLD
       C4 = C4IN*P/POLD
       T = T1N
       H = H1N
       C1IN = C1
       C2IN = C2
       C3IN = C3
       C4IN = C4

111 CALL ILC (PCHECK)
       IF (PCHECK.LT.0.) GO TO 11
       CALL ILCILW (PCHECK)
       IF (PCHECK.LT.0.) GO TO 11

22
CALL LIQUID (PCHECK)
IF (PCHECK,L10,U) GO TO 11
CALL LIQVAP (PCHECK)
IF (PCHECK,L10,U) GO TO 11
CALL VAPOR (PCHECK)
IF (PCHECK,L10,U) GO TO 11
GO TO 1
10 CONTINUE
WRITE (0,1)
10 FORMAT ('//SUXX:******** OPERATIONS COMPLETE ********')
STOP
END
C THE NUMBERS 1, 2, 3, 4 IN THE VARIABLE NAMES REFER TO H2, O2, H2O,
WRITE (0,1111) HL

1111 FORMAT (/1x,'H(E)THALPT) = ',E10.5,'5X,'PRESSURE = ',E10.5)
GO TO 1

50 IF (C1.EQ.0.) C1=0.
   IF (C2.EQ.0.) C2=0.
   IF (C3.EQ.0.) C3=0.
   IF (C4.EQ.0.) C4=0.
   IF (C1.EQ.C2) MFRAC1 = 0.
   IF (C2.EQ.C3) MFRAC2 = 0.
   IF (C3.EQ.C4) MFRAC3 = 0.
   IF (C4.EQ.C1) MFRAC4 = 0.
   WRITE (0,3000)
   WRITE (0,4000) Z,1,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
   WRITE (0,1111) HL
   IF (C1+C2) 55,53,57
   RETURN
53 WRITE (0,50)
60 FORMAT (/1X,'ALL FOLKS EXIT')
   CALL EXIT
60 DELT2 = (15-T1)/41
   C1 = C1P
   C2 = C2P
   C3 = C3P
   C4 = C4P
   T = T5
   H = HP
   Z = ZP
   P = PP
   LFLAG = 1
   GO TO 10
130 PCHLCA = -1.
   RETURN
99 WRITE (0,99)
99 FORMAT (/1X,'AXIAL INCREMENTS HAVE EXCEEDED BED LENGTH')
   CALL EXIT
   END
1110 IF (ICELIQ}
SUBROUTINE ICELIQ (PCHECK)
REAL KC1,KC2,KC3,VMHARVM,M1,M2,M3,M4,MU1VST,MU1,MU2VST,MU2,MU3VST,
       MU4,MU5VST,MU6,MU7VST,MU8,MU9VST,MU10VST,MU11VST,MU12VST,
       MU13VST,MU14VST,MU15VST,MU16VST,MU17VST,MU18VST,MU19VST,
       MU20VST,MU21VST,MU22VST,MU23VST,MU24VST,MU25VST,MU26VST,
       MFRAC1,MFRAC2,MFRAC3,MFRAC4,KP
COMMON /ILUCK/ T,PH,HG,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,
       N2,TOPZM,TSL,HRH,F,AP,PHR,APLHA,APAG,APEXP,APEXP
COMMON /IMAG/ MVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34),
       MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
       CF3V(34),CF3ST(CU),CF4VST(20),VPVST(36),TVSV(36),UHCVST,
       Z(4)

C THE NUMBERS 1,2,3,4 IN THE VARIABLE NAMES REFER TO H2, O2, H2O,
C AND HE RESPECTIVELY
C
WRITE (10,100)
100 FORMAT ((I1,3X,5X,'*********** ICE-LIQUID REGION **********')

C*************** ///
LFLAG = U
HS = H
CJS = C3
W3S = W3
C5L = C5
AP = 1.0

1 CALL UNPAR (MVSZ,1,ZUV,A*KK)
9 CALL UNPAR (APVSZ,1,ZUV,AP*KK)
CALL UNPAR (DELVSZ,1,ZUV,APLHA*KK)
CALL UNPAR (HRH,1,ZUV,APAG*KK)
CALL UNPAR (MU1VST,1,ZUV,MU1*KK)
CALL UNPAR (MU2VST,1,ZUV,MU2*KK)
CALL UNPAR (MU3VST,1,ZUV,MU3*KK)
CALL UNPAR (MU4VST,1,ZUV,MU4*KK)
CALL UNPAR (CF1VST,1,ZUV,CF1*KK)
CALL UNPAR (CF2VST,1,ZUV,CF2*KK)
CALL UNPAR (CF3V,1,ZUV,CF3*KK)
CALL UNPAR (CF4VST,1,ZUV,CF4*KK)
LHV = C1*C3+C4
MUV = C1+C2+C4
SUMV = C1/M1+C2/M2+C4/M4
MU = (MU1+1/M1+MU2+1/M2+MU4+1/M4)/SUMV
MUHARVM = MUV/((C1+1/M1+M2+1/M2+M4+1/M4)
CFBARH = (C1+C2+C4+C5+C6+C7+C8+C9+C5+C6+C7+C8+C9)/MUV
CALL SCRAU (HUV,KC1,KC2,KC3,VG,HC1C1P1,C1C2P2,C3C4P3,TFTP,TPS,CPSV)
C CFBAR
IF (ILV*PS) 11,33,33
33 CALL UNPAR (VPVST,1,ZUV,VP*KK)
TEST = C3*V*TPS/M5
IF (VP*TEST) 1C+11
1C WHILE (ILV*PS)
200 FORMAT (///21X****** 'ATLE HAS CONDENSED OR FROZEN IN THE CATALYST
ASI PARTICL... PROGRAM STOP FOLLOWS ******)
CALL LALT
11 CONTINUE
CALL UNPAR (UHCVST,1,ZUV,DEUHL*KK)
KRRH = U*
HSL = H*UHDF*M5
UW1UZ = - (KRRH*UDEL1+KCI*AP*CICP1)/6
UW2UZ = - (KRRH*UDEL1+M2/(2.4*M1)+KC*AP*CICP2)/6
UW3UZ = (KRRH*UDEL1+M3/(1-KC3V*AP*CICP3V))/6
UW4UZ = -U*
**WPT FOR LIQUID**

SUBROUTINE LIQUID (RCHECK)

REAL  KG1*R2*KC5V*M1*M2*M3*M4*MU1VST*MU1*MU2VST*MU2*M3VST,
       MU3*M4VST*MU4*M5VST*Mu5V*MRAC2*MRAC3*MRAC4*MRAC

COMMON /UCL15//THET, R=+/-1, Z=+/-1, G=+/-1, C=+/-1, M=+/-1, M=+/-1, S=+/-1, T=+/-1,
       M=M1, N=M2, PRIMEZ*NZO*ZETA*ZETAIN

COMMON /ULCES1/AV5Z(99), APV5Z(99), UELV5Z(99), HRV5ST(36), MU1V5ST(34),
       MU2V5ST(34), MU3V5ST(32), MU4VST(34), CF1VST(34), CF2VST(34),
       CF3V1(34), CF35ST(30), CF4V5ST(30), CFVPST(36), CFVPST(36), UCHV5ST

A (24)

C THE NUMBERS 1,2,3,4 IN THE VARIABLE NAMES REFER TO H2, O2, H20,
   AND THE RESPECTIVELY

C

1U0 FORMAT (1i13.9X'************** LIQUID REGION *************')

** **** ///

LFLAG = U
AF = 1U0

CALL U15AR (TV5VPST1, V*, TV*, TL5V, 1)
CALL U15AR (AV5Z1L1, 2*, PM5V, 1)

CALL U15AR (APV5Z, T*, V*, U*, UELTA*KK)
CALL U15AR (HRV5ST1, V*, T*, HKK)
CALL U15AR (MU1V5ST1, V*, MU1K1)
CALL U15AR (MU2V5ST1, V*, MU2K1)
CALL U15AR (MU3V5ST1, V*, MU3K1)
CALL U15AR (MU4V5ST1, V*, MU4K1)
CALL U15AR (CF1VST1, V*, CF1K1)
CALL U15AR (CF2VST1, V*, CF2K1)
CALL U15AR (CF3VST1, V*, CF4K1)

CF3 = CF3

KH5 = C1*C2*+C3*C4

K5 = C1*C2*C3*C4

SUMV = C1+C2+C3/C4

MU5 = (MU5*1/M1+MU5*2/M2+MU5*4/M4)/SUMV

Mu5 = MU5/(C1+C2+C3+C4/KH5)

CF5K1 = M1*1/M1+C2*1/M2+C3*1/M4/C4

CALL UD5AR (R*15K1, C2, KC5V*1HC, C1CP1, C1CP2, C1CP3V, TIP, TIP, TIP, TIP, TIP)

A (24)

IF (11U5.+TIP) 1,11,33

33 CALL U15AR (TV5VPST1, V*, TV*, TP*, TL5V)

IF (TP*+1L5) 1,1,1

10 WHILE (10C5U)

2UU FORMAT (11X'**** RATE HAS CONDENSED OR FROZEN IN THE CATALYTIC
   PARTICLE... PROGRAM STOP FULLUAS *****)

CALL 11

11 CONTINU

CALL U15AR (U15CST, T*, U*, TULHC, 1)

AUHIGH = 0.

AU15 = (1R5UM*DELTA+KC5*AP*C1CP1)/G

AU25 = (1R5UM*DELTA*M2/2*+KC5*AP*C1CP2)/G

AU35 = (1R5UM*DELTA*M2C1KC3V*AP*C1CP3)/G

AU45 = 0.

AU55 = (1R5UM*DELTA+HC*AP*TIP)+ (KC5V*AP*C1CP3V*DELHC))/G

DELTA = CM/15U5

Z15ST = Z15UST

30
IF (C2) 4415.
MFRAC2 = 0.
IF (C4) 0107.
MFRAC4 = 0.
WRITE (0,340)
WRITE (0,460) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
WRITE (0,1411) H,P.
IF (C1*42) 05,55,54
RETURN
WRITE (0,56)
FORMAT (///50X*T0HMAT'S ALL FOLKS )
CALL EX11
DEL1Z = (TL-TT)/UTUZ
T = TL
C1 = C1P
C2 = C2P
C3 = C3P
C4 = C4P
H = HP
Z = ZP
P = PP
LFLAG = 1
GO-TO 150
P_CHECK = -1.
RETURN
WRITE (0,90)
FORMAT (///45X AXIAL INCREMENTS HAVE EXCEEDEDвед LENGTH)
CALL EX11.
WIPT FOR LGVAP
SUBROUTINE LGVAP (P, CHECK)
REAL KC1, KC2, KC3, KM1, KM2, KM3, KM4, MUIVST, MUI, MU2VST, MU2, MU3VST,
MUIVST', MU2VST', MU2', MU3VST',
COMMON /LUCAT/ T1, T2, T3, T4, T5, T6, T7, T8, T9, T10, T11, T12,
COMMON /MUVAR/ MUIVST, MUIVST', MU2VST, MU2VST', MU2', MU3VST',
COMMON /LHF/ LHF1, LHF2, LHF3, LHF4, LHF5, LHF6, LHF7, LHF8,
COMMON /AHF/ AHF1, AHF2, AHF3, AHF4, AHF5, AHF6, AHF7, AHF8,
COMMON /GAM/ GAM1, GAM2, GAM3, GAM4, GAM5, GAM6, GAM7, GAM8,
COMMON /AGM/ AGM1, AGM2, AGM3, AGM4, AGM5, AGM6, AGM7, AGM8,
COMMON /AMF/ AMF1, AMF2, AMF3, AMF4, AMF5, AMF6, AMF7, AMF8,
COMMON /BEX/ BEX1, BEX2, BEX3, BEX4, BEX5, BEX6, BEX7, BEX8,
COMMON /XEX/ XEX1, XEX2, XEX3, XEX4, XEX5, XEX6, XEX7, XEX8,
COMMON /ZETA/ ZETA1, ZETA2, ZETA3, ZETA4, ZETA5, ZETA6, ZETA7, ZETA8,
COMMON /ZETAIN/ ZETAIN1, ZETAIN2, ZETAIN3, ZETAIN4, ZETAIN5, ZETAIN6, ZETAIN7, ZETAIN8,
C THE NUMBERS 1, 2, 3, 4 IN THE VARIABLE NAMES REFER TO H2, O2, H2O,
C AND HE RESPECTIVELY.
C
C
33
C

1U (24)

1U FORMAT ('(1I3,Y10)', TETRAHEDRAL-VAPOUR REGION '**********
**************', '///')
LFLAG = 0
HL = 0
C3V = 0
C3L = 0
W3L = 0
AF = 1
1 CALL UNBAR (AVS, 1, E, 0, APR, KK)
CALL UNBAR (APVS, 1, E, 0, APR, KK)
CALL UNBAR (DEVS, 1, E, 0, DLETA, KK)
CALL UNBAR (HVST, 1, E, 0, HVT, KK)
CALL UNBAR (MUVST, 1, E, 0, MUI, KK)
CALL UNBAR (MU2VST, 1, E, 0, MU2, KK)
CALL UNBAR (MU3VST, 1, E, 0, MU3, KK)
CALL UNBAR (MU4VST, 1, E, 0, MU4, KK)
CALL UNBAR (CF1VST, 1, E, 0, CF1, KK)
CALL UNBAR (CF2VST, 1, E, 0, CF2, KK)
CALL UNBAR (CF3VST, 1, E, 0, CF3, KK)
CALL UNBAR (CF4VST, 1, E, 0, CF4, KK)

RHU = C1+C2+C3+C4
RHUV = C1+C2+C3+C4
SUAV = C1/M1+C2/M2+C3/M3+C4/M4
MU = (MUI+MU1+MU2+MU3+MU4+M3+M4)/SUMV
MBARV = MUV/((C1/M1+C2/M2+C3/M3+C4/M4)
CBARV = (C1+C2+C3+C4)/RHOB
CALL UNBAR (RHOB, 1, E, 0, CBARV, KK)

IF (1105<10PS) 11, 5, 5, 35
CALL UNBAR (VPVST, 1, E, 0, VP, KK)

T31 = CPS*V*K*10PS/M3
IF (VP<1LST) 12, 11, 11
12 WRITE (0, 2J0, 1)

20 U FORMAT ('///')

CALL UNBAR (HVST, 1, E, 0, DELHC, KK)
RHUM = 0
HLV = N+DELHC*W3L
UMUZ = -(NHUM*DELTA1+KC1*AP*CICP1)/E
UN2Z = -(NHUM*DELTA1+M2/2+K2*AP*CICP2)/E
UN3Z = -(NHUM*DELTA1+M3/3+K3*AP*CICP3)/E

11 CONTINUE

400  FORMAT(*d6.9,E10.5/2X,E10.5,2X,E10.5,2X,E10.5,2X,*
       X,E10.5//)
       WRITE (0,500)
       c4')
       WRITE (0,500) MFRAc1, MFRAc2, MFRAc3L, FRAC3v, MFRAc4
600  FORMAT(*32X,'E10.5,2X,E10.5,2X,*E10.5,2X,E10.5//')
       WRITE (0,1111) HP
1111 FORMAT(*10X,'H(ENTHALPY) = ',*E10.5,*5X,'PRESSURE = ',*E10.5)
       GO TO 1

50  IF (C1.LT.0.) C1 = 0.
       IF (C2.LT.0.) C2 = 0.
       IF (C4.LT.0.) C4 = 0.
       IF (C1.LT.0.) C1 = 2.3
2  MFRAc1 = 0.
3  IF (C2) 4/435
4  MFRAc2 = 0.
5  IF (C4) 4/407
6  MFRAc4 = 0.
7  WHILE (0,300)
       WHILE (0,400) Z1 = C1, C2, C3L, C3V, C4
       C3 = C3L + C3V
       FRAC3L = C3L / M3 / (C1 + C2 / M2 + C3L + C3V + C4 / M4)
       WHILE (0,500)
       WHILE (0,600) MFRAc1, MFRAc2, MFRAc3L, FRAC3v, MFRAc4
       IF (C1.LT.0.) 53753, 5
54  KLTUR4
55  WRITE (0,550)
56  FORMAT(*32X, 'DEL(C) = DEL(C3L)')
       CALL EXIT
60  DEL(C) = -C3/DC3LDZ
       C3L = 0
       C1 = C1p
       C2 = C2p
       C3V = C3VP
       C4 = C4p
       H = HP
       Z = ZP
       P = PP

FILAC = -1
       GO TO 20
130  PCMCCK = -1.
       RETURN
90  WHILE (0,90)
90  FORMAT(*45X, 'AXIAL INCREMENTS HAVE EXCEEDED 360 DEG LENGTH')
       CALL EXIT
LWH
C

C THE NUMBERS 1, 2, 3, 4 IN THE VARIABLE NAMES REFER TO H2, O2, H2O,
C AND H, RESPECTIVELY.

C

100 \text{ FORMA} (*-39X-************** VAPOR REGION **********)
C

A

100 \text{ FORMA} (*-39X-************** VAPOR REGION **********)
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100 \text{ FORMA} (*-39X-************** VAPOR REGION **********)
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100 \text{ FORMA} (*-39X-************** VAPOR REGION **********)
C

A
37

```
A = 2/(04.4*A*KHC)
DPUC = DPUC*AF/144.
W1 = C1*KHU
W2 = C2*KHU
W3 = C3*KHU
W4 = C4*KHU
DrHuz = Ktuv*(1./T*(DPUC+1.)/MBARV*UMBRZ+1./T*PTDZ)
RHOFAC = -(1./T*(DPUC+1.)/MBARV*UMBRZ+1./T*PTDZ)
DrHuz = DrHuz*(1.-EXP(-1.)*RHOFAC*DELTZ)/(RHOFAC*DELTZ)
DC1UZ = KHU*UM1UZ+1.*DRMODZ
DC2UZ = KHU*UM2UZ+1.*DRMODZ
DC3UZ = KHU*UM3UZ+1.*DRMODZ
DC4UZ = W4*UM4UZ
C1P = C1
C2P = C2
C3P = C3
C4P = C4
T1 = T
HP = H
ZP = Z
HP = P
C1 = C1+UC1UZ*DELTZ
C2 = C2+UC2UZ*DELTZ
C3 = C3+UC3UZ*DELTZ
C4 = C4+UC4UZ*DELTZ
MFRAC1 = C1/M1/(C1/M1+C2/M2+C3/M3+C4/M4)
MFRAC2 = C2/M2/(C1/M1+C2/M2+C3/M3+C4/M4)
MFRAC3 = C3/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
MFRAC4 = C4/M4/(C1/M1+C2/M2+C3/M3+C4/M4)
IF (C1*LT*U.) C1=U.
IF (C2*LT*U.) C2=U.
IF (C4*LT*U.) C4=U.
IF (C1*LT*2.) C1=2.
MFRAC1 = 0.
MFRAC2 = 0.
MFRAC4 = 0.
H = H+UM4UZ*DELTZ
T = T+ULZ*DELTZ
P = P+UPDEL*DELTZ
IF (LFLAUX.EQ.1) GO TO 40
IF (P.LT.137) GO TO 137
Z = Z+DELTZ
IF (NOKALEQU.EQ.1) GO TO 40
IF (C1+C2).LT.500) GO TO 90
40 WHILE (C1 LT 300)
350 FORMAT (//,1A1,'X',9X,1EM1,P9X,'C1',10X,'C2',10X,'C3',10X,'C4',10X,'C5',10X,
A,'MFRAC1',9X,'MFRAC2',9X,'MFRAC3',9X,'MFRAC4')
WRITE (6,400) Z+T*1.,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
400 FORMAT (/D0,E10.5,2A,E10.5,S9X,'E10.5',S9X,'E10.5',S9X,'E10.5',S9X,'E10.5',S9X,
A,'E10.5',S9X,'E10.5',S9X,'E10.5')
WRITE (6,111) MFRAC1, MFRAC2, MFRAC3, MFRAC4
1111 FORMAT (10X,'HEATCAP',6X,'PRESSURE',6X,'PRESSURE')
IF (LFLAUX.LT.1) GO TO 54
IF (AUX.EQ.2) E10.5,54,1
50 WRITE (6,300)
WRITE (6,400) Z+1.,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
```
WHITE (0,111) MP
NONE = 1
C1CP1 = 0
C1CP2 = 0
C1CP3 = 0
T1TP = 0
DEL1Z = (ZEND-Z)/10.
GO TO 1
60 DEL1Z = ZEND-ZP
Z = ZEND
C1 = CL1
C2 = CL2
C3 = CL3
C4 = CL4
T = T1
H = HP
P = SP
LFLAG = 1
NONE = 1
GO TO 260
150 PCHECK = -1.
54 RETURN
END
DEFINE DF FUNCTION

\[ DF(x+y+z) = 14.744/(x+y+z)^{4.2} \]

C DEFINE DF FUNCTION

\[ KCF(A,B,C,D) = 0.1A/(A*C) + 0.1(B+D) + 0.1A/(A*C) \]

C DEFINE ANALYTIC INTEGRATION FUNCTIONS FROM INTEGRAL EQUATION

\[ Y = \int (\text{expression}) \, d\mu \]

C SET INITIAL VALUES OF MISCL. ITEMS

C SET INITIAL PRODUCT VALUES (H2O)

C SET INITIAL REACTANT VALUES FOR CASE WHEN H2O IS PRIME REACTANT

C (PRIME REACTANT = ONE WHICH IS IN SMALLEST SUPPLY)
MK(2) = M2
PR(1) = 1.
PR(2) = U*0
POWEXP(1) = 0.
POWEXP(2) = 0.
HOM(1) = U.
HOM(2) = U.
RALPH(1) = U.
RALPH(2) = U.
CUEFR(1) = 1.
CUEFR(2) = 5.
HFACTR = 1.
RFACR = 1.
GO TO 210
C ...... SET INITIAL REACTANT VALUES FOR CASE WHEN O2 IS PRIME REACTANT .....
210 CONTINUE
REACTN(1) = O2
REACTN(2) = H2.
CIR(1) = C2
CIR(2) = C1
DUM(1) = DU2
DUM(2) = DU1
MK(1) = M2
MK(2) = M1
PR(1) = U*0
PR(2) = 1.
POWEXP(1) = 0.
POWEXP(2) = 0.
HOM(1) = U.
HOM(2) = U.
RALPH(1) = U.
RALPH(2) = U.
CUEFR(1) = 5.
CUEFR(2) = 1.
HFACTR = 7920.
RFACR = 7920.
210 CONTINUE
C SET INITIAL WEIGHTED AVERAGE FRACTIONS
WAPF1 = 0.
WAPF2 = 0.
WAPR = 0.
WAPR = 0.
WAPF1 = 0.
WAPF2 = 0.
WAPR = 0.
WAPR = 0.
C SET UP INITIALIZATION FOR EACH ENTRY TO *SGRAD*
1 L1FLG = 0.
NPART = 50.
LPI = 1.
LPS = 0.
C INITIALIZE REACTANT PARAMETERS
DU 110 = 1.0
LIR(1) = DUM(1)*14.7/P*(7/492.)*1.823
110 CONTINUE
C INITIALIZE PRODUCT PARAMETERS
UIR(1) = DU1*14.7/P*(7/492.)*1.823
112 DU 114 = 1.0
114 KC(R) = KCB*(U*(K)*MU.*LIR(1)*AP)
LU 119 = 1.0
119 KCP(1) = KCB*(U*(K)*MU.*AP(1)*AP)
HC = 4*(U+L)*LIR(1)*(U*(AP+MU)).**.41

40
Choose initial value of C's for key particle reactant

\[ C_{002} = \text{CIR}(1)/50. \]

\[ DU \ 151 \ 1=1, \ MR \]
\[ UP(1) = UP(T+UP(1), P) \]
\[ UP(1) = UP(1) \]
If (1 \leq 0) go to 151
\[ QU0 = KCR(1)/KCR(1) \]
\[ QU0 = \text{UER}(1) \times \text{MR}(1) \]
\[ CP2(1) = \text{CIR}(1) - (QU0 \times \text{UO} \times \text{CIR}(1) - \text{CPSR}(1)) \]
If (CP2(1) \times LT \times 0) CP2(1) = 0.

\[ DU \ 152 \ 1=1, \ WP \]
\[ UP(1) = UP(T+UP(1), P) \]
\[ WP = KCR(1)/KCR(1) \]
\[ QU0 = \text{UER}(1) \times \text{WP}(1) / (\text{UER}(1) \times \text{MR}(1)) \]
\[ CP2(1) = \text{CIR}(1) - (QU0 \times \text{UO} \times (\text{CPSR}(1) - \text{CIR}(1))) \]
If (CP2(1) \times LT \times 0) CP2(1) = 0.

\[ \text{CALL UNDRM} (HRVST*, T*, TT*, MH1*, KK) \]
\[ HR1 = HR1 \times \text{FACTR} \]
\[ SUM = U* \]

\[ DU \ 160 \ \text{If} (LP1 \times EQ \times 1) \text{go to } \epsilon. \]
\[ DU \ 164 \ \text{TP*P} = \text{TPSP} \]
\[ \text{TPSP} = \text{TP'S} \]

\[ \text{CONTINUE} \]
\[ \text{TP} = 1 - (SUM + HR1 \times KCR(1) + (\text{CIR}(1) - \text{CPSR}(1))) / HC \]
If (TPSP \times LT \times 0) TPSP = 1.
\[ \text{CALL UNDRM} (HRVST*, \text{TPSP}, 0*, MH1*, KK) \]
\[ MH1 = MH1 \times \text{FACTR} \]
\[ UP1(1) = UP(T + UP1(1), P) \]
\[ UP(1) = UP(T + UP(1), P) \]
\[ UP(1) = UP(T + UP1(1), P) \]
\[ UP(1) = UP(1) \]
\[ HR1 = HR1 \]
\[ TMSP = 1 - \text{TP'S} \]
\[ \text{UPUX} = KCR(1) \times \text{UP}(1) \times (\text{CIR}(1) - \text{CPSR}(1)) \]

\[ \text{RETURN} \]

\[ \text{UPDATE X0} \]
\[ \text{GAMMA} = \text{KON}/\text{TP'S} \]
\[ \beta = \text{CPSR}(1) \times \text{HR1} \times \text{UP}(1) / (1 \times \text{TP'S}) \]
\[ KU = \text{ALPHA} \times \text{EXP}(-\text{GAMMA}) \]

\[ \text{CALCULATE X0} \]
\[ XU = \text{XU} \]
\[ XU = A \times L \times \text{UP}(1) / \text{CPSR}(1) \]
\[ XU = XU/A \]
If (XU) 11, 12, 13
\[ XU = U* \]
\[ XU = U* \]
\[ \text{JAD} = \text{JAD} + 1 \]
If (JAD > 10) go to 120
\[ DU \ 120 \ \text{CPSR}(1) = \text{CIR}(1) / (\text{UP}(1) / (A \times KCR(1)) + 1) \]
\[ DU \ 511 \ 1=1, \ MR \]
If (1 \leq 0) go to 11
\[ QU0 = KCR(1)/KCR(1) \]
QUOB = C*F(1) + F(1)/(C*F(1) + MR(1))
CPn(1) = CIR(1) - (QUO*B + CPn(1) - CPSn(1))
IF (CPn(1) = LT1) CPn(1) = 0.

511  CONTINUE

50  512  J=1, NPP

QUOC = C*KCR(1)/KCP(1)
QUOB = C*EFP(1) + MR(1)/(C*EFP(1) + MR(1))
CPn(1) = CIR(1) - (QUO*B + (CPSN(1) - CIR(1))
IF (CPn(1) = LT1) CPn(1) = 0.

512  CONTINUE

UCPUX = CIR(1)/A
TPS = 1/(SUM + H1*UPF(1) + UCPUX)/HC
IF (TPS = LT1) TPS = 1.
CALL UBAR(HRVST1, TPS, H1, KK)
H1 = H1*FAC1R
UPR(1) = UPF(TPS, JUPR(1))
UPR(2) = UPF(TPS, JUPR(2))
DPP(1) = UPF(TPS, JUP(1))
DPn = UPR(1)
UPR = UPR(1)
HRP = H1
TMPN = 1 - TPS
GAMMA = RGM/TPS
DTP = (CPSn(1) + H1*UPF(1))/KPS
K0 = ALPHAKR + EXP(-GAMMA)
WK1 = (GAMMA) LPR(KP)

132  FUMHAT(A/AH, HWE HAVE CALCULATED A NEGATIVE X0 DURING ITERATION
AND '115' / 39X. SET X0 = 0., CALCULATE TPS = '1', 115,' AND CONTINUE
AUX = 1)

GO TO 101

C  INTERKAL FOR CP EQUATION

12  CONTINUE

CALL TRAP2(XUAX1, HXAK, RIESUM)

C  MF 15 INDIKATION FOR CALCULATING CP(X) PROFILE

C  IMP = 1 IMPLIES CONCENTRATION HAS PENETRATED VERY RAPIDLY THRU CATALYST
C  PARTICLES (X0 = 0.)
C  IMP = 2 IMPLIES CONCENTRATION HAS PENETRATED MORE SLOWLY THRU PARTICLES
C  AND A FINE INTEGRATION SUBDIVISION OF THE (X0, A) INTERVAL
C  SHOULD BE USED TO OBTAIN CP(X) PROFILE (X0 = 0.)

10 (IMP = 0 OR U) GO TO 15

GO TO (11, 14), IMP

14  NPAR = 1
XUAX = 0
XU = 0.
GO TO 12

C  CALCULATE HX, CPS.

15  CPSU = U1S(1)
CMCPF = CMCFN
CPSPNP = CPSNP
CPSPN = CPSNL
CPn(1) = CIR(1) - A*IESUM/KCR(1)

822  CPSPN = CPSN(1)
IF (CPn(1) = LT1) CPn(1) = 0.

130  CMCPH = CIR(1) - CPSn(1)
C  CALCULATE HX, CP

13  CONTINUE

GRAU = UCPUA*UPR(1)
FORAD = 2 (1 = TPS)
TPSR = TPSP
TPSP = TPS
TMTPO = TMTPN

51 CONTINUE

TPS = T - (SUM+HR*KC(1)+(CIR(1)-CPSR(1)))/HC
IF (TPS - LT, 0) TPS = 1.
CALL UNBAR (HRV5T1*TPS, 0, HR1*HR1*HR2)
HR1 = HR1*HR1*FACTR
DPR(1) = UTP(1) + (TPS - UMR(1))
DPR(2) = UTP(2) - (TPS - UMR(2))
DPU(1) = UTP(1) + (TPS - UMR(1))
DPU(2) = UTP(2) - (TPS - UMR(2))
DCPUK = KCR(1)/DPU(1)*(CIR(1)-CPSR(1))
TMTPN = T - TPS
GAMMA = KG/TPS
BETA = -CPSR(1)*HR1*DP(1)/(KP*TPS)
KU = ALPHAI*EXP(-GAMMA)

C TEMPERATURE CURVE TRACTION FOR 5% LIMIT
IF (ABS (T/TNPO - 1.0)/TMTN - .05) 41, 41, 817
41 IF (ABS ((EMCPO-CMCPN)/CMCPN) - .05) 70, 70, 817
817 IF (LP1 < LT, 3) GO TO 46
IF (AMAX(CPSR(1), CPSPR, CPSPR) - CPSR) 818, 820, 818
818 IF (AMAX1(CPSR(1), CPSPR, CPSPR) - CPSR) 46, 820, 46
820 IF (AMAX(CE1) = 0, 0) GO TO 820
NXU = 1
ZETA = ZELIUG
WRITE (ORC, 9025)
9025 FORMAT (1/3A1, 'CPSCML CHANGED DIRECTION -- NEW EQ. FOR CPXF USED')
GO TO 136.

40 CPSR(1) = -(CPSR(1) - MAF2 - CPSR(1))
IF (CPSR(1) - LT, 0) CPSR(1) = 0.
IF (NXU = 0, 0) GO TO 157
GO 139
139 CONTINUE
C CALCULATE CPSP'S FOR PRODUCTS
157 GO 140 = 1 NS
GO = KCR(1)/KCP(1)
QUO = KCR(1)/KCP(1)
CPSR(1) = JP1(1) = QUO*UOO*(CPSR(1) - CIR(1))
IF (CPSR(1) - LT, 0) CPSR(1) = 0.
140 CONTINUE
53 DCPUK = KCR(1)/DPU(1)*(CIR(1) - CPSR(1))
CMCPN = CIR(1) - CPSR(1)
HR1 = HR1*HR1
42 LP1 = LP1 +
IF (LP1 = 25) 40, 40, 44
44 CONTINUE
IF (JWAFGE, 1) GO TO 811
WAF1 = WAF1 + 1
JWAF = +
GO TO 813
811 CONTINUE
WAF1 = WAF1 + 0.05
JWAF = Z
GO TO 813
815 IF (WAF1 = 0.045) GO TO 99
C CONVERGENCE WITH PRESENT WEIGHTED AVERAGE FACTORS FOR X0
C
C REPEAT ITERATION PROCEDURE WITH NEW FACTORS
G0 TO 1
99 CONTINUE
810 WRITE (0,99)
98 FORMAT (///,5X,'UNABLE TO FIND SUITABLE X0 AFTER 3 TRIES OF 25 1
A TERTIONS EACH ... SET CPS = 0, AND CONTINUE!')
CPSR(1) = 0.
CPSR(2) = CIR(2)-((UOA*UOO)*(CIR(1)-CPSR(1)))
IF (CPSR(2).LT.0.) CPSR(2) = 0.
CPSR(1) = CIR(1)-((UOC*UOO)*(CPSR(1)-CIR(1)))
IF (CPSR(1).LT.0.) CPSR(1) = 0.
TPS = 1-(SUM+K1*K1)*(CIR(1)-CPSR(1)))/HC
CALL UNDARK (HRVST,1,TPS,1,H1,HP)
K1 = H1*FACTR
K2 = H1*FACTR
K3 = H1*FACTR
K4 = H1*FACTR
K5 = H1*FACTR
DCPSR = K1*(CIR(1)-CPSR(1))
G0 TO 104
C Satisfactory X0 has been found
020 WRITE (0,10)
10 FORMAT (///,6X,'SATISFACTORY X0 FOUND AFTER ,13, ' TRIES! /
A X FOUND AT THIS POINT!')
027 IF (X0A.LT.9999) G0 TO 131
WRITE (0,0)
131 CPSR(1) = 0.
CPSR(2) = CIR(2)-((UOA*UOO)*(CIR(1)-CPSR(1)))
IF (CPSR(2).LT.0.) CPSR(2) = 0.
CPSR(1) = CIR(1)-((UOC*UOO)*(CPSR(1)-CIR(1)))
IF (CPSR(1).LT.0.) CPSR(1) = 0.
TPS = 1-(SUM+K1*K1)*(CIR(1)-CPSR(1)))/HC
CALL UNDARK (HRVST,1,TPS,1,H1,HP)
K1 = H1*FACTR
K2 = H1*FACTR
K3 = H1*FACTR
K4 = H1*FACTR
K5 = H1*FACTR
DCPSR = K1*(CIR(1)-CPSR(1))
WRITE (0,132)
132 FORMAT (///,6X,'X0 Y0/Z0 A GREATER THAN .9999 ... SET CPS = 0, AND CONTINUE /
A A! )
C C CALCULATE GRADIENT
C 131 IF (CPSR(1).GE.134,134,133)
134 IF (PRMLEE.LT.121) G0 TO 133
CICP1 = CIR(1)
CICP2 = CIR(2)-CPSR(2)
K1 = K1
K2 = K1
G0 TO 136
135 CICP1 = CIR(2)-CPSR(2)
CICP2 = CIR(1)
KC1 = KC(2)
KC2 = KC(1)

130 CONTINUE
CICPSV = CIC(1) - CPS(1)
KE3V = KE(1)
TIP = T-TPS
WRITE (9,810) CICPI, CICPSV, TIP
RETURN

133 LP2 = 1
NX = 24
NAM1 = NAM1 + 1
UHA = UHR(1)
CPAR(1, NX1) = CPSR(1)

291 XUA = XUA / A
V = -KCU(1) / UHR(1)

INH1 = 1
K = 2
R1 = 0
R2 = 0
PS1 = 0
PS2 = 0

U=UQA = (1-XUA)/FLOAT(NX)

C CALCULATE PROFILE CURVES FOR INTEGRAND FUNCTIONS
XH = XUA
UH / 70.0 UH = 1, NX1

C CP(X/Al) IS A LINEAR PROFILE DURING FIRST APPROXIMATION
IF (LP2.GT.1) GO TO 664

C CALCULATE CP(X/Al) FOR KEY PARTICLE-REACTANT
CPAR(1, J) = ((XR-XUA)/((1-XUA)**2ETR*CPXR(1, NX1))
IF (CPAR(1, J), U1, U3, U5) CPAR(1, J) = 0.

C CALCULATE CPSR FOR ALL OTHER REACTANTS
664 IF (NX.LE.1) GO TO 158
LU 141 IZ1, IZ2

GU1 = UHR(1) / UHR(1)
GU2 = CLFR(1)*MR(1)/(CLFR(1)*MR(1))
CPAR(1, J) = CPSR(1) + GU1*GU2*(CPAR(1, J) - CPXR(1, NX1))
IF (CPAR(1, J), U1, U3, U5) CPAR(1, J) = 0.

141 CONTINUE
C CALCULATE CPSR FOR PRODUCTS

158 - BU 142 IZ1, IZ2
GU3 = UHR(1) / UHR(1)
GU4 = CLFR(1)*MR(1)/(CLFR(1)*MR(1))
CPAR(1, J) = CPSR(1) + GU3*GU4*(CPAR(1, J) - CPXR(1, NX1))
IF (CPAR(1, J), U1, U3, U5) CPAR(1, J) = 0.

142 CONTINUE

GUOTA = 1.
GUOB = 1.
DO 143 IZ1, IZ2
GUOA = CPXR(1, J)*MR(1)
GUOTA = GUOTA*GUOA

143 CONTINUE

DO 144 IZ1, IZ2
IF (IZ1) 144, 144, 144
144 CONTINUE

1000 PWUA = CPXR(1, J)*MR(1)
GO TO 1002

1001 PWUA = 1.
1002 CONTINUE
144 CONTINUE
CALCULATE GENERALIZING TERM --- (ABSORPTION)

SUMTRM = 0.
SMTRK = 0.
CNUM = BETA*(I.*CPX(1,J)/CIR(1))
C3UNUN = 1.+BETA*(I.*CPX(1,J)/CIR(1))
DU OUT I=1,NJ
RGK = RGK(1)/T
KEP(I) = RGK(I)*CNUM/C3UNUN
KRU(I) = RAHP(I)*EXP(-RGK(I))
IF (KRU(I)) 1000,1004,1003
1005 KRU'RI(I) = KRU(I)*CPX(I,J)**PUWEP(I)*EXP(REXP(I))
GU TO 1007
1004 KRU'RI(I) = 0.
1007 SUMTRK = SUMTRM+KRU'RI(I)
6000 CONTINUE
Do OUT I=1,NP
PGAMMA(I) = PGAM(1)/I
PLAP(I) = PGAMMA(I)*CNUM/C3UNUN
PKU(I) = PAHP(I)*EXP(-RGK(I))
IF (PKU(I)) 1005,1008,1005
1005 PKU'RI(I) = PKU(I)*CPX(I,J)**PUWEP(I)*EXP(REXP(I))
GU TO 1008
1008 PKU'RI(I) = 0.
1008 SMTRK = SMTRK+PKU'RI(I)
6007 CONTINUE
AUSDXU = (SUMTRM+SUMTRK+SMTRK)**PPP
GENEX = 1./AUSDXU
RHE1(J) = A.*QUOTAT*QUOTAT*EXP(GAMMA*BETA*(I.*CPX(1,J)/CPX(1,J)*X1))
RHE1(J) = RHE1(J)*VL**XJL
RHE1(J) = RHE1(J)*MNCTK
DX(J) = XA
AA = AA+DELXOA
770 CONTINUE
-- TAKE INTERVAL FUNCTION HINTS AS CONSTANT VALUE FOR CP(X/AA) AND RHE1(J)
DU 771 JJ=1,INX
CPX(J,J) = (CPX(J,J)+CPX(J,J+1))/2.
RHE(J) = (RHE(J)+RHE(J+1))/2.
771 CONTINUE
XA = XA+DELXOA
C1IK = (A+X1)/(X1)

C INTEGRAL EQUATION FUNCTION
C IOX(I) IS SPECIAL CASE ..., X = XU
DAL = XU
DAU = DAL+DELXU
RK1 = 0.
DU 377 J=1,INX
RK1 = RK1+RHE(J)*EVAL(0)XU)*C1IK*EVAL1(DAL,DXU)
DAL = DAU
DAU = DXU+DELXOA
377 CONTINUE
CPX(J,J) = C1IK(J)-X1/DXU*EVAL1(DAL,DXU)
DAL = DAU
DU 772 J=1,INX
RK1 = RK1+RHE(J)*EVAL1(XI,2,AA)
XU = AA
AA = AA+DELXOA
772 CONTINUE.
R1 = R1*X/XUA-C1RM
XUA = XA
XA = XA+DELR
DU 773 I=INT1+1

PS1 = PS1+RMT(I+1)*LVA-2(XAT*XA)
PS2 = PS2+RMT(I+1)*LVA1(AA+XA)
XA = XA+RMT
XUA = XUA+DELR

773 CONTINUE
R2 = PS1-C1RM*PS2
INT1 = INT1+1
CPS1(X,1) = C1R(I)-AA/UPR(1)*(R1+R2)
IF (CPS1(X,1)>LT.U) CPS1(X) = U
XUA = A/AA
XA = XUA+DELR
K = K+1

R1 = U
R2 = U
PS1 = U
PS2 = U
IF (K.LT.NX) GO TO 779

C CPS1(X,1) IS SPECIAL CASE ... X=A

UXL = XUA
UAU = UXL+DELR
RR1 = U
DU 378 I=INT1+1
RR2 = U
RR1 = RR2+RMT(I+1)*LVA1(UXL*UXU)
UXL = UXL

UAU = UXL+DELR

378 CONTINUE
CPS1(X,1) = C1R(I)-AA/UPR(1)*(1.-C1RM)*RR2
IF (CPS1(X,1) LT 190) 190,10,191
190 CPS1(X,1) = 0.

CPS2(I+1) = CIP(I+1)-U(AA+UOU)*(C1R(I)-CPS2(I))

IF (CPS2(I+1)>LT.U) CPS2(I+1) = 0.
CPS2(I) = CIP(I)-U(AA+UOU)*(CPS2(I)-C1R(I))
IF (CPS2(I)>LT.U) CPS2(I) = 0.
TPS = 1-(SUM+HR1*KCR(I)*(C1R(I)-CPS2(I)))/HC
CALL UNDAR (HKVSTL+TPS*U+HR1*KK)
HR1 = HK1+HC
UPR(1) = UPR(TPS,JKR(I)*P)
UPR(2) = UPR(TPS,JKR(I)*P)
UPR(1) = UPR(TPS,UPR(1)*P)
UPR(2) = UPR(TPS,UPR(2)*P)

192 FORMAT (//CONCENTRATIONS CALCULATED FROM INTEGRATION SECTION IN RELATIVE OR ZERO ... SET CPS = U*AND CONTINUE*)
GO TO 194
C CALCULATE A NEW TPS
194 CONTINUE
HPK = HR1
UPK = UPR(1)
TPS = 1-(SUM+HR1*KCR(I)*(C1R(I)-CPS2(I)))/HC
IF (TPS<LT.U) TPS = 1.
CALL UNDAR (HKVSTL+TPS*U+HR1*KK)
HR1 = HKR1+HC
UPR(1) = UPR(TPS,JKR(I)*P)
UPR(2) = UPR(TPS,JKR(I)*P)

47
DP(1-1) = U*{TP*UP(1)+P)

UCP[1] = CIR(1)/UPA(1)*CIR(1)-CPSR(1)

TMAPO = TMAPI

TMBN = 1-TPS

--- Two passes needed before check on temp. Conc. can be made ---

33 IF (LP<2*EU1) GO TO 27

CMCPO = CMCPI

CMCPI = CIR(1)-CPDX(1)*1

IF (ABS(UPH(1)-TPH(1))/TMHPN = 0.05) 26+62+27

26 IF (ABS(MCMPO-CMCP0)/CMCP = 0.05) 68+88+27

C CALCULATE NEW CPXR(11) PROFILE FOR NEXT PASS

C

77 LU 36 I=1,NA1

IF (MUP(LP2+5)) 34+57,34

C CALCULATE WEIGHTED AVERAGE OF OLD AVERAGED AND CALCULATED PROFILES

34 CPX(1+1) = 0.8*CPX(1)+2.4*CPX(1)

GO TO 50

C AVERAGE PRESENT AND PAST CALCULATED PROFILES EVERY 5TH PASS TO SMOOTH

57 CPXR(11) = (CPX(1)+CPX(1))/2.

C STORE PRESENT CALCULATED PROFILE

50 CPX(1) = CPX(1)

55 CONTINUE

CMCP0 = CIR(1)-CPXR(1+1)

TPR = 1-(SUM/HF*1+CIR(1)+FIR(1)-CPXR(1))/HC

IF (TPR>1.0) TPR = 1.

CALL UNHAO (HNS1,1*TPR,0.0,1*HF1,KK)

HF1 = HF1+FACF1

UPK1(1) = URT(1)/TPR*UPK(1)

UPK2(1) = URT(TPR,UPK(1))*P

UPK1(1) = URT(1)/UPK(1)*P

DCPDX = KCPX(11)/CPDX(1)*CIR(1)-CPXR(1+N1)

TMAPO = TMAPO

TMBN = 1-TPS

LP2 = LP2+1

IF (LP2<50) 19*CPY2,20

WHILE (LP2<85) CPX(1+1)

WHILE (LP2<85) CPX(1+1)

GO TO 10

29 GAMMA = KU/TPR

DELTA = CPXR(1+1)*HF1*UPK(1)/(KP*TPR)

KU = ALPHAK*AEXP(-GAMMA-A)

DO 752 I=2,N1

KUPX = KCPX(11)/KCP(1)

KUPX = KCPX(11)/KCP(1)

CPX(1+1) = CIR(1)-JUCA*KUPX*(CIR(1)-CPXR(1+N1))

IF (CPXR(1+N1)+LUPX) CPXR(1)=0

752 CONTINUE

DO 753 I=1,N1

KUPX = KCPX(11)/KCP(1)

KUPX = KCPX(11)/KCP(1)

CPXR(1+1) = CIR(1)-JUCA*KUPX*(CPXR(1+N1)-CIR(1))

753 CONTINUE

GO TO 29

88 DO 189 I=1,NA1

JPR(1) = TPS-HF1*UPK(1)/(KP*(CPXR(1+N1)-CPX(1))}

CPXR(1+1) = CPX(1+1)
CONTINUE
WRITE (0,79)
FORMAT (10,34X,111)
FINAL

DO 777 I=1,1
WRITE (0,25) REACT(I), REACTN(I), CPX(I)
A = (UX(I)+CPX(I))/17
A = A2

25 FORMAT (10X,9X,34X,111)

777 CONTINUE
WRITE (0,26) CPX
FORMAT (10,34X,111)
A = 13,6H TRIES
A = 45A27

26 FORMAT (10,34X,111)

DO 82 J=1,1
WRITE (0,83) CPX
FORMAT (10,34X,111)
A = 12.5

83 FORMAT (10,34X,111)

DO 185 K=1,1
WRITE (0,185) CPX
FORMAT (10,34X,111)
A = 12.5

185 FORMAT (10,34X,111)

IF (F1F) 240,240,240
C1P1 = CL(1)-C1P1
C1P2 = CL(2)-C1P2
K1 = K1(1)
K2 = K1(2)

240 CONTINUE

C1P3 = C1P1
C1P4 = C1P2
K1 = K1(1)
K2 = K1(2)

241 CONTINUE

C1P5 = C1P3
T1P = T1P-1
WRITE (0,10) C1P1, C1P2, C1P3, C1P4, C1P5, T1P
FORMAT (78X,34X,111)
ASV = ,1S,CL,4,1X,1S,CL,4,1X,1S,CL,4,1X,1S,CL,4,1X,1S,CL,4,1S,ASV
RETURN
END
SUBROUTINE TRAP2 (XL,UX,UP,NP,TRH,IESUM)
C  NUMERICAL INTEGRATION USING TRAPEZIODAL METHOD
C  THIS ROUTINE IS USED WHEN CP(X) PROFILE HAS NOT ALREADY BEEN DETERMINED
REAL ML,M2,M3,M4,KX,KP,KG,KP,MR,MP,MU
COMMON /BLK1/ L,T,H,L2,L3,C2,C3,C4,M1,M2,M3,M4,U01,D02,D03,D04,TS,
          X,CONX,END,U,ULZ,V3,CF3,E1,DELH,F,ALPHA,AGM,AEXP,EXP,
          X,AP,DELTA,CM,KP,MU,PRIME,Z,T1,NX0,ZETA,ZETA1
COMMON /BLK2/ C1,CF31,CF32,CF33,PP,POWER(2),POWER(1),NM(2),PM(1),
          X,K,NM1,NM2,KM1,KM2,ALPHA1,ALPHA,KR,NPR,DP(1),DOP(1)
COMMON /BLK3/ UPH(2),UPD(1),UHR(1),UCR(1),PCXR(2,100),CPXP(2,100),KUP,
          X,AGAME,ARMA,DETA,X1,CGEFH(2),COEFH(1),HFACTR,RFCTR
COMMON /FLAGS/ MM,MM1,MM2,MM3,MM4,MM5,MD,MDA,MD2,MD3,MD4,MD5,
DIMS,NSAMAX,NSAMIN,NSAMATION,NSAMATION1,NSAMATION2,NSAMATION3
C  Define RHT FUNCTION
RHTF(X) = 10.*C*EXP(D*X*(1.-F/G)/(1.+E*(1.-F/G)))
C  Define CP(X) FUNCTION FOR RHT EQUATION
CPH(X,Y) = ((X+Y)/((1.-Y)**2)*ZETA+4)
C  Calculate CP(X) FOR KEY PARTICLE REACTANT FOR RHT1 (INITIAL POINT
C  OF PROFILE) AND FOR RHT2 (FINAL POINT OF PROFILE)
CPX1(1) = CXP(XL,UX,UP,A,CPH(1))
CPX2(1) = CXP(XL,UX,UP,A,CPH(1))
CPX1(2) = CXP(XL,UX,UP,A,CPH(1))
CPX2(2) = CXP(XL,UX,UP,A,CPH(1))
C  Calculate CP(X) FOR PARTICLE PRODUCTS
DO 11 I = 1, NP
   QU4 = UPH(I)/UPD(I)
   QU5 = CGEFH(2)*CPH(2)/(COEFH(1)*MR(I))
   CPX1(I) = CPXP(1)+QU4*QU5*(CPXR(1(I))-CPXR(1(I))
   CPX2(I) = CPXP(2)+QU4*QU5*(CPXR(2(I))-CPXR(2(I))
11 CONTINUE
C  Calculate RHT FOR INITIAL AND FINAL PTS OF CP(X) PROFILE (RHT1 & RHT2)
QUOTA = 1.
QUOTA = 1.
QUOTA = 1.
QUOTA = 1.
DO 12 I = 1, NP
   POW1 = CPX1(I)*MR(I)
   POW2 = CPX2(I)*MR(I)
   QUOTA = QUOTA*POW1
   QUOTA = QUOTA*POW2
12 CONTINUE
DU 13 1=1,4NP
POWA = CPXP1(I)**HP(I)
POWBB = CPXP2(I)**HP(I)
IF (HP(I)) 1000, 1001, 1002

1001 POWDA = 1.
POWBB = 1.

1000 QUOTBA = QUOTBA*POWBA
QUOTBB = QUOTBB*POWBB

13 CONTINUE
C CALCULATE GENERALIZING TERM USED IN RHET (FIRST PT OF CPX PROFILE)
SUMTRM = 0.
SMTERM = 0.

C CALCULATE GENERALIZING TERM (ASSURPTION)
CONNUM = BLAA*(1,-CPXH1(I)/CIR(I))
CONDEN = 1.+BETA*(1,-CPXH1(I)/CIR(I))
DU 09 D = 1,4NP

RGOAMMA(I) = RGM(I)/T
KLXP(I) = RGOAMMA(I)*CONNUM/CONDEN
KKU(I) = KALPH(I)**EXP(-RGOAMMA(I))
IF (CPXH1(I)) GO TO 09

DU 09 KKUTRM(I) = KKU(I)**CPXH1(I)**POWE(I)**EXP(REXP(I))
GO TO 0LU

0LU RNUTRM = 0.
0LU SUMTRM = SUMTRM+KKUTRM(I)
0LU CONTINUE

DU 07 D = 1,4NP
PGAMMA(I) = PGM(I)/T
PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
PKU(I) = PALPH(I)**EXP(-PGAMMA(I))
PKUTRM(I) = PKU(I)**CPXH1(I)**POWE(I)**EXP(REXP(I))
SMTERM = SMTERM+PKUTRM(I)
07 CONTINUE

ASUURD = (ASUR+SUMTRM+SMTERM)**PPP
GENREL = 1./ASUURD

RHE11 = RHE11*(1+QUOTA+QUOTB+GAMMA+BETA+CPXH1(I)*CPXH2(I))

^ GENERAL
RHE11 = RHE11*FACIR

C CALCULATE THE GENERALIZING TERM USED IN RHET (LAST PT OF CPX PROFILE)
SUMTRM = 0.
SMTERM = 0.

C CALCULATE ASSURPTION TERM (*DENOMINATION OF GENERALIZING TERM)
CONNUM = BLAA*(1,-CPXH2(I)/CIR(I))
CONDEN = 1.+BETA*(1,-CPXH2(I)/CIR(I))
DU 414 D = 1,4NP
RGOAMMA(I) = RGM(I)/T
KLXP(I) = RGOAMMA(I)*CONNUM/CONDEN
KKU(I) = KALPH(I)**EXP(-RGOAMMA(I))
IF (KKU(I)**CPXH2(I)) 614, 614, 416

416 KKUTRM(I) = KKU(I)**CPXH2(I)**POWE(I)**EXP(REXP(I))
SUMTRM = SUMTRM+KKUTRM(I)
014 CONTINUE

DU 015 D = 1,4NP
PGAMMA(I) = PGM(I)/T
PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
PKU(I) = PALPH(I)**EXP(-PGAMMA(I))
PKUTRM(I) = PKU(I)**CPXH2(I)**POWE(I)**EXP(REXP(I))
SMTERM = SMTERM+PKUTRM(I)
015 CONTINUE

ASUURD = (ASUR+SUMTRM+SMTERM)**PPP

51
GENERL = 1/ADSURD
KRET2 = RHEK[(KU*QUOTA+QUOTDB*GAMMA*GAMMA*CPXR2(1)+CPXR2(1)+CPXR2(1))]

A = GENERL
KRET2 = KRET2*RFACR

IF (KRET2) I=177777
77
MM = 1
GOTO 77

C
C BEGIN INTEGRATION USING TRAPEZOIDAL METHOD
C
C CALCULATE FIRST AND LAST TERMS OF APPROXIMATING SUM FIRST
4
THM1 = FOPX(XLOWER+KRET1)/2.
THM2 = FOPX(XUPPER+KRET2)/2.

40
DO 5 J=1,N
C CALCULATE CP(X) FOR KEY PARTICLE REACTANTS (TO USE IN KRET TERM)
CPXRK(1) = CPXP(XP1+XOA*CPSR(1))

C CALCULATE CP(X) FOR OTHER REACTANT (TO USE IN KRET)
CPXRK(2) = CPSR(2)+UO1*UO2*(CPXRK(1)-CPXRK(1))

C CALCULATE CP(X) FOR PARTICLE PRODUCTS (TO USE IN KRET)
UV 15 I=1,NP
CPXP(1) = CPSR(1)+UO3*UO4*(CPXRK(1)-CPXRK(1))

15
CONTINUE

C CALCULATE KRET EXPRESSION
QUOTA = 1.
QUO1 = 1.

UV 16 I=1,N
POMA = CPXRK(1)**PK(1)
QUOTA = QUOTA*POMA

16
CONTINUE

UV 17 I=1,NP
POMA = CPXP(1)**PP(1)

IF (PP(1)) 1000,1000,1005
1000
QUOTB = QUOTB*POMA

1005
CONTINUE

C CALCULATE GENERALIZING TERM FOR KRET (FOR INTERMEDIATE PTS ON CPX PROFILE)
SUM1MM = 0.
SUMLMM = 0.

CONNUM = ULI1*CPXRK(1)/CIR(1)
CONDEN = ULI1*UET1*CPXRK(1)/CIR(1)

UV 622 I=1,NK
RKAMMA(1) = RKM(I)/T
REXP(1) = RKAMMA(1)*CONNUM/CONDEN
KKU(1) = RALPH(1)*EXP(-RKAMMA(1))
KKU1RM(1) = KKU(1)*CPXRK(1)**POWER(1)*EXP(REXP(1))

SUMRM = SUMRM+KKU1RM(1)

622
CONTINUE

UV 623 I=1,NP
PKAMMA(1) = PGM(1)/T
PEXP(1) = PKAMMA(1)*CONNUM/CONDEN
PKU(1) = PALPH(1)*EXP(-PKAMMA(1))
P KU1RM(1) = PKU(1)*CPXP(1)**POWER(1)*EXP(PEXP(1))

SUMRM = SUMRM+PKU1RM(1)

623
CONTINUE
ADSURD = (CUMST+SUMRM+SUMLMM)**PPP

GENERL = 1./ADSURD
KRET = NVIDIA*(QUOTA+QUOTDB*GAMMA*GAMMA*CPXR2(1)+CPXR2(1)+CPXR2(1))*GENERL
RHEK = KRET*(RFACR)

IF (UO1*UO1*UO1*UO1*UO1*UO1*UO1) MM = 2
IF (MMM=NE2) GO TO 207
IF (J.UJ, NM) JJJ = JJJ + 1
IF (JJJ.GT.0) RETURN

207 SUM = SUM + FFX(XPH + RHET)
200 XPH = XPH + NN
0 CONTINUE
1 RESUM = H1*(THM1 + SUM + FRM2)
99 RETURN
END
# Table of Heat of Reaction vs Temperature (Deg R)

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# Table of Vapor Pressure (Psia) vs Temperature (Deg R)

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# Table of Temperature (Deg R) vs Vapor Pressure (Psia)

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# Table of Delta Heat of Condensation vs Temperature

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# Delta Heat of Condensation (UHC)

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Four Viscosity Tables Follow

# Table of H2 Viscosity (Lb/ft-sec) vs Temperature (Deg R)

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<th>Temperature (°C)</th>
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<th>Temperature (°C)</th>
<th>H₂ Viscosity (cP)</th>
<th>Temperature (°C)</th>
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**Table of H₂ Viscosity (cP) vs Temperature (°C)**

**Table of O₂ Viscosity (cP) vs Temperature (°C)**

**Table of H₂O Viscosity (cP) vs Temperature (°C)**

**Table of H₂ Specific Heat (BTU/LB-°F) vs Temperature (°F)**

**Table of O₂ Specific Heat (BTU/LB-°F) vs Temperature (°F)**
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**C TABLE OF H₂O (VAPOR) SPECIFIC HEAT (BTU/LB-DEG-R) VS TEMPERATURE**

**DATA (CF3V1(I), I=1..34) / 0., 1., 15., 0.,**

**TEMPERATURES**

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<th>1080.</th>
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<td>3240.</td>
<td>3600.</td>
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**SPECIFIC HEATS OF H₂O (VAPOR)**

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**DATA (CF3ST(I), I=1..16) / 0., 1., 6., 0.,**

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<td>1.24</td>
<td>1.24</td>
<td>1.24</td>
<td>1.24</td>
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**SPECIFIC HEATS OF HELIUM**

ENDU
SUBROUTINE UNBAR(T,IK,XIN,YIN,ZN,ZZ,KK)
DIMENSION T(1),X(1),Y(1),A(1)
C ------------------ MARCH 4, 1961 ------------------
C ------------------ MODIFIED 7/62 ------------------
C ------------------ 7G-10 QUADRTIC AND LINEAR INTERPOLATION ALSO
C
II = IK+1
N = 3
N2= 2

700 IF (T(I1)-T,) 700,101,702
702 IF (T(I1)-T,) 607,701,704
704 N = 1
705 GU 7U 707
706 N = 2
707 N2 = 1
701 II = II+1
702 N1 = N + 1
    GU 5U L = II+1
    IF (T(L) + U*) GU 6U,51
703 KX = T(L)
    ZL = U*
    GU 4U 9Y
51 NX = T(L)
    IF (T(L+1) + U*) GU 52,54
52 NY = 0
    GU 4U 53
54 NX = T(L+1)
55 CONTINUE

KX = 0
KY = 0
AX = XN1
AY = YN1
JO = II+2

J2 = N+1+1

400 IF (XX-T(J1)) 301,300,400
300 C0NTINUE
302 CONTINUE
304 AX = T(J1)
305 CONTINUE
308 JX1 = JZ-N
309 C0NTINUE
301 KX = 1
306 JX1 = JO
307 C0NTINUE
303 JX1 = JZ-N2
304 1500 AX = T(J1)
308 1500 AX = T(J1)
307 1500 AX = T(J1)
306 1500 1500
304 1500 1500
303 1500 1500
302 1500 1500
301 1500 1500
300 1500 1500
309 1500 1500
308 1500 1500
307 1500 1500
306 1500 1500
305 1500 1500
304 1500 1500
303 1500 1500
302 1500 1500
301 1500 1500
300 1500 1500

\begin{verbatim}
712 X(J) = -TAL1
713 X(J) = (X(J+2) - X(J)) * TAL1
  55 CONTINUE
A(I) = A(N+I)
ZZ = 0.
  60 IF (I = 1 + N) THEN
X(J) = U/(A(J) + I(J+1)) * X(J)
ZZ = ZZ + I(J) * X(J)
  59 CONTINUE
IF (I) 9999, 9996, 9999
9999 KK = KK + KT
RETURN
END
\end{verbatim}
**APPENDIX III**

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AXIAL TEMPERATURE AND CHAMBER PRESSURE PROFILES FOR A LOW NOMINAL CHAMBER PRESSURE

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 X 10^4 N/M^2)
FEED MIXTURE RATIO = 1.0 LB O₂ / LB H₂ (1.0 KG O₂ / KG H₂)
FEED TEMPERATURE = 210 DEG R (117 DEG K)
MASS FLOW RATE = 1.28 LB/FT² - SEC (6.25 KG/M² - SEC)  NO HELIUM DILUTION
BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES

FIG. 1

TEMPERATURE IN INTERSTITIAL PHASE, T₁ = DEG K

CHAMBER PRESSURE, P = 10^4 N/M²

CHAMBER PRESSURE, P = PSIA

AXIAL DISTANCE, z = INCHES

AXIAL DISTANCE, z = METERS
AXIAL CONCENTRATION PROFILES FOR A LOW NOMINAL CHAMBER PRESSURE

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89x10^4 N/m^2)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

FEED MIXTURE RATIO = 1.0 LB O_2/LB H_2 (1.0 KG O_2/KG H_2)

NO HELIUM DILUTION

MASS FLOW RATE = 1.28 LB/FT^2-SEC (6.25 KG/M^2-SEC)

BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES
FIG. 3

AXIAL MOLE-FRACTION PROFILES FOR A LOW NOMINAL CHAMBER PRESSURE

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89X10^4 N/M^2)
FEED TEMPERATURE = 210 DEG R (117 DEG K)
FEED MIXTURE RATIO = 1.0 LB O_2 / LB H_2 (1.0 KG O_2 / KG H_2)
NO HELIUM DILUTION
MASS FLOW RATE = 1.28 LB/FT^2 - SEC (6.25 KG/M^2 - SEC)
BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES

AXIAL DISTANCE, z - INCHES

AXIAL DISTANCE, z - METERS
EFFECT OF PROPELLANT FEED TEMPERATURE ON AXIAL TEMPERATURE PROFILES

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 x 10^4 N/m^2)
FEED MIXTURE RATIO = 1.0 LB O_2/LB H_2 (1.0 KG O_2/KG H_2)
MASS FLOW RATE = 1.28 LB/FT^2 - SEC (6.25 KG/M^2 - SEC)
NO HELIUM DILUTION

BED CONFIGURATIONS: ALL 14-18 MESH CATALYST PARTICLES

BED CONFIGURATION: ALL 1/16 IN. SPHERES IN. (0.16 x 10^-2 M)
EFFECT OF STOICHIOMETRY ON AXIAL TEMPERATURE PROFILES

Nominal Chamber Pressure = 10 PSIA (6.89 x 10^4 N/m^2)
Feed Temperature = 210 Deg R (117 Deg K)
Mass Flow Rate = 1.28 lb/ft^2 - sec (6.25 kg/m^2 - sec)

Bed Configuration: All 14-18 mesh catalyst particles

Bed Configuration: All 1/16 in. spheres (0.16 x 10^-2 m)

Feed mixture ratio = 4 \( \frac{lb O_2}{lb H_2} \left( \frac{kg O_2}{kg H_2} \right) \)

Temperature in interstitial phase, \( T_i \), - Deg K

Temperature in interstitial phase, \( T_i \), - Deg K

Axial distance, \( z \), - inches

Axial distance, \( z \), - meters
EFFECT OF HELIUM DILUTION ON AXIAL TEMPERATURE PROFILES

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 x 10^4 N/m^2)
FEED TEMPERATURE = 210 DEG R (117 DEG K)
MASS FLOW RATE = 1.28 LB/FT^2 SEC (6.25 KG/M^2 SEC)
FEED MIXTURE = 1.0 LB O_2/LB H_2 (1.0 KG O_2/KG H_2)

BED CONFIGURATION: ALL 14-18 MESH PARTICLES

BED CONFIGURATION: ALL 1/16 IN. SPHERES (0.16 x 10^-2 M)

TEMPERATURE IN INTERSTITIAL PHASE, T_i - DEG K

HELIUM WEIGHT FRACTION = 0.0

0.10

0.25

0.35

0.50

AXIAL DISTANCE, z - INCHES

AXIAL DISTANCE, z - METERS

FIG. 6
EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES
NO HELIUM DILUTION

NOMINAL CHAMBER PRESSURE = 10 PSIA \((6.89 \times 10^4 \text{ N/m}^2)\)

FEED TEMPERATURE = 210 DEG R \((117 \text{ DEG K})\)

FEED MIXTURE = 1.0 LB \(\text{O}_2/\text{LB H}_2\) \((1.0 \text{ KG } \text{O}_2/\text{KG H}_2)\)

BED CONFIGURATION: ALL 14-18 MESH PARTICLES

BED CONFIGURATION: ALL 1/16 IN. SPHERES \((0.16 \times 10^{-2} \text{ M})\)
EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

Medium Weight - Fraction = 0.25
Nominal Chamber Pressure = 10 PSIA (6.89 X 10^4 N/m^2)
Feed Temperature = 210 Deg R (117 Deg K)
Feed Mixture Ratio = Lb.O_2/Lb.H_2 = 1.0 (19 KG O_2/KG H_2)

Bed Configuration: All 1/16 in. Spheres (0.16 X 10^-2 m)

Temperature in Interstitial Phase, 1 - Dec R

FIG. 8

Bed Configuration: All 14-18 Mesh Particles

Temperature in Interstitial Phase, 1 - Dec K
EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIUM WEIGHT-FRACTION = 0.50

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 x 10^4 N/m^2)
FEED TEMPERATURE = 210 DEG R (117 DEG K)
FEED MIXTURE RATIO = 1.0 LB O_2/LB H_2 (1.0 KG O_2/ KG H_2)

BED CONFIGURATION: ALL 14-18 MESH PARTICLES

BED CONFIGURATION: ALL 1/16 IN. SPHERES (0.16 x 10^-2 M)

AXIAL DISTANCE, z - INCHES
AXIAL DISTANCE, z - METERS
AXIAL TEMPERATURE AND CHAMBER PRESSURE PROFILES FOR A HIGH NOMINAL CHAMBER PRESSURE

NOMINAL CHAMBER PRESSURE = 100 PSIA (6.89 x 10^5 N/m^2)
FEED MIXTURE RATIO = 1.0 LB O_2 / LB H_2 (1.0 KG O_2 / KG H_2)
FEED TEMPERATURE = 210 DEG R (117 DEG K)
MASS FLOW RATE = 5.25 LB/FT^2 - SEC (25.6 KG/M^2 - SEC)
NO HELIUM DILUTION
BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES
AXIAL CONCENTRATION PROFILES FOR A HIGH NOMINAL CHAMBER PRESSURE

NOMINAL CHAMBER PRESSURE = 100 PSIA (6.89 X 10^5 N/M^2)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

MASS FLOW RATE = 5.25 LB/FT^2 - SEC (25.6 KG/M^2 - SEC)

FEED MIXTURE RATIO = 1.0 LB O_2/LB H_2 (1.0 KG O_2/KG H_2)

NO HELIUM DILUTION

BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES
AXIAL MOLE-FRACTION PROFILES FOR A HIGH NOMINAL CHAMBER PRESSURE

NOMINAL CHAMBER PRESSURE = 100 PSIA (6.89 x 10^5 N/M^2)
FEED TEMPERATURE = 210 DEG R (117 DEG K)
FEED MIXTURE RATIO = 1.0 LB O_2/LB H_2 (1.0 KG O_2/KG H_2)
NO HELIUM DILUTION
MASS FLOW RATE = 5.25 LB/FT^2 - SEC (25.6 KG/M^2 - SEC)
BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES

AXIAL DISTANCE, z - INCHES

AXIAL DISTANCE, z - METERS
EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

NO HELIUM DILUTION

NOMINAL CHAMBER PRESSURE = 100 PSIA \( (6.89 \times 10^5 \text{ N/m}^2) \)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

FEED MIXTURE RATIO = 1.0 \( \text{LB O}_2 / \text{LB H}_2 \) (1.0 \( \text{KG O}_2 / \text{KG H}_2 \))

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**BED CONFIGURATION: ALL 14–18 MESH PARTICLES**

- \( \text{LB/FT}^2 \text{ - SEC (KG/M}^2 \text{ - SEC)} \)
  - \( G = 1.05 \) \((5,12)\)
  - \( 2.10 \) \((10,2)\)
  - \( 3.15 \) \((15,4)\)
  - \( 4.20 \) \((20,5)\)
  - \( 5.25 \) \((25,6)\)

---

**BED CONFIGURATION: ALL 1/16 IN. SPHERES (0.16 \( \times 10^{-2} \text{ M)\])**

- \( \text{LB/FT}^2 \text{ - SEC (KG/M}^2 \text{ - SEC)} \)
  - \( G = 1.05 \) \((5,12)\)
  - \( 2.10 \) \((10,2)\)
  - \( 3.15 \) \((15,4)\)
  - \( 4.20 \) \((20,5)\)
  - \( 5.25 \) \((25,6)\)
EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIUM WEIGHT-FRACTION = 0.25

NOMINAL CHAMBER PRESSURE = 100 PSIA (6.89 X 10^5 N/M^2)
FEED TEMPERATURE = 210 DEG R (117 DEG K)
FEED MIXTURE RATIO = 1.0 LB O_2/LB H_2 (1.0 KG O_2/KG H_2)

FIG. 14
EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIX WEIGHT-FRACTION = 0.50

NOMINAL CHAMBER PRESSURE = 100 PSIA \( (6.89 \times 10^5 \text{ N/m}^2) \)

FEED TEMPERATURE = 210 DEG R \( (117 \text{ DEG K}) \)

FEED MIXTURE RATIO = 1.0 LB \( \text{O}_2 \)/LB \( \text{H}_2 \) \( (1.0 \text{ KG} \text{O}_2/\text{KG} \text{H}_2) \)

BED CONFIGURATION: ALL 14–18 MESH PARTICLES

BED CONFIGURATION: ALL 1/16 IN. SPHERES \( (0.16 \times 10^{-2} \text{m}) \)

\[
\begin{align*}
\text{LB/FT}^2 &- \text{SEC} \quad (\text{KG/M}^2 - \text{SEC}) \\
G & = 1.05 \quad (5.12) \\
2.10 & \quad (10.2) \\
3.15 & \quad (15.4) \\
4.20 & \quad (20.5) \\
5.25 & \quad (25.6)
\end{align*}
\]

0 0.002 0.004 0.006 0.008 0.010 0.012

0 0.1 0.2 0.3 0.4 0.5

AXIAL DISTANCE, \( z \) - METERS

AXIAL DISTANCE, \( z \) - INCHES

FIG. 15