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FINAL PROGRESS REPORT

**STUDY OF CATALYTIC REACTORS
FOR HYDROGEN-OXYGEN IGNITION**

by

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prepared for

**NATIONAL AERONAUTICS
AND SPACE ADMINISTRATION**

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Study of Catalytic Reactors for

Hydrogen-Oxygen Ignition

Final Progress Report

August 28, 1968 - May 28, 1969

Contract NASW-1795

TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT	i
FOREWORD	ii
SUMMARY	1
INTRODUCTION	2
DISCUSSION	3
Steady-State Model of Hydrogen-Oxygen Catalytic Ignition System	3
Kinetics Information	8
Results of Calculations	9
Definition of Rate-Controlling Processes	11
REFERENCES	12
LIST OF SYMBOLS	14
APPENDIX I	16
APPENDIX II - LISTING OF STEADY-STATE COMPUTER PROGRAM	20
APPENDIX III - DISTRIBUTION LIST	60
FIGURES	70

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.

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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.

DISCUSSION

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

$$\frac{dw_i^{H_2}}{dz} = -\frac{1}{G} \left\{ r_{\text{hom}} \delta + k_c^{H_2} A_p \left[c_i^{H_2} - (c_p)_s^{H_2} \right] \right\} \quad (1)$$

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

$$\frac{dw_i^{H_2O}}{dz} = \frac{1}{G} \left\{ r_{\text{hom}} \delta \frac{M^{H_2O}}{M^{H_2}} - k_c^{H_2O(v)} A_p \left[c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)} \right] \right\} \quad (3)$$

$$\frac{dw_i^{\text{He}}}{dz} = 0 \quad (4)$$

The rates of change of species concentrations with axial distance are then given by

$$\frac{dc_i^J}{dz} = \rho_i \frac{dw_i^J}{dz} + w_i^J \frac{d\rho_i}{dz} \quad (5)$$

where

$$\begin{aligned} \frac{1}{\rho_i} \frac{d\rho_i}{dz} \left[1 - w_i^{\text{H}_2\text{O}(s)} - w_i^{\text{H}_2\text{O}(l)} \right] &= \frac{dw_i^{\text{H}_2\text{O}(s)}}{dz} + \frac{dw_i^{\text{H}_2\text{O}(l)}}{dz} \\ &+ \frac{\rho_i^{(v)}}{\rho_i} \left[\frac{1}{P} \frac{dP}{dz} + \frac{1}{\bar{M}^{(v)}} \frac{d\bar{M}^{(v)}}{dz} - \frac{1}{T_i} \frac{dT_i}{dz} \right] \end{aligned} \quad (6)$$

and

$$\frac{1}{\bar{M}^{(v)}} \frac{d\bar{M}^{(v)}}{dz} = - \left[\frac{\sum_{\text{(vapor)}} \frac{dw_i^J}{dz} / M^J}{\sum_{\text{(vapor)}} \frac{w_i^J}{M^J}} \right] \quad (7)$$

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

$$h_c = .74 \bar{C}_f^{(v)} G \left(\frac{G}{A_D \mu} \right)^{-.41} \quad (8)$$

$$k_c^J = \frac{.61G}{\rho_i^{(v)}} \left(\frac{\mu}{\rho_i^{(v)} D_{i^J}} \right)^{-.667} \left(\frac{G}{A_D \mu} \right)^{-.41} \quad (9)$$

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

$$\begin{aligned} \frac{dh_i}{dz} = & -\frac{l}{G} \left\{ H r_{\text{hom}} \delta + h_c A_p [T_i - (T_p)_s] \right. \\ & \left. + k_c^{H_2O(v)} A_p [c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)}] [\Delta H^f + \Delta H^c] \right\} \end{aligned} \quad (10)$$

In this "ice region"

$$\frac{dw_i^{H_2O}}{dz} = \frac{dw_i^{H_2O(s)}}{dz} \quad (11)$$

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

$$\begin{aligned} \frac{dh_i}{dz} = & -\frac{l}{G} \left\{ H r_{\text{hom}} \delta + h_c A_p [T_i - (T_p)_s] \right. \\ & \left. + k_c^{H_2O(v)} A_p [c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)}] \left[\Delta H^c + \Delta H^f \left(\frac{h_i - h_i^{(s)}}{h_i^{(s-\ell)} - h_i^{(s)}} \right) \right] \right\} \end{aligned} \quad (12)$$

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

$$\frac{dw_i^{H_2O(s)}}{dz} = \frac{dw_i^{H_2O}}{dz} \left[\frac{h_i^{(s-\ell)} - h_i}{h_i^{(s-\ell)} - h_i^{(s)}} \right] - \frac{l}{(h_i^{(s-\ell)} - h_i^{(s)})} \frac{dh_i}{dz} \quad (13)$$

$$\frac{dw_i^{H_2O(l)}}{dz} = \frac{dw_i^{H_2O}}{dz} \left[\frac{h_i - h_i^{(s)}}{h_i^{(s-\ell)} - h_i^{(s)}} \right] + \frac{l}{(h_i^{(s-\ell)} - h_i^{(s)})} \frac{dh_i}{dz} \quad (14)$$

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

$$h_i^{(s-l)} = h_i(z) + \Delta H^f w_i^{H_2O(s)}(z) \quad (15)$$

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

$$\begin{aligned} \frac{dh_i}{dz} = & -\frac{1}{G} \left\{ H r_{\text{hom}} \delta + h_c A_p [T_i - (T_p)_s] \right. \\ & \left. + k_c^{H_2O(v)} A_p [c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)}] [\Delta H^c] \right\} \end{aligned} \quad (16)$$

In this "liquid region"

$$\frac{dw_i^{H_2O}}{dz} = \frac{dw_i^{H_2O(l)}}{dz} \quad (17)$$

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

$$\begin{aligned} \frac{dh_i}{dz} = & -\frac{1}{G} \left\{ H r_{\text{hom}} \delta + h_c A_p [T_i - (T_p)_s] \right. \\ & \left. + k_c^{H_2O(v)} A_p [c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)}] \left[\Delta H^c \left(\frac{h_i - h_i^{(l)}}{h_i^{(l-v)} - h_i^{(l)}} \right) \right] \right\} \end{aligned} \quad (18)$$

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

$$\frac{dw_i^{H_2O(l)}}{dz} = \frac{dw_i^{H_2O}}{dz} \left[\frac{h_i^{(l-v)} - h_i}{h_i^{(l-v)} - h_i^{(l)}} \right] - \frac{1}{(h_i^{(l-v)} - h_i^{(l)})} \frac{dh_i}{dz} \quad (19)$$

$$\frac{dw_i^{H_2O(v)}}{dz} = \frac{dw_i^{H_2O}}{dz} \left[\frac{h_i - h_i^{(l)}}{h_i^{(l-v)} - h_i^{(l)}} \right] + \frac{1}{(h_i^{(l-v)} - h_i^{(l)})} \frac{dh_i}{dz} \quad (20)$$

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

$$h_i^{(l-v)} = h_i(z) + \Delta H^c w_i^{H_2O(l)}(z) \quad (21)$$

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

$$\frac{dh_i}{dz} = -\frac{1}{G} \left\{ H r_{\text{hom}} \delta + h_c A_p [T_i - (T_p)_s] \right\} \quad (22)$$

and

$$\frac{dw_i^{H_2O}}{dz} = \frac{dw_i^{H_2O(v)}}{dz} \quad (23)$$

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

$$r_{\text{hom}} = 0.16 \times 10^{14} c_i^{\text{H}_2} c_i^{\text{O}_2} e^{-35,800/T_i} \text{ lbs H}_2 \text{ reacted/ft}^3\text{-sec}$$

$$(\text{=} 0.10 \times 10^{13} c_i^{\text{H}_2} c_i^{\text{O}_2} e^{-19,889/T_i} \text{ kg H}_2 \text{ reacted/m}^3\text{-sec}) \quad (24)$$

where the concentrations are in lb/ft³ (kg/m³) and T_i 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 on 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.

$$\begin{aligned}
 r_{\text{het}} &= \alpha c_p^{\text{H}_2} (c_p^{\text{O}_2})^{0.8} e^{-5000/T_p} \quad \text{lbs H}_2 \text{ reacted / ft}^3\text{-sec} \\
 &(\ = 0.11 \alpha c_p^{\text{H}_2} (c_p^{\text{O}_2})^{0.8} e^{-2778/T_p} \quad \text{kg H}_2 \text{ reacted / m}^3\text{-sec}
 \end{aligned}
 \tag{25}$$

where T_p is in deg R (deg K). The rate constant, α , is specific to the type and structure of the platinum family metal employed.

It was originally intended to estimate α for a particular catalyst by using the steady-state program to find the value of α 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 α 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, α , 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 ($6.89 \times 10^4 \text{ N/m}^2$), 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/ft²-sec (6.25 kg/m²-sec). In order to accommodate this rather high flow rate in this low pressure system, the upstream chamber pressure was taken as 30 psia ($2.07 \times 10^5 \text{ N/m}^2$) (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. ($0.16 \times 10^{-2} \text{ m}$) 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. (0.16×10^{-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 $0.26 \text{ lb/ft}^2\text{-sec}$ ($1.27 \text{ kg/m}^2\text{-sec}$) to $1.28 \text{ lb/ft}^2\text{-sec}$ ($6.25 \text{ kg/m}^2\text{-sec}$) 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 $5.24 \text{ lb/ft}^2\text{-sec}$ ($25.6 \text{ kg/m}^2\text{-sec}$). The nominal chamber pressure was taken as 100 psia ($6.89 \times 10^5 \text{ N/m}^2$) 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. (0.16×10^{-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 $1.05 \text{ lb/ft}^2\text{-sec}$ ($5.12 \text{ kg/m}^2\text{-sec}$) and $5.25 \text{ lb/ft}^2\text{-sec}$ ($25.6 \text{ kg/m}^2\text{-sec}$). 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.

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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, lb/ft^3 (kg/m^3)
c_p	Reactant concentration in gas phase within the porous catalyst particle, lb/ft^3 (kg/m^3)
C_F	Specific heat of fluid in the interstitial phase, $\text{Btu}/\text{lb-deg R}$ ($\text{Cal}/\text{kg-deg K}$)
\bar{C}_F	Average specific heat of fluid in the interstitial phase, $\text{Btu}/\text{lb-deg R}$ ($\text{Cal}/\text{kg-deg K}$)
D_i	Diffusion coefficient of reactant gas in the interstitial phase, ft^2/sec (m^2/sec)
D_p	Diffusion coefficient of reactant gas in the porous particle, ft^2/sec (m^2/sec)
G	Mass flow rate, $\text{lb}/\text{ft}^2\text{-sec}$ ($\text{kg}/\text{m}^2\text{-sec}$)
h_i	Enthalpy, Btu/lb (Cal/kg)
$h_i^{(s)}$	Enthalpy at the Ice/Ice-Liquid interface, Btu/lb (Cal/kg)
$h_i^{(s-l)}$	Enthalpy at the Ice-Liquid/Liquid interface, Btu/lb (Cal/kg)
$h_i^{(l)}$	Enthalpy at the Liquid/Liquid-Vapor interface, Btu/lb (Cal/kg)
$h_i^{(l-v)}$	Enthalpy at the Liquid-Vapor/Vapor interface, Btu/lb (Cal/kg)
h_c	Heat transfer coefficient, $\text{Btu}/\text{ft}^2\text{-sec-deg R}$ ($\text{Cal}/\text{m}^2\text{-sec-deg K}$)
H	Heat of reaction, Btu/lb (Cal/kg)
ΔH^c	Heat of condensation, Btu/lb (Cal/kg)
ΔH^f	Heat of fusion, Btu/lb (Cal/kg)
k_c	Mass transfer coefficient, ft/sec (m/sec)
K_p	Thermal conductivity of the porous catalyst particle, $\text{Btu}/\text{ft-sec-deg R}$ ($\text{Cal}/\text{m-sec-deg K}$)

H910721

M	Molecular weight, lb/lb mole (kg/kg mole)
\bar{M}	Average molecular weight, lb/lb mole (kg/kg mole)
P	Chamber pressure, psia (N/m^2)
r_{het}	Rate of (heterogeneous) chemical reaction on the catalyst surfaces, lb/ft ³ -sec (kg/m ³ -sec)
r_{hom}	Rate of (homogeneous) chemical reaction in the interstitial phase, lb/ft ³ -sec (kg/m ³ -sec)
T	Temperature, deg R (deg K)
w_i	Weight fraction of reactant in interstitial phase
x	Radial distance from the spherical catalyst particle, ft (m)
z	Axial distance, ft (m)
α	Catalytic reaction rate constant
δ	Interparticle void fraction
μ	Viscosity of interstitial fluid, lb/ft-sec (kg/m-sec)
ρ_i	Density of interstitial fluid, lb/ft ³ (kg/m ³)

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

H ₂ O(s)	Refers to water in the solid phase
H ₂ O(l)	Refers to water in the liquid phase
H ₂ O(v)	Refers to water in the vapor phase
J	Refers to chemical species (e.g. H ₂ , O ₂ , H ₂ O, He)
(v)	Refers to vapor phase

APPENDIX I

Generalization to Multireactant Systems of the Integral Method
used to Evaluate the Effects of Heat and Mass Diffusion
on Reaction Rates in Porous Catalyst Particles

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

$$D_p \nabla^2 c_p - r_{het} = 0 \quad (I-1)$$

$$K_p \nabla^2 T_p - H r_{het} = 0 \quad (I-2)$$

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

$$D_p \left(\frac{dc_p}{dx} \right)_s = k_c [c_i - (c_p)_s] \quad (I-3)$$

$$H D_p \left(\frac{dT_p}{dx} \right)_s = h_c [T_i - (T_p)_s] \quad (I-4)$$

Using Eqs. (I-1) and (I-2), Prater (Ref. 14) has pointed out that temperature and concentration are related quite simply by

$$T_p - (T_p)_s = -\frac{H D_p}{K_p} \left[(c_p)_s - c_p \right]. \quad (\text{I-5})$$

The use of this relationship enables the reaction rate, r_{het} , 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 $r_{het} = r_{het}(c_p)$, 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

$$c_p(x) = c_i - \left[\frac{1}{x} - \frac{a k_c - D_p}{a^2 k_c} \right] \int_0^x \xi^2 \frac{r_{het}(c_p)}{D_p} d\xi - \int_x^a \left[\frac{1}{\xi} - \frac{a k_c - D_p}{a^2 k_c} \right] \xi^2 \frac{r_{het}(c_p)}{D_p} d\xi \quad (\text{I-6})$$

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_{het} , 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



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

$$D_p^A \nabla^2 c_p^A - r_{het}^A(c_p^A, c_p^B, \dots, c_p^T, \dots, T_p) = 0 \quad (\text{I-7})$$

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

$$\begin{array}{c} c_p^B - (c_p)_s^B \\ \vdots \end{array} = \frac{bM^B}{aM^A} \frac{D_p^A}{D_p^B} \begin{array}{c} [c_p^A - (c_p)_s^A] \\ \vdots \end{array} \quad (\text{I-15})$$

$$\begin{array}{c} c_p^T - (c_p)_s^T \\ \vdots \end{array} = \frac{tM^T}{aM^A} \frac{D_p^A}{D_p^T} \begin{array}{c} [(c_p)_s^A - c_p^A] \\ \vdots \end{array} \quad (\text{I-16})$$

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

$$\begin{array}{c} c_i^B - (c_p)_s^B \\ \vdots \end{array} = \frac{bM^B}{aM^A} \frac{k_c^A}{k_c^B} \begin{array}{c} [c_i^A - (c_p)_s^A] \\ \vdots \end{array} \quad (\text{I-17})$$

$$\begin{array}{c} c_i^T - (c_p)_s^T \\ \vdots \end{array} = \frac{tM^T}{aM^A} \frac{k_c^A}{k_c^T} \begin{array}{c} [(c_p)_s^A - c_i^A] \\ \vdots \end{array} \quad (\text{I-18})$$

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_{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

WIPT FOR READIN

REAL M1,M2,M3,M4,MU,KP

COMMON /BLOCK1/ T,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,

~~X ZCON,ZEND,G,DHDZ,W3,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,~~

~~X A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETA IN~~

COMMON /BLOCK2/ CONST,PPP,POWERP(2),POWERP(1),KGM(2),PGM(1),

~~X KALPH(2),PALPH(1),KGM,ALPHAK,NR,NP,DOR(2),DOP(1)~~

COMMON /BLOCK3/ DPK(2),DPP(1),KGR(2),KGP(1),CPSR(2),CPSP(1),CIR(2)

COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)

~~X MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),~~

~~X CF3V(34),CF3S(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST~~

~~X (24)~~

DIMENSION TITLE(14)

DATA END /'END'/'

C

~~C THE NUMBERS 1,2,3,4 IN THE VARIABLE NAMES REFER TO H2, O2, H2O,~~

C

~~AND HE RESPECTIVELY~~

C

KP = 0.4 E-4

DELHF = 145.4

CF3L = 1.0

~~k = 10.73~~

1 READ (5,100) TITLE

100 FORMAT (14A6)

IF (TITLE(1)-END) 20,10,26

26 WRITE (6,200) TITLE

200 FORMAT (1H1,14A6//)

~~READ (5,250) PRIME~~

250 FORMAT (A2)

30 READ (5,300) T,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,

~~X ZCON,ZEND,ALPHA,ALXP,BEXP,AGM,ALPHAK,ZETA IN~~

300 FORMAT (8E10.5)

WRITE (6,400)

400 FORMAT (/11X,'T',11X,'P',11X,'H',10X,'C1',10X,'C2',10X,'C3

~~X',10X,'C4',10X,'M1',10X,'M2')~~

WRITE (6,500) T,P,H,C1,C2,C3,C4,M1,M2

500 FORMAT (/6X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,

~~XE10.5,2X,E10.5,2X,E10.5,2X,E10.5)~~

WRITE (6,600)

600 FORMAT (/10X,'M3',10X,'M4',9X,'D01',9X,'D02',9X,'D03',9X,'D04',10

~~X',TS',9X,'ZCON',8X,'ZEND',8X,'ALPHA')~~

WRITE (6,700) M3,M4,D01,D02,D03,D04,TS,ZCON,ZEND,ALPHA

700 FORMAT (/6X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,

~~AE10.5,2X,E10.5,2X,E10.5,2X,E10.5)~~

WRITE (6,800)

800 FORMAT (/9X,'AEXP',8X,'BEXP',9X,'AGM',7X,'ALPHAK',8X,'ZETA')

WRITE (6,900) ALXP,BEXP,AGM,ALPHAK,ZETA IN

900 FORMAT (/6X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,

READ (5,950) NOFZ

950 FORMAT (1I2)

NZTBL = 2*NOFZ+4

~~NOFZ4 = NOFZ+4~~

NOFZ5 = NOFZ+1

READ (5,20) (AVSZ(I),I=1,4)

20 FORMAT (4E6.4)

READ (5,21) (AVSZ(I),I=5,NOFZ4)

21 FORMAT (10E6.4)

~~READ (5,21) (AVSZ(I),I=NOFZ5,NZTBL)~~

```

READ (5,20) (APVSZ(1),I=1,4)
READ (5,21) (APVSZ(1),I=5,NOFZ4)
READ (5,21) (APVSZ(1),I=NOFZ5,NZTBL)
READ (5,20) (DELVSZ(1),I=1,4)
READ (5,21) (DELVSZ(1),I=5,NOFZ4)
READ (5,21) (DELVSZ(1),I=NOFZ5,NZTBL)
WRITE (6,9,9)
999 FORMAT (//,55X,13H A VS Z TABLE)
WRITE (6,22) (AVSZ(1),I=1,4)
22 FORMAT (40A,4E13.5)
WRITE (6,23) (AVSZ(1),I=5,NOFZ4)
23 FORMAT (1X,10E13.5)
WRITE (6,23)
25 FORMAT ( / )
WRITE (6,23) (AVSZ(1),I=NOFZ5,NZTBL)
WRITE (6,24)
24 FORMAT ( / )
WRITE (6,997)
997 FORMAT (54X,14H AP VS Z TABLE)
WRITE (6,22) (APVSZ(1),I=1,4)
WRITE (6,23) (APVSZ(1),I=5,NOFZ4)
WRITE (6,23)
WRITE (6,23) (APVSZ(1),I=NOFZ5,NZTBL)
WRITE (6,24)
WRITE (6,9,5)
995 FORMAT (52X,17H DELTA VS Z TABLE)
WRITE (6,22) (DELVSZ(1),I=1,4)
WRITE (6,23) (DELVSZ(1),I=5,NOFZ4)
WRITE (6,23)
WRITE (6,23) (DELVSZ(1),I=NOFZ5,NZTBL)
PIN = P
TIN = T
HIN = H
C1IN = C1
C2IN = C2
C3IN = C3
C4IN = C4
GO TO 111
11 PCHECK = 0.
POLD = PIN
P = PIN*5.
WRITE (6,13) P
13 FORMAT ('1# ////////////// 22X 'PRESSURE HAS GONE NEGATIVE --- RAISE
X INPUT PRESSURE TO P = 'E10.4,' PSIA AND START OVER' )
PIN = P
C1 = C1IN*P/POLD
C2 = C2IN*P/POLD
C3 = C3IN*P/POLD
C4 = C4IN*P/POLD
T = TIN
H = HIN
C1IN = C1
C2IN = C2
C3IN = C3
C4IN = C4
111 CALL ICE (PCHECK)
IF (PCHECK.LT.0.) GO TO 11
CALL ICELIQ (PCHECK)
IF (PCHECK.LT.0.) GO TO 11

```

```
CALL LIQUID (PCHECK)
IF (PCHECK.LT.0.) GO TO 11
CALL LIQVAP (PCHECK)
IF (PCHECK.LT.0.) GO TO 11
CALL VAPOR (PCHECK)
IF (PCHECK.LT.0.) GO TO 11
GO TO 1
10 CONTINUE
WRITE (6,601)
601 FORMAT (///5X,'***** OPERATIONS COMPLETE *****')
STOP
END
```

WIPT FOR ICE

SUBROUTINE ICE (PCHECK)

REAL KC1,KC2,KC3,MBARV,M1,M2,M3,M4,MU1VST,MU1,MU2VST,MU2,MU3VST,
X MU3,MU4VST,MU4,MU,MFRAC1,MFRAC2,MFRAC3,MFRAC4,KP
~~COMMON /BLOCK1/ F,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,~~
X ZCON,ZLND,G,DHCZ,H3,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,
X A,AP,DELTA,C3V,KP,MU,PRIME,Z,IX0,ZETA,ZETA1IN
COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
X ,MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
X CF3VST(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
X (24)

C
C THE NUMBERS 1,2,3,4 IN THE VARIABLE NAMES REFER TO H2, O2, H2O,
C AND H₂O₂ RESPECTIVELY
C

WRITE (0,100)

~~100 FORMAT (11,41X, '***** ICE REGION *****')~~

~~X**' ///~~

LFLAG = 0

Z = 0.

AT = 1.0

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)

WRITE (0,300)

WRITE (0,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4

1 CALL UNBAR (AVSZ,1,Z,0.,A,KK)

~~CALL UNBAR (APVSZ,1,T,0.,AP,KK)~~

CALL UNBAR (DELVSZ,1,2,0.,DELTA,KK)

CALL UNBAR (HRVST,1,T,0.,HR,KK)

CALL UNBAR (MU1VST,1,T,0.,MU1,KK)

CALL UNBAR (MU2VST,1,T,0.,MU2,KK)

CALL UNBAR (MU3VST,1,T,0.,MU3,KK)

~~CALL UNBAR (MU4VST,1,T,0.,MU4,KK)~~

CALL UNBAR (CF1VST,1,T,0.,CF1,KK)

CALL UNBAR (CF2VST,1,T,0.,CF2,KK)

CALL UNBAR (CF3ST,1,1,0.,CF3S,KK)

CF3 = CF3S

CALL UNBAR (CF4VST,1,T,0.,CF4,KK)

~~RHO = C1+C2+C3+C4~~

RHOV = C1+C2+C4

SUMV = C1/M1+C2/M2+C4/M4

MU = (MU1*C1/M1+MU2*(C2/M2+MU4*C4/M4))/SUMV

MBARV = RHOV/(C1/M1+C2/M2+C4/M4)

CFBAR = (CF1*C1+CF2*C2+CF3*C3+CF4*C4)/RHO

~~CALL SUBAD (RHO,KC1,KC2,KC3,HG,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,~~

~~X CFCAR)~~

IF (1105.-TPS) 11,03,33

33 CALL UNBAR (VPVST,1,TPS,0.,VF,KK)

TEST = CFS3V*KR*TPS/M3

IF (VP-TEST) 12,11,11

~~12 WRITE (0,200)~~

200 FORMAT (///20X,'***** WATER HAS CONDENSED OR FROZEN IN THE CATALY
XST PARTICLE ... PROGRAM STOP FOLLOWS *****')

CALL EXIT

11 CONTINUE

CALL UNBAR (DHCVST,1,T,0.,DELLHC,KK)

RHOV = 0.

```

DW1DZ = -(RHO1*DELTA+KC1*AP*CICP1)/G
DW2DZ = -(RHO1*DELTA*M2/(2.*M1)+KC2*AP*CICP2)/G
DW3DZ = -(RHO1*DELTA*M3/M1-KC3V*AP*CICP3V)/G
DW4DZ = 0.
DHDZ = -((TK*RHO1*DELTA+HC*AP*TIPT)+(KC3V*AP*CICP3V*(DELHF+DELHC))
^
)/G
DELTZ = ZCON/DHDZ
ZTEST = ZEND/10.
IF (DELTZ.GT.ZTEST) DELTZ = ZTEST
DUDZ = DFDL/CFBAR
DMBRDZ = (-MBAKV)*((DW1DZ/M1+DW2DZ/M2+DW4DZ/M4)/(W1/M1+W2/M2+W4/M4
^
))
DPDZ = ((DELTA-1.)/DELTA**5)*(1.75+(75.*MU*(1.-DELTA))/(A*G))*(G**
^
2./104.4*A*RHO)
DPDZ = DPDZ*AF/144.
W1 = C1/RHO
W2 = C2/RHO
W3 = C3/RHO
W4 = C4/RHO
DRHODZ = (RHO/(1.-W3))*(DW3DZ+RHOV/RHO*(1./P*DPDZ+1./MBAKV*DMBRDZ-
^
1./F*DTDZ))
RHOFAC = (-1./(1.-W3))*(DW3DZ+RHOV/RHO*(1./P*DPDZ+1./MBAKV*DMBRDZ
^
-1./F*DTDZ))
DRHODZ = DRHODZ*((1.-EXP(-RHOFAC*DELTZ))/(RHOFAC*DELTZ))
DC1DZ = RHO*DW1DZ+W1*DRHODZ
DC2DZ = RHO*DW2DZ+W2*DRHODZ
DC3DZ = RHO*DW3DZ+W3*DRHODZ
DC4DZ = W4*DRHODZ
C1P = C1
C2P = C2
C3P = C3
C4P = C4
T1 = T
HP = H
ZF = Z
PP = P
20 C1 = C1+DC1DZ*DELTZ
C2 = C2+DC2DZ*DELTZ
C3 = C3+DC3DZ*DELTZ
C4 = C4+DC4DZ*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)
H = H+DHDZ*DELTZ
MFRAC4 = C4/M4/(C1/M1+C2/M2+C3/M3+C4/M4)
Z = Z+DELTZ
P = P+DPDZ*DELTZ
IF (P) 100,107,107
107 IF (LFLAG.EQ.1) GO TO 50
T = T+DUDZ*DELTZ
IF (C1.LT.0..OR.C2.LT.0..OR.C4.LT.0.) GO TO 50
IF (Z.GT.ZEND) GO TO 99
IF (TS=1) GO TO 40
40 WRITE (0,300)
300 FORMAT (///11X,'Z',9X,'TEMP',9X,'C1',10X,'C2',10X,'C3',10X,'C4',8X
^
,'MFRAC1',5X,'MFRAC2',5X,'MFRAC3',5X,'MFRAC4')
WRITE (0,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
400 FORMAT (//5X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,
^
E10.5,2X,E10.5,2X,E10.5,2X,E10.5)

```

```

WRITE (6,1111) H,P
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) 2,2,3
2 MFRAC1 = 0.
3 IF (C2) 4,4,5
4 MFRAC2 = 0.
5 IF (C4) 6,6,7
6 MFRAC4 = 0.
7 WRITE (6,300)
WRITE (6,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
WRITE (6,1111) H,P
IF (C1*C2) 53,53,54
54 RETURN
53 WRITE (6,50)
56 FORMAT (/758X,'16M THAT'S ALL FOLKS -)
CALL EXIT
60 DELT2 = (15-T)/DTDZ
C1 = C1P
C2 = C2P
C3 = C3P
C4 = C4P
T = TP
H = HP
Z = ZP
P = PP
LFLAG = 1
GO TO 20
136 PCHECK = -1.
RETURN
99 WRITE (6,90)
98 FORMAT (/10X,'AXIAL INCREMENTS HAVE EXCEEDED BED LENGTH')
CALL EXIT
END
WIPI FOR ICELIQ

```


SUBROUTINE ICELIQ (PCHECK)

```

REAL KC1,KC2,KC3V,MBARV,M1,M2,M3,M4,MU1VST,MU1,MU2VST,MU2,MU3VST,
X MU3,MU4VST,MU4,MU,MFRAC1,MFRAC2,MFRAC4,KP
COMMON /BLOCK1/ G,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,
X ZCON,ZEND,G,DHDZ,W3,CF3L,K,DELHF,ALPHA,AGM,AEXP,BEXP,
X A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETA1N
COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
X MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
X CF3V(34),CF3S(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
X (24)

```

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

WRITE (6,100)

100 FORMAT (11,3BX '***** ICE-LIQUID REGION *****')

X '***** / / /')

LFLAG = 0

HS = H

C3S = C3

W3S = W3

C3L = 0.

AP = 1.0

```

1 CALL UNBAR (AVSZ,1,2,0.,A,KK)
CALL UNBAR (APVSZ,1,2,0.,AP,KK)
CALL UNBAR (DELVSZ,1,2,0.,DELTA,KK)
CALL UNBAR (HRVST,1,1,0.,H,K,KK)
CALL UNBAR (MU1VST,1,T,0.,MU1,KK)
CALL UNBAR (MU2VST,1,T,0.,MU2,KK)
CALL UNBAR (MU3VST,1,T,0.,MU3,KK)
CALL UNBAR (MU4VST,1,T,0.,MU4,KK)
CALL UNBAR (CF1VST,1,T,0.,CF1,KK)
CALL UNBAR (CF2VST,1,T,0.,CF2,KK)
CALL UNBAR (CF3S,1,T,0.,CF3S,KK)
CALL UNBAR (CF4VST,1,T,0.,CF4,KK)

```

RHO = C1+C2+C3+C4

RHOV = C1+C2+C4

SUMV = C1/M1+C2/M2+C4/M4

MU = (MU1*C1/M1+MU2*C2/M2+MU4*C4/M4)/SUMV

MBARV = RHOV/(C1/M1+C2/M2+C4/M4)

CFBAR = (CF1*C1+CF2*C2+CF3S*C3S+CF3L*C3L+CF4*C4)/RHO

```

CALL SGRA (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,
X CFBAR)

```

IF (1105.-TPS) 11,33,33

```

33 CALL UNBAR (VPVST,1,TPS,0.,VP,KK)
TEST = CPS3V*R*TPS/M3
IF (VP-TEST) 12,11,11

```

12 WRITE (6,200)

200 FORMAT (//20X,'***** WATER HAS CONDENSED OR FROZEN IN THE CATALY
AST PARTICLE ... PROGRAM STOP FOLLOWS *****')

CALL EXIT

11 CONTINUE

```

CALL UNBAR (DHCVST,1,T,0.,DELHC,KK)

```

RHOM = 0.

HSL = H+DELHF*W3S

DW1DZ = -(RHOM*DELTA+KC1*AP*CICP1)/G

DW2DZ = -(RHOM*DELTA+M2/(2.*M1)+KC2*AP*CICP2)/G

DW3DZ = (RHOM*DELTA*M3/M1-KC3V*AP*CICP3V)/G

DW4DZ = 0.

```

DW3SDZ = DW3SDZ*((HSL-H)/(HSL-HS)-(1./(HSL-HS)*DHDZ))
DW3LDZ = DW3LDZ*((H-HS)/(HSL-HS)+(1./(HSL-HS)*DHDZ))
DHDZ = -((HR*RHOM*DELTA*HC*AP*TI*TP)+(KC3V*AP*E1CP3V*(DELHC+DELHF*
X ((H-HS)/(HSL-HS)))))/G
DELTAZ = ZCON/DHDZ
ZTEST = ZEND/10.
IF (DELTAZ.GT.ZTEST) DELTAZ = ZTEST
DMBRDZ = (-MBAKV)*((DW1DZ/M1+DW2DZ/M2+DW4DZ/M4)/(W1/M1+W2/M2+W4/M4
X ))
DPDZ = ((DELTA-1.)/DELTA**3)*(1.75+(75.*MU*(1.-DELTA))/(A*G))*(G**
X 2./(04.4*A*RHG))
DPDZ = DPDZ*AF/144.
W1 = C1/RHO
W2 = C2/RHO
W3S = C3S/RHO
W3L = C3L/RHO
W4 = C4/RHO
DRHODZ = (RHO/(1.-W3S-W3L))*(DW3SDZ+DW3LDZ+RHOV/RHO*(1./P*DPDZ+1./
A MBAKV*DMBRDZ))
RHOFAC = (-1./(1.-W3S-W3L))*(DW3SDZ+DW3LDZ+RHOV/RHO*(1./P*DPDZ+1./
A MBAKV*DMBRDZ))
DRHODZ = DRHODZ*((1.-EXP(-RHOFAC*DELTAZ))/(RHOFAC*DELTAZ))
DC1DZ = RHO*DW1DZ+W1*DRHODZ
DC2DZ = RHO*DW2DZ+W2*DRHODZ
DC3SDZ = RHO*DW3SDZ+W3S*DRHODZ
DC3LDZ = RHO*DW3LDZ+W3L*DRHODZ
DC4DZ = W4*DRHODZ
C1P = C1
C2P = C2
C3SP = C3S
C3LP = C3L
C4P = C4
HP = H
ZP = Z
PP = P
20 C1 = C1+DC1DZ*DELTAZ
C2 = C2+DC2DZ*DELTAZ
C3L = C3L+DC3LDZ*DELTAZ
C4 = C4+DC4DZ*DELTAZ
MFRAC1 = C1/M1/(C1/M1+C2/M2+C3/M3+C4/M4)
MFRAC2 = C2/M2/(C1/M1+C2/M2+C3/M3+C4/M4)
FRAC3L = C3L/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
MFRAC4 = C4/M4/(C1/M1+C2/M2+C3/M3+C4/M4)
H = H+DMDZ*DELTAZ
Z = Z+DELTAZ
P = P+DPDZ*DELTAZ
IF (P) 136,137,137
137 IF (LFLAG.EQ.1) GO TO 50
C3S = C3S+DC3SDZ*DELTAZ
FRAC3S = C3S/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
C3 = C3S+C3L
IF (C1.LT.U..OR.C2.LT.U..OR.C4.LT.U.) GO TO 50
IF (Z.GT.ZEND) GO TO 99
IF (C3S) 00,50,40
40 WRITE (0,300)
300 FORMAT (///11X,'Z',9X,'TEMP',11X,'C1',10X,'C2',10X,'C3S',9X,'C3L',
A9X,'C4')
WRITE (0,400) Z,T,C1,C2,C3S,C3L,C4
400 FORMAT (10X,E10.5,2X,E10.5,4X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,

```

```

x E10.5//)
WRITE (6,500)
500 FORMAT (34X,'MFRAC1',6X,'MFRAC2',6X,'MFRAC3S',5X,'MFRAC3L',5X,'MFR
AC4')
WRITE (6,600) MFRAC1,MFRAC2,FRAC3S,FRAC3L,MFRAC4
600 FORMAT (32X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5/)
WRITE (6,1111) H,P
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) 2,2,3
2 MFRAC1 = 0.
3 IF (C2) 4,4,5
4 MFRAC2 = 0.
5 IF (C4) 6,6,7
6 MFRAC4 = 0.
7 WRITE (6,300)
WRITE (6,400) Z,T,C1,C2,C3S,C3L,C4
C3 = C3S+C3L
FRAC3S = C3S/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
WRITE (6,500)
WRITE (6,600) MFRAC1,MFRAC2,FRAC3S,FRAC3L,MFRAC4
WRITE (6,1111) H,P
IF (C1*C2) 53,53,54
54 RETURN
53 WRITE (6,50)
50 FORMAT (/7,58X,'***** ALL FOLKS *****')
CALL EX11
60 DELT2 = -C3SP/DC350Z
C3S = 0.
C1 = C1P
C2 = C2P
C3L = C3LP
C4 = C4P
H = HP
Z = ZP
P = PP
LFLAG = 1
GO TO 20
106 PCHECK = -1.
RETURN
99 WRITE (6,90)
90 FORMAT ('0' // 45X 'AXIAL INCREMENTS HAVE EXCEEDED BED LENGTH')
CALL EX11
END

```

WIPT FOR LIQUID

SUBROUTINE LIQUID (PCHECK)

REAL KC1,KC2,KC3V,MBARV,M1,M2,M3,M4,MU1VST,MU1,MU2VST,MU2,MU3VST,
A MU3,MU4VST,MU4,MU,MFRAC1,MFRAC2,MFRAC3,MFRAC4,KP
~~COMMON /BLOCK1/ F,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,~~
X ZCON,ZEND,G,DHDZ,G3,CF3L,K,DELHF,ALPHA,AGM,AEXP,BEXP,
X A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETA1N
COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
X ,MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
X CF3V(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
X (24)

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

WRITE (0,100)

~~100 FORMAT ('I=39X ***** LIQUID REGION *****')~~

~~A***** ///~~

LFLAG = 0

AF = 1.0

CALL UNBAR (TVSVP,1,T,U,TL,KK)

1 CALL UNBAR (AVSZ,1,Z,0,AP,KK)

~~CALL UNBAR (APVSZ,1,Z,0,AP,KK)~~

CALL UNBAR (DELVSZ,1,Z,0,DELTA,KK)

CALL UNBAR (HRVST,1,T,U,HR,KK)

CALL UNBAR (MU1VST,1,T,U,MU1,KK)

CALL UNBAR (MU2VST,1,T,U,MU2,KK)

CALL UNBAR (MU3VST,1,T,U,MU3,KK)

~~CALL UNBAR (MU4VST,1,T,U,MU4,KK)~~

CALL UNBAR (CF1VST,1,T,U,CF1,KK)

CALL UNBAR (CF2VST,1,T,U,CF2,KK)

CALL UNBAR (CF4VST,1,T,U,CF4,KK)

CF3 = CF3L

RHO = C1+C2+C3+C4

~~RHOV = C1+C2+C4~~

SUMV = C1/M1+C2/M2+C4/M4

MU = (MU1*C1/M1+MU2*C2/M2+MU4*C4/M4)/SUMV

MBARV = RHOV/(C1/M1+C2/M2+C4/M4)

CFBAR = (CF1*C1+CF2*C2+CF3*C3+CF4*C4)/RHO

CALL SUBAU (RHO,KC1,C2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,
X CFBAR)

IF (1105.-TPS) 11,00,33

33 CALL UNBAR (VPVST,1,TPS,0,VP,KK)

TLST = CPS3V*R*TPS/M3

IF (VP-TEST) 12,11,11

12 WRITE (0,200)

~~200 FORMAT ('//20X ***** WATER HAS CONDENSED OR FROZEN IN THE CATALY
ST PARTICLE ... PROGRAM STOP FOLLOWS *****')~~

CALL EXIT

11 CONTINUE

CALL UNBAR (DHCVST,1,T,U,DELHC,KK)

RHOM = 0.

~~DW1UZ = -(RHOM*DELTA+KC1*AP*CICP1)/G~~

~~DW2UZ = -(RHOM*DELTA*M2/(2.*M1)+KC2*AP*CICP2)/G~~

~~DW3UZ = (RHOM*DELTA*M3/M1-KC3V*AP*CICP3V)/G~~

~~DW4UZ = 0.~~

~~DHDZ = -(HR*RHOM*DELTA+HC*AP*TITP)+(KC3V*AP*CICP3V*DELHC)/G~~

~~DELTA = ZCON/DHDZ~~

~~ZTEST = ZEND/10.~~

```

IF (DELTA.GT.ZTEST) DELTA = ZTEST
DTDZ = DHDZ/CFBAR
DMBRDZ = (-MBARV)*((DW1DZ/M1+DW2DZ/M2+DW4DZ/M4)/(W1/M1+W2/M2+W4/M4
^
^
DPDZ = ((DELTA-1.)/DELTA**3)*(1.75+(75.*MU*(1.-DELTA))/(A*G))*(G**
^
^
2./(6+.4*A*KHC))
DPDZ = DPDZ*AF/144.
P = P+DPDZ*DELTA
IF (P) 130,137,137
137 W1 = C1/RHO
W2 = C2/RHO
W3 = C3/RHO
W4 = C4/RHO
DRHODZ = (RHO/(1.-n3))*(DW3DZ+RHOV/RHO*(1./P*DPDZ+1./MBARV*DMBRDZ-
^
^
1./T*DTDZ))
RHOFAC = (-1./(1.-n3))*(DW3DZ+RHOV/RHO*(1./P*DPDZ+1./MBARV*DMBRDZ
^
^
-1./T*DTDZ))
DRHODZ = DRHODZ*((1.-EXP(-RHOFAC*DELTA))/(RHOFAC*DELTA))
DC1DZ = RHO*DW1DZ+n1*DRHODZ
DC2DZ = RHO*DW2DZ+n2*DRHODZ
DC3DZ = RHO*DW3DZ+n3*DRHODZ
DC4DZ = W4*DRHODZ
C1P = C1
C2P = C2
C3P = C3
C4P = C4
TT = T
HP = H
ZP = Z
PP = P
20 C1 = C1+DC1DZ*DELTA
C2 = C2+DC2DZ*DELTA
C3 = C3+DC3DZ*DELTA
C4 = C4+DC4DZ*DELTA
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)
H = H+DHDZ*DELTA
Z = Z+DELTA
IF (C1.LT.0..OR.C2.LT.0..OR.C4.LT.0.) GO TO 50
IF (LFLAG.EQ.1) GO TO 50
T = T+DTDZ*DELTA
IF (Z.GT.ZEND) GO TO 99
IF (TL=1) 30,50,40
40 WRITE (0,300)
300 FORMAT (7F7.1X,1Z1.9X,1LE11.9X,1C1.10X,1C2.10X,1C3.10X,1C4.8X,
^
^
X,MFRAC1.5X,MFRAC2.5X,MFRAC3.5X,MFRAC4.5)
WRITE (0,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
400 FORMAT (1/6X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,
^
^
A E10.5,2X,E10.5,2X,E10.5,2X,E10.5)
WRITE (0,1111) H,P
1111 FORMAT (1/10X,'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) 2,2,3
2 MFRAC1 = 0.

```

```

3   IF (C2) 4,4,5
4   MFRAC2 = 0.
5   IF (C4) 6,6,7
6   MFRAC4 = 0.
7   WRITE (6,300)
   WRITE (6,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
   WRITE (6,1111) H,P
   IF (C1*C2) 53,53,54
54  RETURN
53  WRITE (6,50)
56  FORMAT (///50X,16HTHAT'S ALL FOLKS )
   CALL EXIT
60  DELIZ = (FL-TT)/DTDZ
   T = TL
   C1 = C1P
   C2 = C2P
   C3 = C3P
   C4 = C4P
   H = HP
   Z = ZP
   P = PP
   LFLAG = 1
   GO TO 20
130 PCHECK = -1.
   RETURN
99  WRITE (6,90)
90  FORMAT (4'D'//45X 'AXIAL INCREMENTS HAVE EXCEEDED USED LENGTH')
   CALL EXIT
   END

```

```

QIPT FOR LIQVAP
SUBROUTINE LIQVAP (PCHECK)
REAL KC1,KC2,KC3V,MBARV,M1,M2,M3,M4,MU1VST,MU1,MU2VST,MU2,MU3VST,
X MU4VST,MU4,MU3V,MU,MFRAC1,MFRAC2,MFRAC4,KP
COMMON /BLOCK1/ F,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS
X ZCON,ZEND,G,UHDZ,W3,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,
X AP,AP,DELFA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETA1N
COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
X MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
C THE NUMBERS 1,2,3,4 IN THE VARIABLE NAMES REFER TO H2, O2, H2O,
C AND HE RESPECTIVELY
C
X CF3VST(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
C
X (24)
WRITE (0,100)
100 FORMAT ('1-37X ***** LIQUID-VAPOR REGION *****
^*****' ///)
LFLAG = 0
HL = 11
C3V = 0.
C3L = C3
W3L = W3
AF = 1.0
1 CALL UNBAR (AVSZ,1,2,0.,AP,KK)
CALL UNBAR (APVSZ,1,2,0.,AP,KK)
CALL UNBAR (DELVSZ,1,2,0.,DELTA,KK)
CALL UNBAR (HRVST,1,T,0.,HR,KK)
CALL UNBAR (MU1VST,1,T,0.,MU1,KK)
CALL UNBAR (MU2VST,1,T,0.,MU2,KK)
CALL UNBAR (MU3VST,1,T,0.,MU3V,KK)
CALL UNBAR (MU4VST,1,T,0.,MU4,KK)
CALL UNBAR (CF1VST,1,T,0.,CF1,KK)
CALL UNBAR (CF2VST,1,T,0.,CF2,KK)
CALL UNBAR (CF3VST,1,T,0.,CF3V,KK)
CALL UNBAR (CF4VST,1,T,0.,CF4,KK)
RHO = C1+C2+C3+C4
RHOV = C1+C2+C3V+C4
SUMV = C1/M1+C2/M2+C3V/M3+C4/M4
MU = (MU1*C1/M1+MU2*C2/M2+MU3V*C3V/M3+MU4*C4/M4)/SUMV
MBARV = RHOV*(C1/M1+C2/M2+C3V/M3+C4/M4)
CFBAR = (CF1*C1+CF2*C2+CF3L*C3L+CF3V*C3V+CF4*C4)/RHO
CALL SUBRD (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,
X CFBAR)
IF (1100.-TPS) 11,33,33
33 CALL UNBAR (VPVST,1,TPS,0.,VP,KK)
TEST = CPS3V*K*TPS/M3
IF (VP-TEST) 12,11,11
12 WRITE (0,200)
200 FORMAT ('//2UX, ***** WATER HAS CONDENSED OR FROZEN IN THE CATALY
AST PARTICLE .... PROGRAM STOP FOLLOWS *****')
CALL EXIT
11 CONTINUE
CALL UNBAR (DHCVST,1,T,0.,DELHC,KK)
RHOM = 0.
HLV = H+DELHC*W3L
DW1DZ = -(RHOM*DELTA+KC1*AP*CICP1)/G
DW2DZ = -(RHOM*DELTA*M2/(2.*M1)+KC2*AP*CICP2)/G
DW3DZ = -(RHOM*DELTA*M3/M1-KC3V*AP*CICP3V)/G

```

```

DW4DZ = 0
DW3LDZ = DW3DZ*((HLV-H)/(HLV-HL))-(1./(HLV-HL))*DHDZ)
DW3VDZ = DW3DZ*((H-HL)/(HLV-HL))+((1./(HLV-HL))*DHDZ)
DHDZ = -((HK*RHOM*DELTA+HC*AP*TITP)+(KC3V*AP*CICP3V*(DELHC*((H-HL)
/((HLV-HL)))))/G
DELIZ = ZCON/DHDZ
ZTEST = ZEND/10
IF (DELIZ.GT.ZTEST) DELIZ = ZTEST
DMBRDZ = (-MBARV)*((1-W1DZ/M1+DW2DZ/M2+DW3VDZ/M3+DW4DZ/M4)/(W1/M1+
W2/M2+W3V/M3+W4/M4)
DPDZ = ((DELTA-1.)/DELTA**3)*(1.75+(75.*MU*(1.-DELTA))/(A*6))*(6**
2./(04.4*A*RHO))
DPDZ = DPDZ*AF/144.
W1 = C1/RHO
W2 = C2/RHO
W3L = C3L/RHO
W3V = C3V/RHO
W4 = C4/RHO
DRHODZ = (RHO/(1.-W3L))*((DW3LDZ+RHOU/RHO*(1./P*DPDZ+1./MBARV*
DMBRDZ))
RHOFAC = (-1./(1.-W3L))*((DW3LDZ+RHOU/RHO*(1./P*DPDZ+1./MBARV*
DMBRDZ))
DRHODZ = DRHODZ*((1.-EXP(-RHOFAC*DELIZ))/(RHOFAC*DELIZ))
DC1DZ = RHO*DW1DZ+W1*DRHODZ
DC2DZ = RHO*DW2DZ+W2*DRHODZ
DC3LDZ = RHO*DW3LDZ+W3L*DRHODZ
DC3VDZ = RHO*DW3VDZ+W3V*DRHODZ
DC4DZ = W4*DRHODZ
C1P = C1
C2P = C2
C3LP = C3L
C3VP = C3V
C4P = C4
HP = H
ZP = Z
PP = P
20 C1 = C1+DC1DZ*DELTA
C2 = C2+DC2DZ*DELTA
C3V = C3V+DC3VDZ*DELTA
C4 = C4+DC4DZ*DELTA
MFRAC1 = C1/M1/(C1/M1+C2/M2+C3/M3+C4/M4)
MFRAC2 = C2/M2/(C1/M1+C2/M2+C3/M3+C4/M4)
FRAC3V = C3V/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
MFRAC4 = C4/M4/(C1/M1+C2/M2+C3/M3+C4/M4)
H = H+DHDZ*DELIZ
Z = Z+DELIZ
P = P+DPDZ*DELIZ
IF (P) 136,137,137
137 IF (C1.LT.0..OR.C2.LT.0..OR.C4.LT.0.) GO TO 50
IF (LFLAG.EQ.1) GO TO 50
C3L = C3L+DC3LDZ*DELTA
FRAC3L = C3L/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
C3 = C3L+C3V
IF (Z.GT.ZEND) GO TO 99
IF (C3L) 60,50,40
40 WRITE (0,300)
300 FORMAT (//11X,'Z',9X,'TEMP',11X,'C1',10X,'C2',10X,'C3L',9X,'C3V',
A9X,'C4')
WRITE (0,400) Z,T,1,C2,C3L,C3V,C4

```



```

400  FORMAT (/6X,E10.5,2X,E10.5,4X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,
      XE10.5//)
      WRITE (6,500)
500  FORMAT (34X,'MFRAC1',6X,'MFRAC2',6X,'MFRAC3L',5X,'MFRAC3V',5X,'MFR
      AC4'//)
      WRITE (6,600) MFRAC1,MFRAC2,FRAC3L,FRAC3V,MFRAC4
600  FORMAT (32X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5//)
      WRITE (6,1111) H,P
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) 2,2,3
2  MFRAC1 = 0.
3  IF (C2) 4,4,5
4  MFRAC2 = 0.
5  IF (C4) 6,6,7
6  MFRAC4 = 0.
7  WRITE (6,300)
      WRITE (6,400) Z,T,C1,C2,C3L,C3V,C4
      C3 = C3L+C3V
      FRAC3L = C3L/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
      WRITE (6,500)
      WRITE (6,600) MFRAC1,MFRAC2,FRAC3L,FRAC3V,MFRAC4
      WRITE (6,1111) H,P
      IF (C1*C2) 53,53,54
54  RETURN
53  WRITE (6,50)
56  FORMAT (/7/58X,'BIBBIANAT'S ALL FOLKS ')
      CALL EXIT
60  DELFZ = -C3LP/DC3L0Z
      C3L = 0.
      C1 = C1P
      C2 = C2P
      C3V = C3VP
      C4 = C4P
      H = HP
      Z = ZP
      P = PP
      LFLAG = 1
      GO TO 20
130  PCHECK = -1.
      RETURN
99  WRITE (6,90)
90  FORMAT ('0' // 45X 'AXIAL INCREMENTS HAVE EXCEEDED BED LENGTH')
      CALL EXIT
      END

```

WIPT FOR VAPOR

SUBROUTINE VAPOR (PCHECK)

```
REAL KC1,KC2,KC3V,M1,ARV,M1,M2,M3,M4,MU1VST,MU1,MU2VST,MU2,MU3VST,  
X MU3,MU4VST,MU4,MU,MFRAC1,MFRAC2,MFRAC3,MFRAC4,KP  
COMMON /BLOCK1/ T,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,  
X ZCON,ZEND,G,DHDZ,W3,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,  
X A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETA1N  
COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)  
X MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),  
X CF3VST(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST  
X (24)
```

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

WRITE (6,100)

~~100 FORMAT (1,39X,'***** VAPOR REGION *****'
X '*****' //)~~

LFLAG = 0

NONE = 0

AF = 1.0

EPS = 1. E-5

~~1 CALL UNBAR (AVSZ,1,2,0.,A,KK)~~

CALL UNBAR (APVSZ,1,2,0.,AP,KK)

CALL UNBAR (DELVSZ,1,2,0.,DELTA,KK)

CALL UNBAR (HRVST,1,T,0.,HK,KK)

CALL UNBAR (MU1VST,1,T,0.,MU1,KK)

CALL UNBAR (MU2VST,1,T,0.,MU2,KK)

CALL UNBAR (MU3VST,1,T,0.,MU3,KK)

CALL UNBAR (MU4VST,1,T,0.,MU4,KK)

CALL UNBAR (CF1VST,1,T,0.,CF1,KK)

CALL UNBAR (CF2VST,1,T,0.,CF2,KK)

CALL UNBAR (CF3VST,1,T,0.,CF3V,KK)

CF3 = CF3V

~~CALL UNBAR (CF4VST,1,T,0.,CF4,KK)~~

RHO = C1+C2+C3+C4

RHOV = RHO

SUMV = C1/M1+C2/M2+C3/M3+C4/M4

MU = (MU1*C1/M1+MU2*C2/M2+MU3*C3/M3+MU4*C4/M4)/SUMV

MBARV = RHOV/(C1/M1+C2/M2+C3/M3+C4/M4)

~~CFBAR = (CF1*C1+CF2*C2+CF3*C3+CF4*C4)/RHO~~

IF (NONE.EQ.1) GO TO 22

CALL SGRAU (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,GPS3V,
X CFBAR)

~~22 CALL UNBAR (DHCVST,1,T,0.,DELHC,KK)~~

RHOM = ALPHA*C1**AEXP*C2**BEXP*EXP(-AGM/T)

~~DW1DZ = -(RHOM*DELTA+KC1*AP*CICP1)/G~~

DW2DZ = -(RHOM*DELTA*M2/(2.*M1)+KC2*AP*CICP2)/G

DW3DZ = (RHOM*DELTA*M3/M1-KC3V*AP*CICP3V)/G

DW4DZ = 0.

DHDZ = -(HK*RHOM*DELTA+HC*AP*TITP)/G

IF (NONE.EQ.1) GO TO 23

DELTAZ = ZCON/DHDZ

ZTEST = ZEND/10.

IF (DELTAZ.GT.ZTEST) DELTAZ = ZTEST

~~23 DTDZ = DHDZ/CFBAR~~

DMBRDZ = (-MBARV)*((DW1DZ/M1+DW2DZ/M2+DW3DZ/M3+DW4DZ/M4)/(W1/M1+W2
X /M2+W3/M3+W4/M4))

~~DPDZ = ((DELTA-1.)ZDELTA**3)*(1.75+(75.*MU*(1.-DELTA)))/(A*G))*G**~~

```

      X      2./(04.4*A*RHO)
DPDZ = DPDZ*AF/144.
W1 = C1/RHO
W2 = C2/RHO
W3 = C3/RHO
W4 = C4/RHO
DRHODZ = RHOV*(1./P*DPDZ+1./MBARV*DMBRDZ-1./T*DTDZ)
RHOFAC = -(1./P*DPDZ+1./MBARV*DMBRDZ-1./T*DTDZ)
DRHODZ = DRHODZ*((1.-EXP(-RHOFAC*DELTZ))/(RHOFAC*DELTZ))
DC1DZ = RHO*DW1DZ+W1*DRHODZ
DC2DZ = RHO*DW2DZ+W2*DRHODZ
DC3DZ = RHO*DW3DZ+W3*DRHODZ
DC4DZ = W4*DRHODZ
C1P = C1
C2P = C2
C3P = C3
C4P = C4
TT = T
HP = H
ZP = Z
PP = P
20  C1 = C1+DC1DZ*DELTZ
    C2 = C2+DC2DZ*DELTZ
    C3 = C3+DC3DZ*DELTZ
    C4 = C4+DC4DZ*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.0.) C1=0.
    IF (C2.LT.0.) C2=0.
    IF (C4.LT.0.) C4=0.
    IF (C1) 2,2,3
2   MFRAC1 = 0.
3   IF (C2) 4,4,5
4   MFRAC2 = 0.
5   IF (C4) 6,6,7
6   MFRAC4 = 0.
7   H = H+DHDZ*DELTZ
    T = T+DTDZ*DELTZ
    P = P+DPDZ*DELTZ
    IF (LFLAG.EQ.1) GO TO 40
    IF (P) 136,137,137
137 Z = Z+DELTZ
    IF (NONE.EQ.1) GO TO 40
    IF (C1*C2) 50,50,51
51  IF (ZEND-Z) 60,40,40
40  WRITE (0,300)
300 FORMAT (///11X,'Z',9X,'TEMP',9X,'C1',10X,'C2',10X,'C3',10X,'C4',8X
X,'MFRAC1',6X,'MFRAC2',6X,'MFRAC3',6X,'MFRAC4')
    WRITE (0,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
400 FORMAT (/0X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,
X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5)
    WRITE (0,111) H,P
111 FORMAT(/10X,'H(LNTEMP) = ',E10.5,5X,'PRESSURE = ',E10.5)
    IF (LFLAG.EQ.1) GO TO 54
    IF (ABS(ZEND-Z)-EPS) 54,54,1
50  WRITE (0,300)
    WRITE (0,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4

```

```
WRITE (0,111) H,P
NONE = 1
C1CP1 = 0.
C1CP2 = 0.
C1CP3V = 0.
T1TP = 0.
DELIZ = (ZEND-Z)/10.
60 GO TO 1
DELIZ = ZEND-ZP
Z = ZEND
C1 = C1P
C2 = C2P
C3 = C3P
C4 = C4P
T = T1
H = HP
P = PP
LFLAG = 1
NONE = 1
60 GO TO 20
130 PCHECK = -1.
54 RETURN
END
```

```

QIPT FOR SGRAD
SUBROUTINE SGRAD (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,
  X   CPS3V,CFBAR)
REAL   KC1,KC2,KC3V,M1,M2,M3,M4,MU,K0,KP,KCR,KCP,MR,MP,KGM
COMMON /BLOCK1/ T,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,
  X   ZCON,ZEND,G,DHDZ,W3,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,
  X   A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETA IN
COMMON /BLOCK2/ CONST,PPP,POWERP(2),POWERP(1),KGM(2),PGM(1),
  X   KALPH(2),PALPH(1),KGM,ALPHA,K,NR,NP,DOR(2),DOP(1)
COMMON /BLOCK3/ DUP(2),DUP(1),KCR(2),KCP(1),CPSR(2),CPSP(1),CIR(2)
  X   CIP(1),MK(2),MP(1),PR(2),PP(1),CPXR(2,100),CPXP(1,100),K0,
  X   XUA,GAMMA,BETA,NA1,COEFR(2),COEFP(1),HFACTR,RFACTR
COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
  X   MU2VST(34),MU3VST(34),MU4VST(34),CF1VST(34),CF2VST(34),
  X   CF3VST(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
  X   (24)
COMMON /FLAGS/ MMM,JUU
DIMENSION CPOX(100),PCPOX(100),DX(100),RHET(100),DIR(2),DIP(1),
  X   IPX(100),RGAMMA(2),PGAMMA(1),REXP(2),
  X   IEXP(1),RK0(2),PK0(1),RKUTRM(2),PK0TRM(1)
DIMENSION REACTN(2),PRODUCT(1)
C   DEFINE DF FUNCTION
  DPF(X,Y,Z) = 14.7*(1/2*(1/492.))**1.623*(1.-EXP(-.0672*Z*492./
  X   (14.7*x)))
C   DEFINE KC FUNCTION
  KCF(A,B,C,D,E) = .01*A/B*(C/(B*D))**-.607*(A/(E*C))**-.41
C   DEFINE ANALYTIC INTEGRATION FUNCTIONS FROM INTEGRAL EQUATION
  EVAL1(A,B) = B**3/3.-A**3/3.
  EVAL2(A,B) = B**2/2.-A**2/2.
C   ..... SET INITIAL VALUES OF MISCL. ITEMS .....
  KTEMP = 1
  JUU = 1
  NR = 2
  NP = 1
  CONST = 1.
  PPP = 0.
  KGM = 5000.
  NXU = 0
  ZETA = 1.0
C   ..... SET INITIAL PRODUCT VALUES (H2O) .....
  PRODUCT(1) = 'H2O'
  CIP(1) = C3V
  DUP(1) = D03
  MP(1) = M3
  FP(1) = 0.
  POWERP(1) = 0.
  PGM(1) = 0.
  PALPH(1) = 0.
  COEFP(1) = 1.
  IF (PRIME.EQ.'H2') GO TO 215
C   ..... SET INITIAL REACTANT VALUES FOR CASE WHEN H2 IS PRIME REACTANT .....
C   (PRIME REACTANT = ONE WHICH IS IN SMALLEST SUPPLY)
  REACTN(1) = 'H2'
  REACTN(2) = 'O2'
  CIR(1) = C1
  CIR(2) = C2
  DOR(1) = D01
  DOR(2) = D02
  MK(1) = M1

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```

MR(2) = M2
PR(1) = 1.
PR(2) = 0.8
POWERR(1) = 0.
POWERR(2) = 0.
RGM(1) = 0.
RGM(2) = 0.
RALPH(1) = 0.
RALPH(2) = 0.
COEFR(1) = 1.
COEFR(2) = .5
HFACTR = 1.
RFACTR = 1.
GO TO 210
C ..... SET INITIAL REACTANT VALUES FOR CASE WHEN O2 IS PRIME REACTANT .....
215 CONTINUE
REACTN(1) = 'O2'
REACTN(2) = 'H2'
CIR(1) = C2
CIR(2) = C1
DUR(1) = DU2
DUR(2) = DU1
MR(1) = M2
MR(2) = M1
PR(1) = 0.8
PR(2) = 1.
POWERR(1) = 0.
POWERR(2) = 0.
RGM(1) = 0.
RGM(2) = 0.
RALPH(1) = 0.
RALPH(2) = 0.
COEFR(1) = .5
COEFR(2) = 1.
HFACTR = 0.120
RFACTR = 7.930
210 CONTINUE
C SET INITIAL WEIGHTED AVERAGE FRACTIONS
WAF1 = .8
WAF2 = .2
JWAF = 0
XU = 0.
JXU = 0
C SET UP INITIALIZATION FOR EACH ENTRY TO 'SGRAD'
1 LIFLG = 0
NPART = 50
LPI = 1
IPSP = 0.
C INITIALIZE REACTANT PARAMETERS
DO 110 I=1,NR
DIR(I) = DUR(I)*14.7/P*(T/492.)**1.823
110 CONTINUE
C INITIALIZE PRODUCT PARAMETERS
DIP(1) = DUP(1)*14.7/P*(T/492.)**1.823
112 DO 114 I=1,NR
114 KGR(I) = KCF(G,RHO,MU,DIR(I),AP)
DO 115 I=1,NP
115 KCP(I) = KCF(G,RHO,MU,DIP(I),AP)
HC = .7400*CFBAR*(U/(AP*MU))**-.41

```

```

C
C  INITIALIZATION COMPLETE ... NOW LOCATE SUITABLE X0
C
C  CHOOSE INITIAL VALUE OF CPS FOR KEY PARTICLE REACTANT
3002 CPSR(1) = CIR(1)/50.
      DO 151 I=1,NR
      DPR(1) = DPF(T,DUR(I),P)
      DPRP = DPR(1)
      IF (I.EQ.1) GO TO 151
      QUQA = KCR(1)/KCR(1)
QUQB = COEFR(I)*MR(1)/(COEFR(1)*MR(1))
      CPSR(I) = CIR(1)-(QUQA*QUQB*(CIR(1)-CPSR(1)))
      IF (CPSR(I).LT.0.) CPSR(I)=0.
151  CONTINUE
      DO 152 I=1,NP
      DPP(I) = DPF(T,DUP(I),P)
QUQC = KCR(1)/KCP(1)
      QUQD = COEFP(I)*MP(1)/(COEFP(1)*MR(1))
      CPSP(I) = CIP(1)-(QUQC*QUQD*(CPSR(1)-CIR(1)))
      IF (CPSP(I).LT.0.) CPSP(I)=0.
152  CONTINUE
      CMCPN = CIR(1)-CPSR(1)
CALL UNBAR (HRVST,I,T,0.,HR1,KK)
      HR1 = HR1*HFACTR
      SUM = 0.
680  IF (LP1.EQ.1) GO TO 8.
40   TPSP = TPSP
      TPSP = TPS
6     CONTINUE
      TPS = 1-(SUM+HR1*KCR(1)+(CIR(1)-CPSR(1)))/HC
      IF (TPS.LT.0.) TPS = 1.
      CALL UNBAR (HRVST,I,TPS,0.,HR1,KK)
      HR1 = HR1*HFACTR
      DPR(1) = DPF(TPS,DUR(1),P)
DPR(2) = DPF(TPS,DUR(2),P)
      DPR(1) = DPF(TPS,DUP(1),P)
      DPRP = DPR(1)
      HRP = HR1
      TMTPN = 1-TPS
      UCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
C  RETURN POINT IN ITERATION SCHEME TO OBTAIN X0
01   GAMMA = K0M/TPS
      BETA = -CPSR(1)*HR1+DPR(1)/(KP*TPS)
      KU = ALPHA*EXP(-GAMMA)
C  CALCULATE X0
      XUP = XU
X0 = -A-ZETA+CPSR(1)/UCPDX
      X0A = XU/A
      IF (X0) 11,12,12
11   X0 = 0.
      X0A = 0.
      XUP = 0.
JX0 = JX0+1
      IF (JX0.GT.10) GO TO 120
      GO TO 12
120  CPSR(1) = CIR(1)/(DPR(1)/(A*KCR(1))+1.)
      DO 511 I=1,NR
      IF (I.EQ.1) GO TO 511
QUQA = KCR(1)/KCR(1)

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      QUOB = COEFR(I)*MR(I)/(COEFR(1)*MR(1))
      CPSR(I) = CIR(I)-(QUOA*QUOB*(CIR(1)-CPSR(1)))
      IF (CPSR(I).LT.0.) CPSR(I)=0.
511 CONTINUE
DO 512 I=1,HP
      QUOC = KCR(1)/KCP(1)
      QUOD = COEFP(I)*MP(I)/(COEFR(1)*MR(1))
      CPSP(I) = CIP(I)-(QUOC*QUOD*(CPSR(1)-CIR(1)))
      IF (CPSP(I).LT.0.) CPSP(I)=0.
512 CONTINUE
UCPDX = CIR(1)/A
      TPS = 1-(SUM+HR1*UPR(1)*UCPDX)/HC
      IF (TPS.LT.0.) TPS = 1.
      CALL UQBAR (HRVST,1,TPS,0.,HR1,KK)
      HR1 = HR1*MFACIR
      UPR(1) = UPF(TPS,UPR(1),P)
UPR(2) = UPF(TPS,UPR(2),P)
      DPP(1) = UPF(TPS,DPP(1),P)
      DPA = UPR(1)
      DPRP = UPR(1)
      HRP = HR1
      TMTPN = 1-TPS
GAMMA = KGM/TPS
      BETA = -CPSR(1)*HR1*UPR(1)/(KP*TPS)
      KU = ALPHAK*EXP(-GAMMA)
      WRITE (6,102) LP1,TPS
132 FORMAT (A//37A,'WE HAVE CALCULATED A NEGATIVE X0 DURING ITERATION
XNO',10,' / 39X,'SET X0 = 0. , CALCULATE TPS = ',E11.5,' , AND CONTIN
XUE 1)
      GO TO 101
C INTEGRATE FOR CP EQUATION
12 CONTINUE
      CALL TRAP2 (XOA,1.,NFART,RIESUM)
C MFM IS KHEI INDICATOR FOR CALCULATING CP(X) PROFILE
C MFM=0 IMPLIES CURRENT CP(X) PROFILE O.K.
C MFM=1 IMPLIES CONCENTRATION HAS PENETRATED VERY RAPIDLY THRU CATALYST
C PARTICLES (X0 = 0.)
C MFM=2 IMPLIES CONCENTRATION HAS PENETRATED MORE SLOWLY THRU PARTICLES
C AND A FINER INTEGRATION SUBDIVISION OF THE (X0,A) INTERVAL
C SHOULD BE USED TO OBTAIN CP(X) PROFILE (X0 = 0.)
IF (MFM.EQ.0.) GO TO 15
      GO TO (11,14), MFM
14 NFART = 100
      X0 = 0.
      XOA = 0.
      GO TO 12
C CALCULATE NEW CPS
15 CPSO = CPSR(1)
      CMCPN = CMCPN
      CPSKPP = CPSRP
      CPSRP = CPSCAL
      CPSR(1) = CIR(1)-A*RIESUM/KCR(1)
822 CPSCAL = CPSR(1)
      IF (CPSR(1).LT.0.) CPSR(1)=0.
130 CMCPN = CIR(1)-CPSR(1)
C CALCULATE NEW TP
13 CONTINUE
      GRAD = UCPDX*UPR(1)
TGRAD = HC*(1-TPS)

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```

TPSP = TPSP
TPSP = TPS
TMIP0 = TMIPN
51 CONTINUE
TPS = T - (SUM(HR1*KCR(1)*(CIR(1)-CPSR(1)))/HC
IF (TPS.LT.0.) TPS = 1.
CALL UNBAR (HRVST,1,TPS,0.,HR1,KK)
HR1 = HR1*IFACTR
DPR(1) = DPF(TPS,DUR(1),P)
DPR(2) = DPF(TPS,DUR(2),P)
DPP(1) = DPF(TPS,DUP(1),P)
DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
TMTPN = T-TPS
GAMMA = KG0/TPS
BETA = -CPSR(1)*HR1*LPR(1)/(KP*TPS)
KU = ALPHA0*EXP(-GAMMA)
C TEST TEMPERATURE CONCENTRATION FOR 5% LIMIT
IF (ABS((T-TMIP0)-TMTPN)/TMTPN) = .05) 41,41,817
41 IF (ABS((CMCPO-CMCPN)/CMCPN) = .05) 70,70,817
817 IF (LP1.LT.3) GO TO 46
IF (AMINI(CPSR(1),CPSRP,CPSRPP)-CPSRP) 818,820,818
818 IF (AMAX1(CPSR(1),CPSRP,CPSRPP)-CPSRP) 46,820,46
820 IF (NX0.EQ.1) GO TO 825
NX0 = 1
ZETA = ZETA1N
WRITE (0,825)
825 FORMAT (//5X,'CPSR01 CHANGED DIRECTION -- NEW EQ. FOR CPXF USED')
GO TO 216.
40 CPSR(1) = (CPSR(1)*WAF2+CPS0*WAF1)
IF (CPSR(1).LT.0.) CPSR(1)=0.
IF (NR.EQ.1) GO TO 157
DO 139 I=2,NR
QUOA = KCR(1)/KCR(I)
QUOB = COEFR(1)*MR(1)/(COEFR(I)*MR(I))
CPSR(1) = CIR(1) - (QUOA*QUOB*(CIR(1)-CPSR(1)))
IF (CPSR(1).LT.0.) CPSR(1)=0.
139 CONTINUE
C CALCULATE CPS'S FOR PRODUCTS
157 DO 140 I=1,NP
QUOC = KCR(1)/KCP(I)
QUOD = COEFR(I)*MR(I)/(COEFR(1)*MR(1))
CPSP(I) = CIP(I) - (QUOC*QUOD*(CPSR(1)-CIR(1)))
IF (CPSP(I).LT.0.) CPSP(I)=0.
140 CONTINUE
53 DCPDX = KCR(1)/DPRP*(CIR(1)-CPSR(1))
CMCPN = CIR(1)-CPSR(1)
HR1 = HRP
42 LP1 = LP1+1
IF (LP1-25) 40,40,44
44 CONTINUE
IF (JWAF.GE.1) GO TO 811
WAF1 = WAF1+.1
JWAF = 1
GO TO 815
811 CONTINUE
WAF1 = WAF1+.05
JWAF = 2
GO TO 815
815 IF (WAF1.GT..950) GO TO 99

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      WAF2 = 1.-WAF1
C     NO CONVERGENCE WITH PRESENT WEIGHTED AVERAGE FACTORS FOR X0
C     REPEAT ITERATION PROCEDURE WITH NEW FACTORS
      GO TO 1
99 CONTINUE
810 WRITE (0,90)
98  FORMAT (//15X,'UNABLE TO FIND SUITABLE X0 AFTER 3 TRIES OF 25 I
      ALTERATIONS EACH ... SET CPS = 0. AND CONTINUE')
      CPSR(1) = 0.
      CPSR(2) = CIR(2)-(GUOA*GUOB*(CIR(1)-CPSR(1)))
IF (CPSR(2).LT.0.) CPSR(2) = 0.
      CPSP(1) = CIP(1)-(GUOC*GUOD*(CPSR(1)-CIR(1)))
      IF (CPSP(1).LT.0.) CPSP(1) = 0.
      TPS = 1-(SUM+HR1*KCR(1)*(CIR(1)-CPSR(1)))/HC
      CALL UNBAR (HRVST,1,TPS,0.,HR1,KK)
      HR1 = HR1*FACIR
DPR(1) = DPF(TPS,DUR(1),P)
      DPR(2) = DPF(TPS,DUR(2),P)
      DPP(1) = DPF(TPS,DUP(1),P)
      DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
      GO TO 104
C     SATISFACTORY X0 HAS BEEN FOUND
020 NX0 = 0
70  WRITE (0,10) LP1,X0
10  FORMAT (///40X,'SATISFACTORY X0 FOUND AFTER',I3,' TRIES' /
      X      57X,'X0 =',E12.5)
      IF (NAG.NE.2) GO TO 027
      WRITE (0,020)
020 FORMAT (//5X,'CPSCAL CHANGED DIRECTION USING NEW CPXF EQ. USE
      X X0 FOUND AT THIS POINT')
027  IF (X0A.LT..9995) GO TO 131
      CPSR(1) = 0.
      CPSR(2) = CIR(2)-(GUOA*GUOB*(CIR(1)-CPSR(1)))
      IF (CPSR(2).LT.0.) CPSR(2) = 0.
CPOX(NX1) = 0.
      CPSP(1) = CIP(1)-(GUOC*GUOD*(CPSR(1)-CIR(1)))
      IF (CPSP(1).LT.0.) CPSP(1) = 0.
      TPS = 1-(SUM+HR1*KCR(1)*(CIR(1)-CPSR(1)))/HC
      CALL UNBAR (HRVST,1,TPS,0.,HR1,KK)
      HR1 = HR1*FACIR
DPR(1) = DPF(TPS,DUR(1),P)
      DPR(2) = DPF(TPS,DUR(2),P)
      DPP(1) = DPF(TPS,DUP(1),P)
      DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
      WRITE (0,130)
133  FORMAT (// 30X 'X0/A GREATER THAN .9995 .. SET CPS = 0. AND CONTIN
      ADE' )
C
C     CALCULATE GRADIENT
C
131  IF (CPSR(1)) 134,134,135
134  IF (PRIME.NE.'H2') GO TO 135
CICP1 = CIR(1)
      CICP2 = CIR(2)-CPSR(2)
      KC1 = KCR(1)
      KC2 = KCR(2)
      GO TO 135
135  CICP1 = CIR(2) -CPSR(2)
CICP2 = CL(1)

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      KC1 = KCR(2)
      KC2 = KCR(1)
130  CONTINUE
      C1CP3V = C1P(1)-CPSP(1)
      KC3V = KCP(1)
      TITP = 1-TPS
      WRITE (6,610) C1CP1,C1CF2,C1CP3V,TITP
      RETURN
133  LP2 = 1
      NX = 24
      NX1 = NX+1
      NAM1 = NX-1
      DPA = DPR(1)
      CPXR(1,NX1) = CPSR(1)
291  XOA = X0/A
      V = -KCR(1)/DPR(1)
      INFI = 1
      K = 2
      R1 = 0.
      R2 = 0.
      PS1 = 0.
      PS2 = 0.
      DELXOA = (1.-XOA)/FLOAT(NX)
C   CALCULATE PROFILE CURVES FOR INTEGRAND FUNCTIONS
      XA = XOA
      DO 70 J=1,NX1
C   CP(X/A) IS A LINEAR PROFILE DURING FIRST APPROXIMATION
      IF (LP2.GT.1) GO TO 664
C   CALCULATE CP(X) FOR KEY PARTICLE REACTANT
      CPXR(1,J) = ((XA-XOA)/(1.-XOA))**ZETA*CPXR(1,NX1)
      IF (CPXR(1,J).LT.0.) CPXR(1,J)=0.
C   CALCULATE CPS'S FOR REMAINING REACTANTS
664  IF (NR.EQ.1) GO TO 158
      DO 141 I=2,NR
QUO1 = DPR(I)/DPR(1)
      QUO2 = COEFR(I)*MR(I)/(COEFR(1)*MR(1))
      CPXR(1,J) = CPSR(1) + QUO1*QUO2*(CPXR(1,J)-CPXR(1,NX1))
      IF (CPXR(1,J).LT.0.) CPXR(1,J)=0.
141  CONTINUE
C   CALCULATE CPS'S FOR PRODUCTS
158  DO 142 I=1,NR
      QUO3 = DPR(1)/DPP(1)
      QUO4 = COEFP(1)*MP(1)/(COEFR(1)*MR(1))
      CPXP(1,J) = CPSP(1) + QUO3*QUO4*(CPXR(1,NX1)-CPXR(1,J))
      IF (CPXP(1,J).LT.0.) CPXP(1,J)=0.
142  CONTINUE
      QUO1A = 1.
      QUO1B = 1.
      DO 143 I=1,NR
      POWA = CPXR(1,J)**MR(I)
      QUO1A = QUO1A*POWA
143  CONTINUE
DO 144 I=1,NR
      IF (PP(I)) 1000,1001,1000
1000  POWB = CPXP(1,J)**MP(I)
      GO TO 1002
1001  POWB = 1.
1002  QUO1B = QUO1B*POWB
144  CONTINUE

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C   CALCULATE GENERALIZING TERM ---- (ABSORPTION)
      SUMTRM = 0.
      SMTERM = 0.
      CONNUM = BETA*(1.-CPXR(1,J)/CIR(1))
      CONDEN = 1.+BETA*(1.-CPXR(1,J)/CIR(1))
      DO 606 I=1,NR
      RGAMMA(I) = RGM(I)/T
      REXP(I) = RGAMMA(I)*CONNUM/CONDEN
      RKU(I) = RALPH(I)*EXP(-RGAMMA(I))
      IF (RKU(I)) 1003,1004,1003
1003 RKUTRM(I) = RKU(I)*CPXR(I,J)**POWERK(I)*EXP(REXP(I))
      GO TO 1007
1004 RKUTRM(I) = 0.
1007 SUMTRM = SUMTRM+RKUTRM(I)
606 CONTINUE
      DO 607 I=1,NP
      PGAMMA(I) = PGM(I)/T
      PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
      PKU(I) = PALPH(I)*EXP(-PGAMMA(I))
      IF (PKU(I)) 1005,1006,1005
1005 PKUTRM(I) = PKU(I)+CPXR(I,J)**POWERP(I)*EXP(PEXP(I))
      GO TO 1008
1006 PKUTRM(I) = 0.
1008 SMTERM = SMTERM+PKUTRM(I)
607 CONTINUE
      ADSORB = (CONST+SUMTRM+SMTERM)**PPP
      GENERE = 1./ADSORB
      RHET(J) = X0*QUOTA*QUOTB*EXP(GAMMA*BETA*(1.-CPXR(1,J)/CPXR(1,NX1))
      /((1.+BETA*(1.-CPXR(1,J)/CPXR(1,NX1))))
      RHET(J) = RHET(J)*GENERE
      RHET(J) = RHET(J)*RFACFR
      DX(J) = XA
      XA = XA+DELXOA
770 CONTINUE
C   TAKE INTERVAL FUNCTION MIDPTS AS CONSTANT VALUE FOR CP(X/A) AND RHET
      DO 771 J=1,NX
      CPXR(1,J) = (CPXR(1,J)+CPXR(1,J+1))/2.
      RHET(J) = (RHET(J)+RHET(J+1))/2.
771 CONTINUE
      XA = X0A+DELXOA
      CTRM = (A*V+1.)/(A*V)
C   INTEGRAL EQUATION FOLLOWS
C   CPOX(1) IS SPECIAL CASE ... X=X0
      DXL = X0A
      DXU = DXL+DELXOA
      RR1 = 0.
DO 377 I=1,NX
      RR1 = RR1+RHET(I)*(EVAL2(DXL,DXU)-CTRM*EVAL1(DXL,DXU))
      DXL = DXU
      DXU = DXU+DELXOA
377 CONTINUE
      CPOX(1) = CIR(1)-A*A/DPI(1)*RR1
IF (CPOX(1).LT.0.) CPOX(1)=0.
C   SOLVE GENERAL EQUATION OF TWO INTEGRALS FOR CP(X/A)
769 DO 772 I=1,NH1
      RI = RI+RHET(I)*EVAL1(X0A,XA)
      X0A = XA
      XA = XA+DELXOA
772 CONTINUE

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R1 = R1*(1./XOA-CIRM)
XAD = XA
XA = XA-DELXOA
DO 773 I=INI1,NAM1
PS1 = PS1+RHET(I+1)*EVAL2(XA,XAD)
PS2 = PS2+RHET(I+1)*EVAL1(XA,XAD)
XA = XAU
XAD = XAD+DELXOA
773 CONTINUE
R2 = PS1-CIRM*PS2
INI1 = INI1+1
CPOX(K) = CIRM(1)-A*A/DPK(1)*(R1+R2)
IF (CPOX(K).LT.U.) CPOX(K)=U.
XOA = XU/A
XA = XOA+DELXOA
K = K+1
K1 = U.
K2 = U.
PS1 = U.
PS2 = U.
IF (K.LE.NX) GO TO 769
C CPOX(NX1) IS SPECIAL CASE ... X=A
DXL = XOA
DXU = DXL+DELXOA
KR2 = U.
DO 578 I=1,NX
RR2 = KR2+RHET(I)*EVAL1(DXL,DXU)
DXL = DXU
DXU = DXU+DELXOA
578 CONTINUE
CPOX(NX1) = CIRM(1)-A*A/UPR(1)*(1.-CIRM)*RR2
IF (CPOX(NX1)) 190,190,191
190 CPOX(NX1) = 0.
CPSR(1) = U.
CPSR(2) = CIRM(2)-(QU(A+QUO)*CIRM(1)-CPSR(1))
IF (CPSR(2).LT.U.) CPSR(2) = 0.
CPSP(1) = CIP(1)-(QU(C*QUO)*CPSR(1)-CIRM(1))
IF (CPSP(1).LT.U.) CPSP(1) = 0.
TPS = 1-(SUM+HR1*ACR(1)*(CIRM(1)-CPSR(1)))/HC
CALL UNBAR (HRVST,1,TPS,U.,HR1,KK)
HR1 = HR1*HFACIR
DPR(1) = DPF(TPS,DUR(1),P)
DPR(2) = DPF(TPS,DUR(2),P)
DPP(1) = DPF(TPS,DUP(1),P)
UCPX = KCR(1)/DPR(1)*(CIRM(1)-CPSR(1))
WRITE (6,192)
192 FORMAT (//10X,CONCENTRATIONS CALCULATED FROM INTEGRATION SECTION IN
NEGATIVE OR ZERO ... SET CPS = U. AND CONTINUE)
GO TO 194
C CALCULATE A NEW TPS
191 CONTINUE
HRP = HR1
DPRP = DPR(1)
TPS = 1-(SUM+HR1*KCR(1)*(CIRM(1)-CPSR(1)))/HC
IF (TPS.LT.U.) TPS = 1.
CALL UNBAR (HRVST,1,TPS,U.,HR1,KK)
HR1 = HR1*HFACIR
DPR(1) = DPF(TPS,DUR(1),P)
DPR(2) = DPF(TPS,DUR(2),P)

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DPP(1) = DPF(TPS,DUP(1),P)
DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
TMFPO = TMFPI
TMFPI = T-TPS
C TWO PASSES NEEDED BEFORE CHECK ON TEMP, CONC CAN BE MADE
33 IF (LP2.EQ.1) GO TO 27
CMCPO = CMCPH
CMCPN = CIR(1)-CPOX(1,NX1)
IF (ABS(TMFP0-TMFPI)/TMFPI - .05) 26,26,27
26 IF (ABS(CMCPO-CMCPN)/CMCPN - .05) 88,88,27
C
C CALCULATE NEW CPXR(1,I) PROFILE FOR NEXT PASS
C
27 DO 55 I=1,NX1
IF (MOD(LP2,5)) 34,57,34
C CALCULATE WEIGHTED AVERAGE OF OLD AVERAGED AND CALCULATED PROFILES
34 CPXR(1,I) = .8*CPXR(1,I)+.2*CPOX(I)
GO TO 50
C AVERAGE PRESENT AND PAST CALCULATED PROFILES EVERY 5TH PASS TO SMOOTH
57 CPOX(1) = (CPOX(1)+PCPOX(1))/2.
C STORE PRESENT CALCULATED PROFILE
50 PCPOX(1) = CPOX(1)
55 CONTINUE
CMCPH = CIR(1)-CPXR(1,NX1)
TPS = T-(SUM+HR1*KCR(1)*(CIR(1)-CPSR(1)))/HC
IF (TPS.LT.0.) TPS = 1.
CALL UNOAR (HRVST,1,TPS,0.,HR1,KK)
HR1 = HR1*IFACTR
DPR(1) = DPF(TPS,DUR(1),P)
DPR(2) = DPF(TPS,DUR(2),P)
DPP(1) = DPF(TPS,DUP(1),P)
DCPDX = KCR(1)/DPRP*(CIR(1)-CPXR(1,NX1))
TMFPO = TMFPI
TMFPI = T-TPS
LP2 = LP2+1
IF (LP2-50) 29,29,50
30 WRITE (6,10) CPOX(NX1)
10 FORMAT (//51X,52HUNABLE TO CONVERGE ON CPS IN 50 TRIES ... CP(X/
XA) =E12.5)
WRITE (6,83) GRAD,IGRAD
GO TO 26
29 GAMMA = KGR/TPS
BETA = -CPXR(1,NX1)*HR1*DPR(1)/(KP*TPS)
KU = ALPHA*K*EXP(-GAMMA)
DO 752 I=2,NR
QUOA = KCR(1)/KCR(I)
QUOB = COEFF(1)*MR(1)/(COEFF(1)*MR(I))
CPSR(1) = CIR(1)-(QUOA*QUOB*(CIR(1)-CPXR(1,NX1)))
IF (CPSR(1).LT.0.) CPSR(I)=0.
752 CONTINUE
DO 753 I=1,NP
QUOC = KCR(1)/KCP(1)
QUOD = COEFF(1)*P(I)/(COEFF(1)*MR(1))
CPS(1) = CIP(1)-(QUOC*QUOD*(CPXR(1,NX1)-CIR(1)))
753 CONTINUE
GO TO 291
88 DO 180 I=1,NX1
TPX(I) = TPS-HR1*DPR(1)/KP*(CPXR(1,NX1)-CPOX(1))
CPXR(1,I) = CPOX(I)

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180 CONTINUE
WRITE (6,779)
779 FORMAT ('///34X,'REACTANT AND PRODUCT CONCENTRATION PROFILES FOR
X(FINAL ITERATION)')
DO 777 I=1,I
WRITE (6,23) REACTN(I),REACTN(I),REACTN(I),REACTN(I),REACTN(I),
X (UX(I),CPXR(I,J),J=1,NX1)
23 FORMAT ('///11X,'X/A',9X,'CPX',9X,'X/A',9X,'CPX',9X,'X/A',9X,'CPX',
X 9X,'X/A',9X,'CPX',9X,'X/A',9X,'CPX' /
X 21X,A6,4(18X,A6) / (5X,10E12.6) )
777 CONTINUE
WRITE (6,82) LP2,CPOX(NX1)
82 FORMAT ('///41X,34HCONCENTRATION GRADIENT FOUND AFTER,13,6H TRIES /
X 45X,27HC(X) AT PARTICLE SURFACE =,E12.5 )
DCPJDX = DCPDX*UPR(1)
TGRAD = HC*(T-TPS)
WRITE (6,83) DCPDX,TGRAD
83 FORMAT (46X,'KCR(1)*(CIR(1)-CPSR(1)) =',E12.5 / 54X,'HC*(T-TPS) =',
X,E12.5)
WRITE (6,105) DCPDX
105 FORMAT ('50X,'SLOPE =',E12.5)
IF (PRIML.NE.'H2') GO TO 240
CICP1 = CIR(1)-CPXR(1,NX1)
CICP2 = CIR(2)-CPXR(2,NX1)
KC1 = KCR(1)
KC2 = KCR(2)
GO TO 241
240 CICP1 = CIR(2)-CPXR(2,NX1)
CICP2 = CIR(1)-CPXR(1,NX1)
KC1 = KCR(2)
KC2 = KCR(1)
241 CONTINUE
CICP3V = CIF(1) - CPXP(1,NX1)
KC3V = KCP(1)
CPS3V = CPXP(1,NX1)
TITP = 1 - IFS
WRITE (6,810) CICP1,CICP2,CICP3V,TITP
810 FORMAT ('/5X,'C1-CP31 = ',E10.5,10X,'C2-CPS2 = ',E10.5,10X,'C3V-CPS
X3V = ',E10.5,10X,'1-TPS = ',E10.5/)
28 RETURN
END

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DIPT FOR TRAP2
SUBROUTINE TRAP2 (XLOWER,XUPPER,NPART,RIESUM)
C NUMERICAL INTEGRATION USING TRAPEZOIDAL METHOD
C THIS ROUTINE IS USED WHEN CP(X) PROFILE HAS NOT ALREADY BEEN DETERMINED
REAL M1,M2,M3,M4,KU,KP,KGR,KCP,MR,MP,MU
COMMON /BLOCK1/ T,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,
X ZCON,ZEND,G,DHDZ,W3,CF3E,R,DELHF,ALPHA,AGM,AEXP,BEXP,
X A,AP,DELTA,CJV,KP,MU,PRIME,Z,NX0,ZETA,ZETA1N
COMMON /BLOCK2/ CONST,PPP,POWER(2),POWERP(1),RGM(2),PGM(1),
X RALPH(2),PALPH(1),KGM,ALPHAK,NR,NP,DOR(2),DOP(1)
COMMON /BLOCK3/ DPR(2),DPP(1),KGR(2),KCP(1),CPSR(2),CPSP(1),CIR(2),
X CIP(1),MR(2),MP(1),PR(2),PP(1),CPXR(2,100),CPXP(1,100),KU,
X XOA,GAMMA,DELTA,NX1,COEFR(2),COEFP(1),HFACTR,RFACTR
COMMON /FLAGS/ MMM,JJJ
DIMENSION RGGAMMA(2),PGAMMA(1),REXP(2),
X PEXP(1),RKO(2),PKO(1),RKOTRM(2),PKOIRM(1),
X CPXR1(2),CPXR2(2),CPXP1(1),CPXP2(1),CPXRR(2),CPXPP(1)
C DEFINE RHET FUNCTION
RHEIF(A,B,C,D,E,F,G) = A*B*C*EXP(D*E*(1.-F/G)/(1.+E*(1.-F/G)))
C DEFINE INTEGRAND FUNCTION
FOFX(X,R) = X**2*R
C DEFINE CP(X) FUNCTION FOR RHET EQUATION
CPXF(X,Y,Z) = ((X-Y)/(1.-Y))**ZETA*Z
MMM = 0
NM = 25
IF (NPART.LT.100) NM=50
N = NPART-1
PART = NPART
HH = (XUPPER-XLOWER)/PART
XPH = XLOWER+HH
SUM = 0.
C CALCULATE CP(X) FOR KEY PARTICLE REACTANT FOR RHET1 (INITIAL POINT
C OF PROFILE) AND FOR RHET2 (FINAL POINT OF PROFILE)
CPXR1(1) = CPXF(XLOWER,XOA,CPSR(1))
CPXR2(1) = CPXF(XUPPER,XOA,CPSR(1))
IF (CPXR1(1).LT.0.) CPXR1(1)=0.
IF (CPXR2(1).LT.0.) CPXR2(1)=0.
QUO1 = DPR(1)/DPR(2)
QUO2 = COEFR(2)*MR(2)/(COEFR(1)*MR(1))
CPXR1(2) = CPSR(2)+QUO1*QUO2*(CPXR1(1)-CPSR(1))
CPXR2(2) = CPSR(2)+QUO1*QUO2*(CPXR2(1)-CPSR(1))
C CALCULATE CP(X) FOR PARTICLE PRODUCTS
DO 11 I=1,NP
QUO3 = DPR(1)/DPP(1)
QUO4 = COEFP(1)*MP(1)/(COEFR(1)*MR(1))
CPXP1(1) = CPSP(1)+QUO3*QUO4*(CPSR(1)-CPXR1(1))
CPXP2(1) = CPSP(1)+QUO3*QUO4*(CPSR(1)-CPXR2(1))
11 CONTINUE
C CALCULATE RHET FOR INITIAL AND FINAL PTS OF CP(X) PROFILE (RHET1 & RHET2)
QUOTAA = 1.
QUOTAB = 1.
QUOTBA = 1.
QUOTBB = 1.
DO 12 I=1,NR
POWAA = CPXR1(1)**PR(I)
POWAB = CPXR2(1)**PR(I)
QUOTAA = QUOTAA*POWAA
QUOTAB = QUOTAB*POWAB
12 CONTINUE

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DO 13 I=1,NP
POWBA = CPXR1(1)**PP(I)
POWBB = CPXR2(1)**PP(I)
IF (PP(1)) 1000,1001,1000
1001 POWBA = 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 (ADSORPTION)
CONNUM = BETA*(1.-CPXR1(1)/CIR(1))
CONDEN = 1.+BETA*(1.-CPXR1(1)/CIR(1))
DO 606 I=1,NR
RGAMMA(I) = RGM(I)/T
REXP(I) = RGAMMA(I)*CONNUM/CONDEN
RKU(I) = RALPH(I)*EXP(-RGAMMA(I))
IF (CPXR1(1)) 608,608,609
609 RKUTRM(I) = RKU(I)*CPXR1(1)**POWER(I)*EXP(REXP(I))
GO TO 610
608 RKUTRM(I) = 0.
610 SUMTRM = SUMTRM+RKUTRM(I)
606 CONTINUE
* DO 607 I=1,NP
PGAMMA(I) = PGM(I)/T
PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
PKU(I) = PALPH(I)*EXP(-PGAMMA(I))
PKUTRM(I) = PKU(I)*CPXR1(1)**POWER(I)*EXP(PEXP(I))
SMTERM = SMTERM+PKUTRM(I)
607 CONTINUE
ADSORB = (CONST+SUMTRM+SMTERM)**PPP
GENEAL = 1./ADSORB
RHET1 = RHET*(KU,QUOTAA*QUOTBA,GAMMA,BETA,CPXR1(1),CPXR2(1))*
A GENEAL
RHET1 = RHET1*RFACIR
C CALCULATE THE GENERALIZING TERM USED IN RHET (LAST PT OF CPX PROFILE)
SUMTRM = 0.
SMTERM = 0.
C CALCULATE ADSORPTION TERM (DENOMINATOR OF GENERALIZING TERM)
CONNUM = BETA*(1.-CPXR2(1)/CIR(1))
CONDEN = 1.+BETA*(1.-CPXR2(1)/CIR(1))
DO 614 I=1,NR
RGAMMA(I) = RGM(I)/T
REXP(I) = RGAMMA(I)*CONNUM/CONDEN
RKU(I) = RALPH(I)*EXP(-RGAMMA(I))
IF (RKU(I)*CPXR2(1)) 614,614,416
416 RKUTRM(I) = RKU(I)*CPXR2(1)**POWER(I)*EXP(REXP(I))
SUMTRM = SUMTRM+RKUTRM(I)
614 CONTINUE
DO 615 I=1,NP
PGAMMA(I) = PGM(I)/T
PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
PKU(I) = PALPH(I)*EXP(-PGAMMA(I))
PKUTRM(I) = PKU(I)*CPXR2(1)**POWER(I)*EXP(PEXP(I))
SMTERM = SMTERM+PKUTRM(I)
615 CONTINUE
ADSORB = (CONST+SUMTRM+SMTERM)**PPP

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      GENERL = 1./ADSORB
      RHET2 = RHETF(KU,QUOTAB,QUOTBB,GAMMA,BETA,CPXR2(1),CPXR2(1))*
      ^ - - - GENERL
      RHET2 = RHET2*RFAC1R
      IF (RHET2) 77,77,4
77   MMM = 1
      GO TO 99
C
C   BEGIN INTEGRATION USING TRAPEZOIDAL METHOD
C
C   CALCULATE FIRST AND LAST TERMS OF APPROXIMATING SUM FIRST
4    TRM1 = FOFX(XLOWER,RHET1)/2.
      TRM2 = FOFX(XUPPER,RHET2)/2.
40   DO 8 J=1,N
C   CALCULATE CP(X) FOR KEY PARTICLE REACTANTS (TO USE IN RHET TERM)
      CPXRR(1) = CPXF(XPR1,XOA,CPSR(1))
C   CALCULATE CP(X) FOR OTHER REACTANT (TO USE IN RHET)
      CPXRR(2) = CPSR(2)*QUO1*QUO2*(CPXRR(1)-CPSR(1))
C   CALCULATE CP(X) FOR PARTICLE PRODUCTS (TO USE IN RHET)
      DO 15 I=1,NP
      CPXPP(1) = CPSR(1)+QUO3*QUO4*(CPSR(1)-CPXRR(1))
15   CONTINUE
C   CALCULATE RHET EXPRESSION
      QUOTA = 1.
      QUOTB = 1.
      DO 16 I=1,NK
      POWA = CPXRR(I)**PK(I)
      QUOTA = QUOTA*POWA
16   CONTINUE
      DO 17 I=1,NP
      POWB = CPXPP(I)**PP(I)
      IF (PP(I)) 1005,1005,1005
1005 POWB = 1.
1005 QUOTB = QUOTB*POWB
17   CONTINUE
C   CALCULATE GENERALIZING TERM FOR RHET (FOR INTERMEDIATE PTS ON CPX PROFILE)
      SUMTRM = 0.
      SMTERM = 0.
      CONNUM = BETA*(1.-CPXRR(1)/CIR(1))
      CONDEN = 1.+BETA*(1.-CPXRR(1)/CIR(1))
      DO 622 I=1,NK
      RGAMMA(I) = RGM(I)/T
      REXP(I) = RGAMMA(I)*CONNUM/CONDEN
      RKU(I) = RALPH(I)*EXP(-RGAMMA(I))
      RKUTRM(I) = RKU(I)*CPXRR(I)**POWERK(I)*EXP(REXP(I))
      SUMTRM = SUMTRM+RKUTRM(I)
622  CONTINUE
      DO 623 I=1,NP
      PGAMMA(I) = PGM(I)/T
      PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
      PKU(I) = PALPH(I)*EXP(-PGAMMA(I))
      PKUTRM(I) = PKU(I)*CPXPP(I)**POWERP(I)*EXP(PEXP(I))
      SMTERM = SMTERM+PKUTRM(I)
623  CONTINUE
      ADSORB = (CONST+SUMTRM+SMTERM)**PPP
      GENERL = 1./ADSORB
      RHET = RHETF(KU,QUOTA,QUOTB,GAMMA,BETA,CPXRR(1),CPXR2(1))*GENERL
      RHET = RHET*RFAC1R
      IF (J.EQ.N AND RHET.LE.0.) MMM=2

```

```
IF (MMH.NE.2) GO TO 207
IF (J.EQ.NM) JJJ=JJJ+1
IF (JJJ.GT.5) RETURN
207 SUM = SUM+FOFX(XPH,RHET)
200 XPH = XPH+HH
6 CONTINUE
RISUM = HTI*(TRM1+SUM+TRM2)
99 RETURN
END
```

WIPT FOR TABLES

BLOCK DATA

REAL MU1VST, MU2VST, MU3VST, MU4VST

COMMON /TABLES/ AVSZ(99), APVSZ(99), DELVSZ(99), HRVST(36), MU1VST(34)

X MU2VST(34), MU3VST(32), MU4VST(34), CF1VST(34), CF2VST(34),

X CF3VST(34), CF3ST(20), CF4VST(20), VPVST(36), TVSVP(36), DHCVST

X (24)

C

C TABLE OF HEAT OF REACTION W.R.T. H2 VS TEMPERATURE (DEG R)

DATA (HRVST(I), I=1,36) / 0., 1., 16., 0.,

C

TEMPERATURES

X 0. , 180. , 360. , 720. , 1080. , 1440. ,

X 1800. , 2160. , 2520. , 2880. , 3240. , 3600. ,

X 3960. , 4320. , 4680. , 5040. ,

C

HEATS OF REACTION

X -5.096E+4, -5.128E+4, -5.141E+4, -5.182E+4, -5.223E+4, -5.259E+4,

X -5.298E+4, -5.314E+4, -5.333E+4, -5.349E+4, -5.361E+4, -5.370E+4,

X -5.379E+4, -5.386E+4, -5.392E+4, -5.398E+4 /

C

C TABLE OF VAPOR PRESSURE (PSIA) VS TEMPERATURE (DEG R)

DATA (VPVST(I), I=1,36) / 0., 1., 16., 0.,

C

TEMPERATURES

X 513. , 562. , 586. , 622. , 653. , 688. ,

X 727. , 768. , 788. , 818. , 842. , 877. ,

X 905. , 927. , 1005. , 1155. ,

C

PRESSURES

X 0.2 , 1.0 , 2.0 , 5.0 , 10. , 20. ,

X 40. , 75. , 100. , 150. , 200. , 300. ,

X 400. , 500. , 1000. , 3000. /

C

C TABLE OF TEMPERATURE (DEG R) VS VAPOR PRESSURE (PSIA)

DATA (TVSVP(I), I=1,36) / 0., 1., 16., 0.,

C

PRESSURES

X 0.2 , 0.5 , 1.0 , 2.0 , 3.5 , 5.0 ,

X 7.5 , 10. , 15. , 20. , 25. , 30. ,

X 40. , 50. , 75. , 100. ,

C

TEMPERATURES

X 513. , 540. , 562. , 586. , 608. , 622. ,

X 640. , 653. , 673. , 688. , 700. , 710. ,

X 727. , 741. , 768. , 788. /

C

C TABLE OF DELTA HEAT OF CONDENSATION VS TEMPERATURE

DATA (DHCVST(I), I=1,24) / 0., 1., 10., 0.,

C

TEMPERATURES

X 513. , 562. , 586. , 622. , 653. , 688. ,

X 710. , 741. , 768. , 788. ,

C

DELTA HEATS OF CONDENSATION (DHC)

X 1064. , 1036. , 1022. , 1001. , 982. , 960. ,

X 945. , 924. , 904. , 889. /

C

C

C

..... FOUR VISCOSITY TABLES FOLLOW

C TABLE OF H2 VISCOSITY (LB/FT-SEC) VS TEMPERATURE (DEG R)

DATA (MU1VST(I), I=1,34) / 0., 1., 15., 0.,

C

TEMPERATURES

X 180. , 360. , 720. , 1080. , 1440. , 1800. ,

X 2160. , 2520. , 2880. , 3240. , 3600. , 3960. ,

X 4320. , 4680. , 5040. ,

C H2 VISCOSITIES
 X 2.54 E-6, 4.47 E-6, 7.30 E-6, 9.54 E-6, 11.48 E-6, 13.29 E-6,
 X 14.97 E-6, 16.54 E-6, 18.04 E-6, 19.47 E-6, 20.84 E-6, 22.16 E-6,
 X 23.45 E-6, 24.68 E-6, 25.89 E-6/

C TABLE OF O2 VISCOSITY (LB/FT-SEC) VS TEMPERATURE (DEG R)
 DATA (MU2VSI(I), I=1,34) / 0., 1., 15., 0.,

C TEMPERATURES
 X 180., 360., 720., 1080., 1440., 1800.,
 X 2160., 2520., 2880., 3240., 3600., 3960.,
 X 4320., 4680., 5040.,

C O2 VISCOSITIES
 X 5.15 E-6, 9.94 E-6, 17.24 E-6, 22.94 E-6, 27.87 E-6, 32.30 E-6,
 X 36.33 E-6, 40.10 E-6, 43.74 E-6, 47.29 E-6, 50.65 E-6, 53.90 E-6,
 X 57.03 E-6, 60.08 E-6, 63.03 E-6/

C TABLE OF H2O (VAPOR) VISCOSITY (LB/FT-SEC) VS TEMPERATURE (DEG R)
 DATA (MU3VSI(I), I=1,32) / 0., 1., 15., 0.,

C TEMPERATURES
 X 360., 720., 1080., 1440., 1800., 2160.,
 X 2520., 2880., 3240., 3600., 3960., 4320.,
 X 4680., 5040.,

C H2O (VAPOR) VISCOSITIES
 X 5.18 E-6, 9.62 E-6, 14.44 E-6, 19.35 E-6, 24.10 E-6, 28.67 E-6,
 X 32.99 E-6, 37.07 E-6, 40.92 E-6, 44.60 E-6, 48.11 E-6, 51.49 E-6,
 X 54.73 E-6, 57.87 E-6/

C TABLE OF HE VISCOSITY (LB/FT-SEC) VS TEMPERATURE (DEG R)
 DATA (MU4VSI(I), I=1,34) / 0., 1., 15., 0.,

C TEMPERATURES
 X 180., 360., 720., 1080., 1440., 1800.,
 X 2160., 2520., 2880., 3240., 3600., 3960.,
 X 4320., 4680., 5040.,

C HE VISCOSITIES
 X 6.71 E-6, 10.54 E-6, 16.50 E-6, 21.43 E-6, 25.80 E-6, 29.79 E-6,
 X 33.50 E-6, 37.01 E-6, 40.34 E-6, 43.52 E-6, 46.58 E-6, 49.54 E-6,
 X 52.40 E-6, 55.17 E-6, 57.87 E-6/

..... FIVE SPECIFIC HEAT TABLES FOLLOW

C TABLE OF H2 SPECIFIC HEAT (BTU/LB-DEG R) VS TEMPERATURE (DEG R)
 DATA (CF1VSI(I), I=1,34) / 0., 1., 15., 0.,

C TEMPERATURES
 X 900., 1080., 1260., 1440., 1620., 1800.,
 X 2160., 2520., 2880., 3240., 3600., 3960.,
 X 4320., 4680., 5040.,

C SPECIFIC HEATS OF H2
 X 3.467, 3.474, 3.487, 3.509, 3.539, 3.577,
 X 3.670, 3.772, 3.872, 3.966, 4.050, 4.126,
 X 4.193, 4.253, 4.306 /

C TABLE OF O2 SPECIFIC HEAT (BTU/LB-DEG R) VS TEMPERATURE (DEG R)
 DATA (CF2VSI(I), I=1,34) / 0., 1., 15., 0.,

C TEMPERATURES
 X 180., 360., 720., 1080., 1440., 1800.,
 X 2160., 2520., 2880., 3240., 3600., 3960.,
 X 4320., 4680., 5040.,

C SPECIFIC HEATS OF O2

X	.217	, .217	, .224	, .239	, .251	, .260
X	.266	, .270	, .274	, .278	, .281	, .285
X	.288	, .291	, .294	/		

C
C TABLE OF H2O (VAPOR) SPECIFIC HEAT (BTU/LB-DEG R) VS TEMPERATURE
DATA (CF3V1(I), I=1,34) / 0., 1., 15., 0.,

C
TEMPERATURES

X	180.	, 360.	, 720.	, 1080.	, 1440.	, 1800.
X	2160.	, 2520.	, 2880.	, 3240.	, 3600.	, 3960.
X	4320.	, 4680.	, 5040.	/		

C
SPECIFIC HEATS OF H2O (VAPOR)

X	.4400	, .4411	, .453	, .480	, .512	, .546
X	.579	, .609	, .636	, .659	, .678	, .694
X	.709	, .721	, .731	/		

C
C TABLE OF H2O (SOLID) SPECIFIC HEAT VS TEMPERATURE
DATA (CF3ST(I), I=1,16) / 0., 1., 6., 0.,

C
TEMPERATURES

X	200.	, 300.	, 350.	, 400.	, 450.	, 491.4
---	------	--------	--------	--------	--------	---------

C
SPECIFIC HEATS OF H2O (SOLID)

X	.227	, .320	, .367	, .415	, .462	, .502
---	------	--------	--------	--------	--------	--------

C
C TABLE OF HE SPECIFIC HEAT (BTU/LB-DEG R) VS TEMPERATURE (DEG R)
DATA (CF4VST(I), I=1,16) / 0., 1., 6., 0.,

C
TEMPERATURES

X	180.	, 720.	, 1800.	, 2880.	, 3960.	, 5040.
---	------	--------	---------	---------	---------	---------

C
SPECIFIC HEATS OF HELIUM

X	1.24	, 1.24	, 1.24	, 1.24	, 1.24	, 1.24
---	------	--------	--------	--------	--------	--------

END

SUBROUTINE UNBAR (T,IK,XIN,YIN,ZZ,KK) -
 DIMENSION T(1),X(6),Y(6),A(6)

UNBAR002
 UNBAR004
 UNBAR005
 UNBAR006
 UNBAR007
 UNBAR008
 UNBAR009
 UNBAR010
 UNBAR011
 UNBAR012
 UNBAR013
 UNBAR014
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 UNBAR016
 UNBAR017
 UNBAR018
 UNBAR019
 UNBAR020
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 UNBAR052
 UNBAR053
 UNBAR054
 UNBAR055
 UNBAR056
 UNBAR057
 UNBAR058
 UNBAR059
 UNBAR060

```

C ----- MARCH 4, 1961 -----
C ----- MODIFIED 7/62 -----
C ----- TO DO QUADRATIC AND LINEAR INTERPOLATION ALSO -----
C
      II = IK+1
      N = 3
      N2 = 2
      IF (T(II)-3.) 700,701,702
700  IF (T(II)+0.) 60,701,704
704  IF (T(II)-2.) 705,706,701
705  N = 1
      GO TO 707
706  N = 2
707  N2 = 1
701  II = II+1
702  N1 = N + 1
      DO 50 L = 11,II
      IF ( T(L) + 0. ) 60,60,51
50  KK = -1
      ZZ = 0.
      GO TO 9999
51  IX = T(L)
      IF (T(L+1) + 0. ) 60,52,50
52  NY = J
      GO TO 53
50  NY = T(L+1)
53  CONTINUE
      KK = 0
      KY = 0
      XX = X11
      YY = Y11
      J1 = 11+2
      J2 = IX+1,1
      IF(XX-T(J1))301,300,400
400  DO 302 J=J1,J2
      IF (XA-T(J)) 304,304,302
302  CONTINUE
309  KK = 2
      XX = T(J2)
308  JX1 = J2-N
      GO TO 305
301  KK = 1
      XX = T(J1)
306  JX1 = J1
      GO TO 305
304  IF (J-J1-1) 301,300,307
307  IF (J-J2) 303,300,309
303  JX1 = J-N2
305  CONTINUE
      XINT = XX
      IF (NY) 1500, 1500, 3000
1500  DO 1599 L=1,N1
      X(L) = T(JX1)
      LY = JX1 + IX
      Y(L) = T(LY)
1599  JX1 = JX1+1
      I = 1

```

	GO TO 54	UNBAR061
3000	J1 = J1+NX	UNBAR062
	J2 = J2+NY	UNBAR063
	IF (YY-T(J1)) 311,316,401	UNBAR064
401	DO 312 J=J1,J2	UNBAR065
	IF (YY-T(J)) 314,314,312	UNBAR066
312	CONTINUE	UNBAR067
319	KY = 0	UNBAR068
	YY = T(J2)	UNBAR069
318	JY1 = J2-N	UNBAR070
	GO TO 315	UNBAR071
311	KY = 3	UNBAR072
	YY = T(J1)	UNBAR073
316	JY1 = J1	UNBAR074
	GO TO 315	UNBAR075
314	IF (J-J1-1) 311,316,317	UNBAR076
317	IF (J-J2) 313,318,319	UNBAR077
313	JY1 = J-N2	UNBAR078
315	CONTINUE	UNBAR079
	JX2 = JX1	UNBAR080
	LY = JY1 + NY*(JX2-II-1)	UNBAR081
	LY1 = LY	UNBAR082
	DO 3099 L=1,N1	UNBAR083
	X(L) = T(JX2)	UNBAR084
	Y(L) = T(LY1)	UNBAR085
	LY1 = LY1+NY	UNBAR086
3099	JX2 = JX2+1	UNBAR087
	I = 0	UNBAR088
	GO TO 54	UNBAR089
3098	Y(1) = ZZ	UNBAR090
	DO 4400 I=1,N	UNBAR091
	LY1 = LY+I	UNBAR092
	Y(I+1) = 0.	UNBAR093
	DO 4000 MM=1,N1	UNBAR094
	Y(I+1) = Y(I+1) + I*(LY1)*X(MM)	UNBAR095
4050	LY1 = LY1+NY	UNBAR096
4400	CONTINUE	UNBAR097
	DO 4199 L=1,N1	UNBAR098
	X(L) = T(JY1)	UNBAR099
4199	JY1 = JY1+1	UNBAR100
	XINT = Y	UNBAR101
	I = 1	UNBAR102
54	U = 1.	UNBAR103
	X(N+2) = X(1)	UNBAR104
	X(N+3) = X(2)	UNBAR105
	DO 55 J=1,N1	UNBAR106
	A(J+1) = X(J+1) - X(J)	UNBAR107
	TPAL1 = XINT - X(J)	UNBAR108
	IF (TPAL1) 57,56,57	UNBAR109
58	ZZ = Y(J)	UNBAR110
	X(1) = 0.	UNBAR111
	X(2) = 0.	UNBAR112
	X(3) = 0.	UNBAR113
	X(4) = 0.	UNBAR114
	X(J) = 1.0	UNBAR115
	GO TO 59	UNBAR116
57	U = U * TPAL1	UNBAR117
	GO TO (711,712,713) ,N	UNBAR118
711	X(J) = TPAL1/A(J+1)	UNBAR119


```

      GO TO 55
712  X(J) = -TPAL1
      GO TO 55
713  X(J) = (X(J+2)-X(J))*TPAL1
55   CONTINUE
      A(1) = A(N+2)
      ZZ = 0.
      DO 56 J=1,N1
        X(J) = D/(A(J)+A(J+1)* X(J))
      ZZ = ZZ + Y(J)* X(J)
56   CONTINUE
59   IF (I) 5098,5098,9999
9999 KK = KK+KY
      RETURN
      END

```

```

UNBAR120
UNBAR121
UNBAR122
UNBAR123
UNBAR124
UNBAR125
UNBAR126
UNBAR127
UNBAR128
UNBAR129
UNBAR130
UNBAR131
UNBAR132
UNBAR133

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FINOE 61.

APPENDIX III

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

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

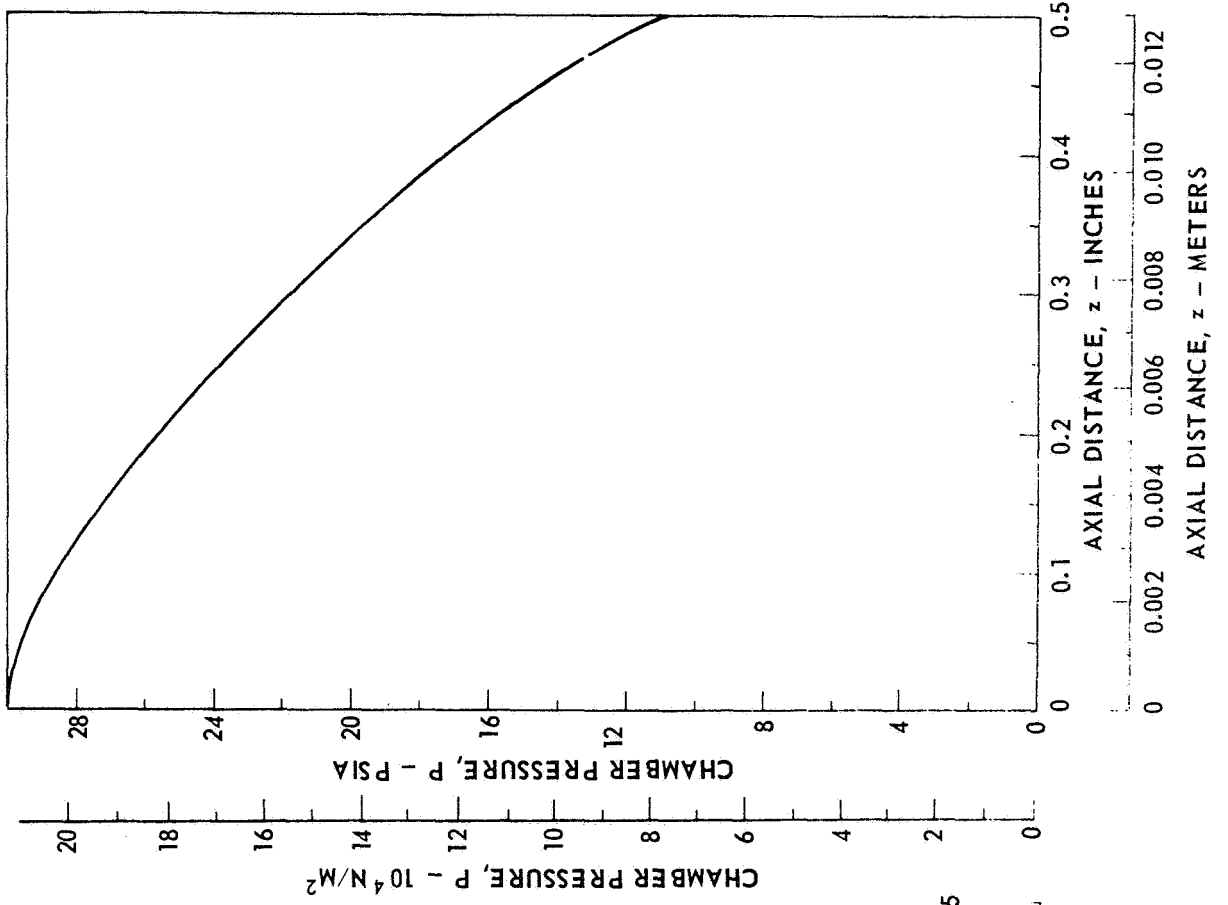
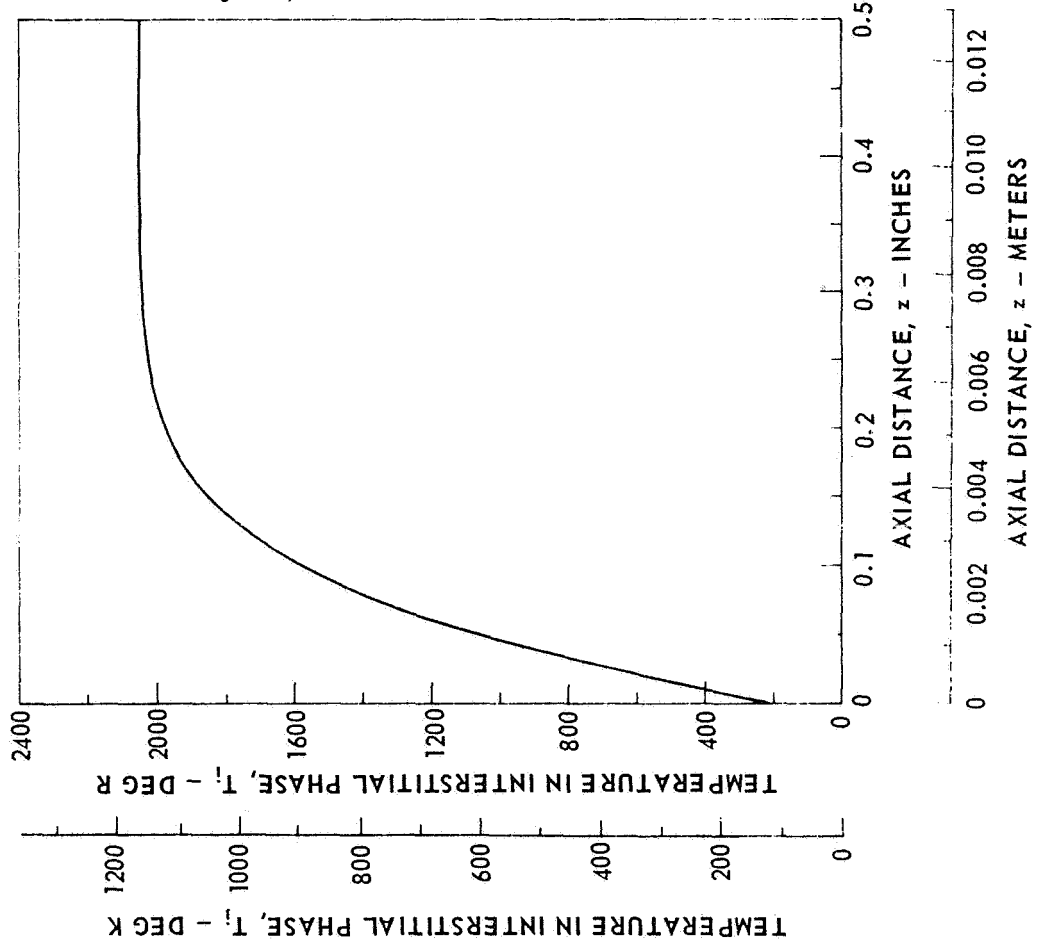
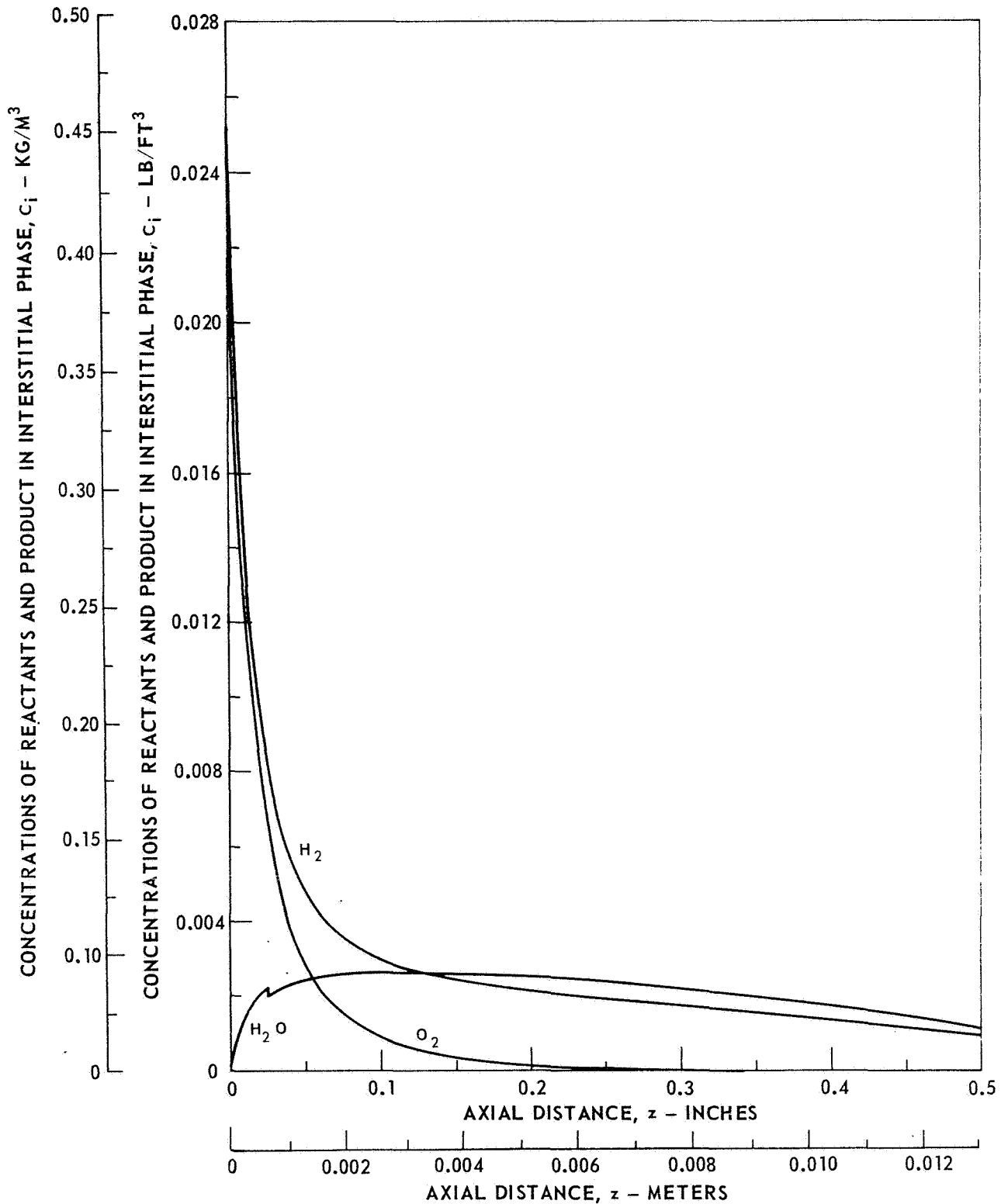


FIG. 1

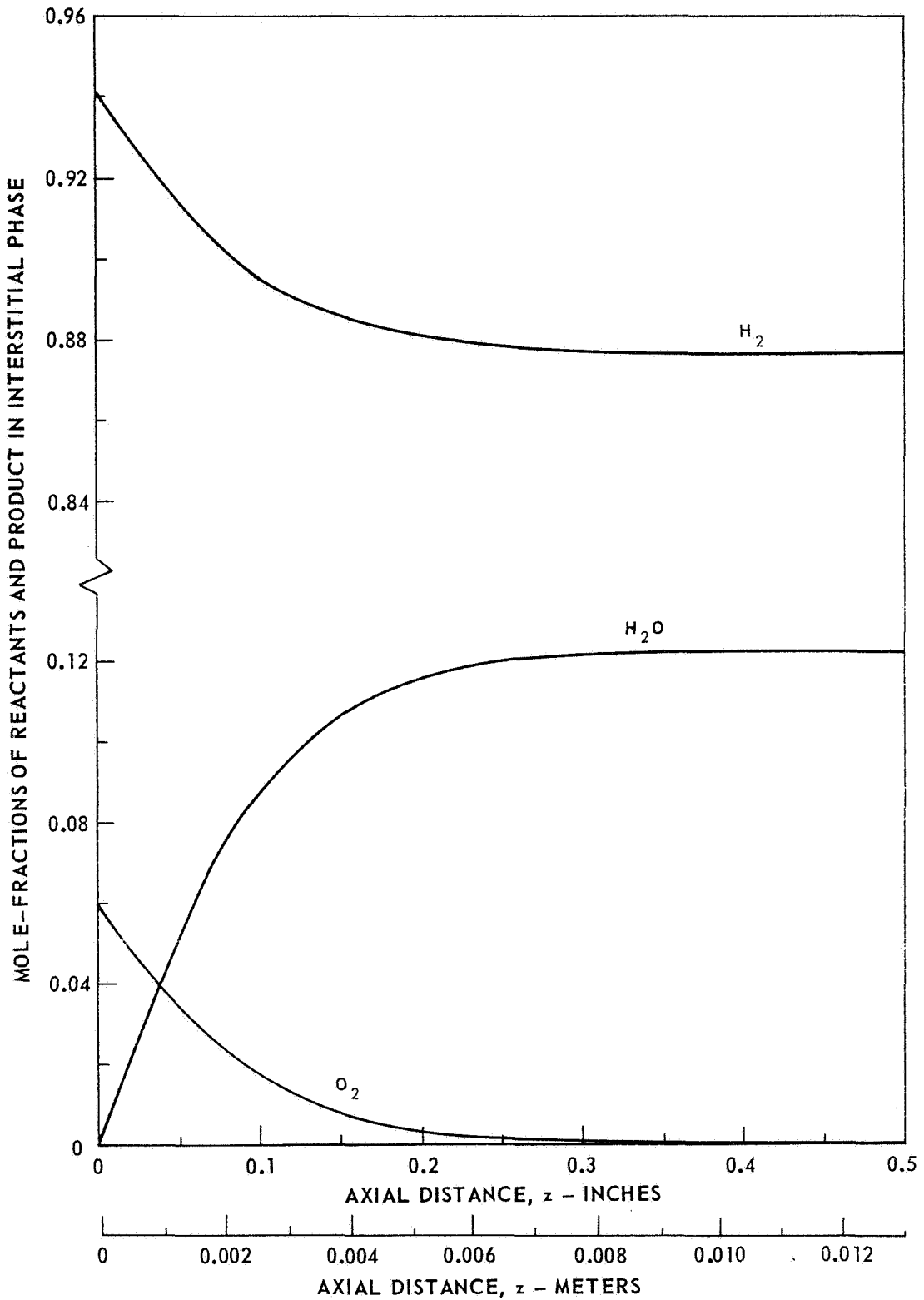
AXIAL CONCENTRATION PROFILES FOR A LOW NOMINAL CHAMBER PRESSURE

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



AXIAL MOLE-FRACTION PROFILES FOR A LOW NOMINAL CHAMBER PRESSURE

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



EFFECT OF PROPELLANT FEED TEMPERATURE ON AXIAL TEMPERATURE PROFILES

H910721

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

FEED MIXTURE RATIO = 1.0 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)

MASS FLOW RATE = 1.28 LB/FT² - SEC (6.25 KG/M^2 - SEC)

NO HELIUM DILUTION

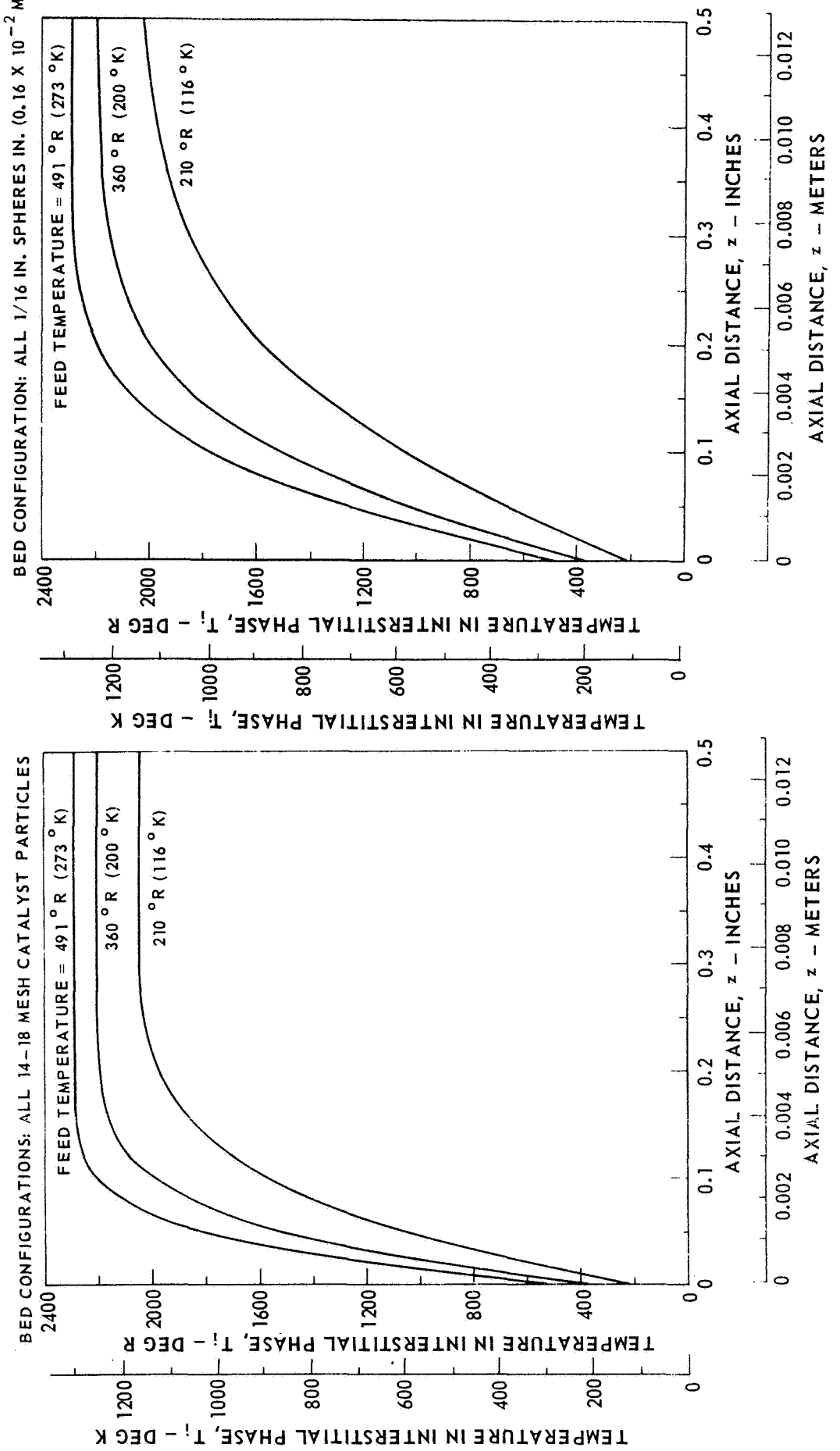


FIG. 4

EFFECT OF STOICHIOMETRY ON AXIAL TEMPERATURE PROFILES

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 X 10⁴ N/M²)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

MASS FLOW RATE = 1.28 LB/FT² - SEC (6.25 KG/M² - SEC)

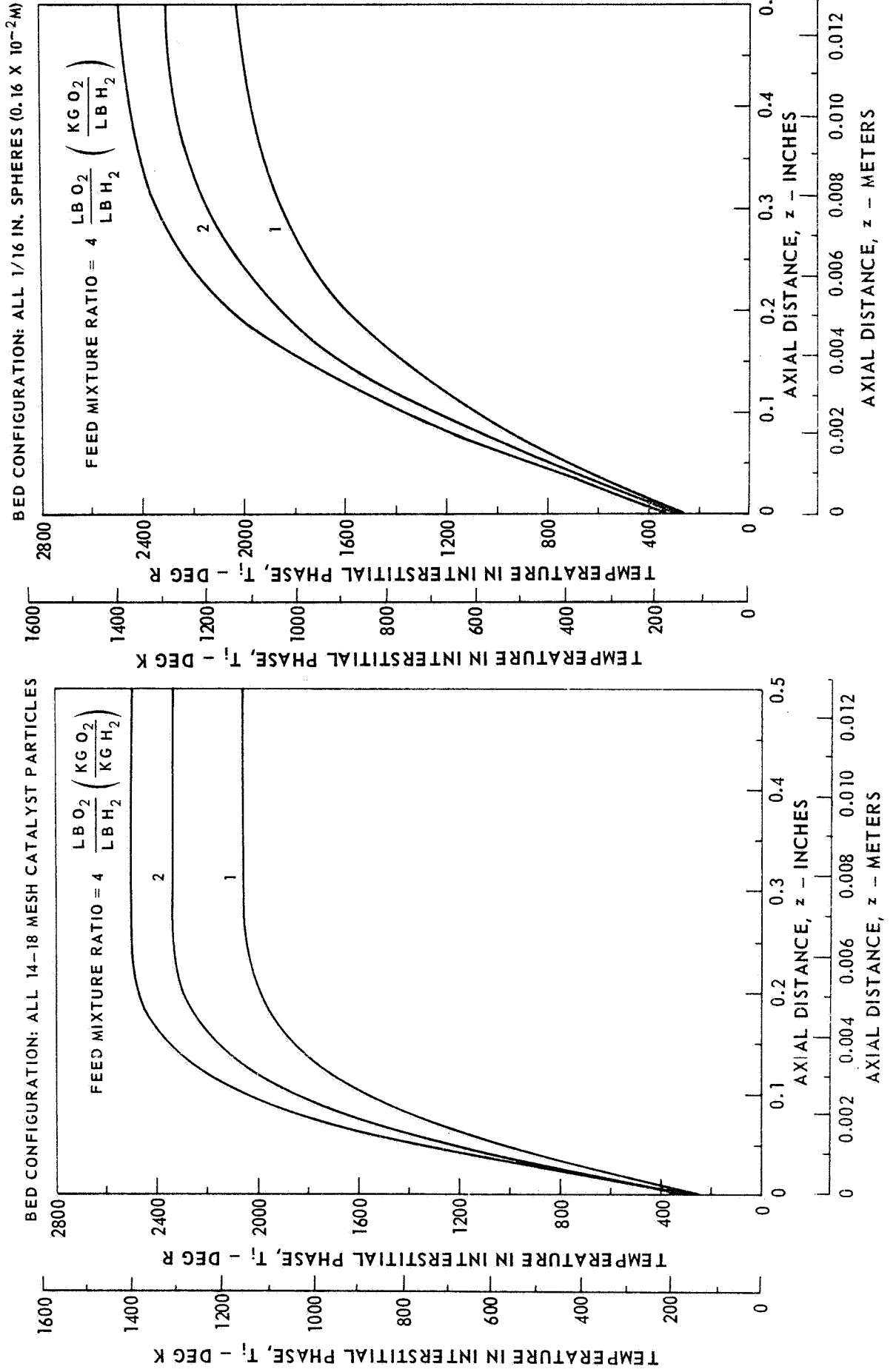


FIG. 5

EFFECT OF HELIUM DILUTION ON AXIAL TEMPERATURE PROFILES

H910721

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

FEED TEMPERATURE = 210 DEG R (117 DEG K)

MASS FLOW RATE = 1.28 LB/FT² - SEC (6.25 KG/M² - SEC)

FEED MIXTURE = 1.0 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)

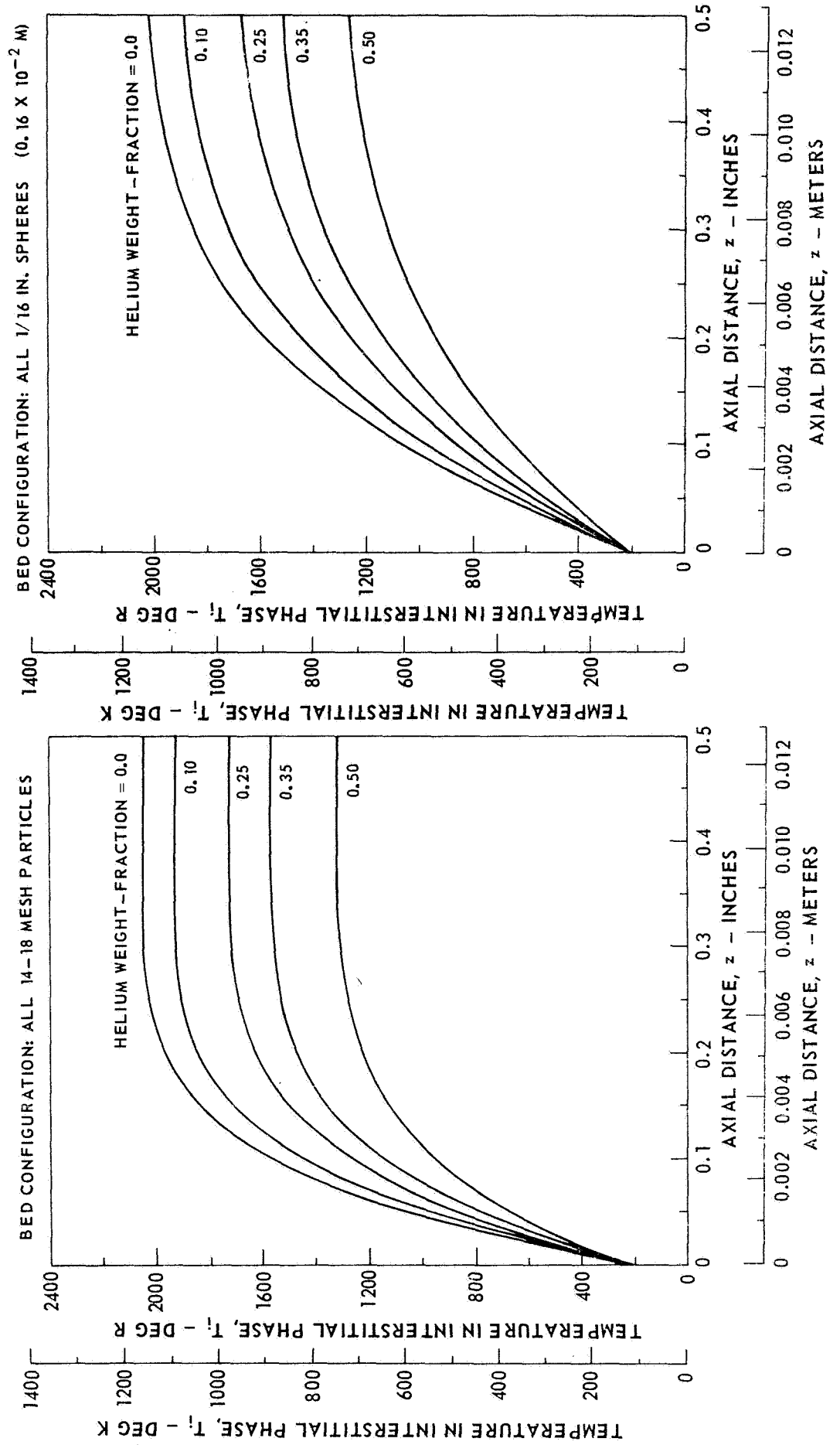


FIG. 6

EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

H9 10721

NO HELIUM DILUTION

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

FEED TEMPERATURE = 210 DEG R (117 DEG K)

FEED MIXTURE = 1.0 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)

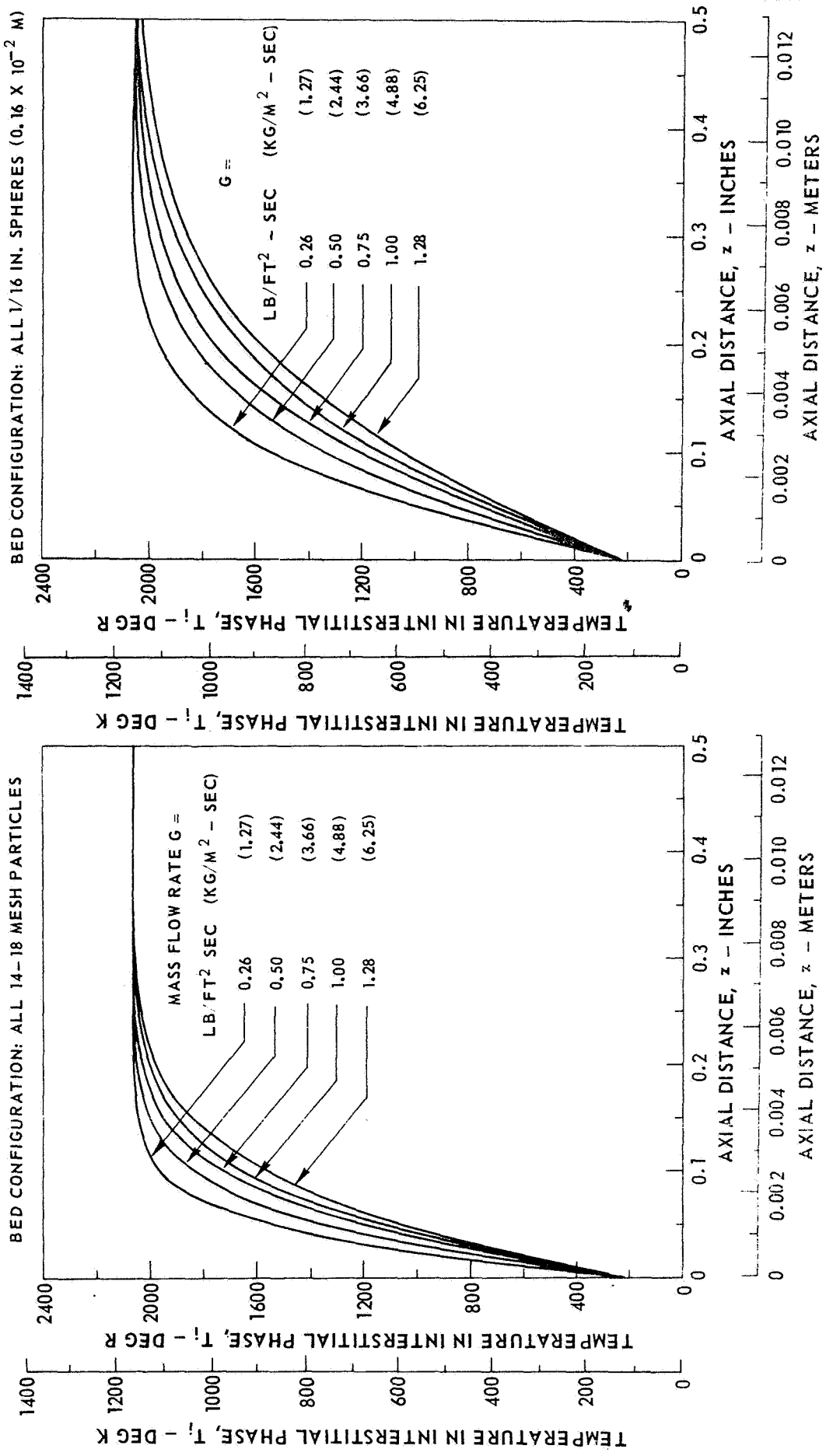


FIG. 7

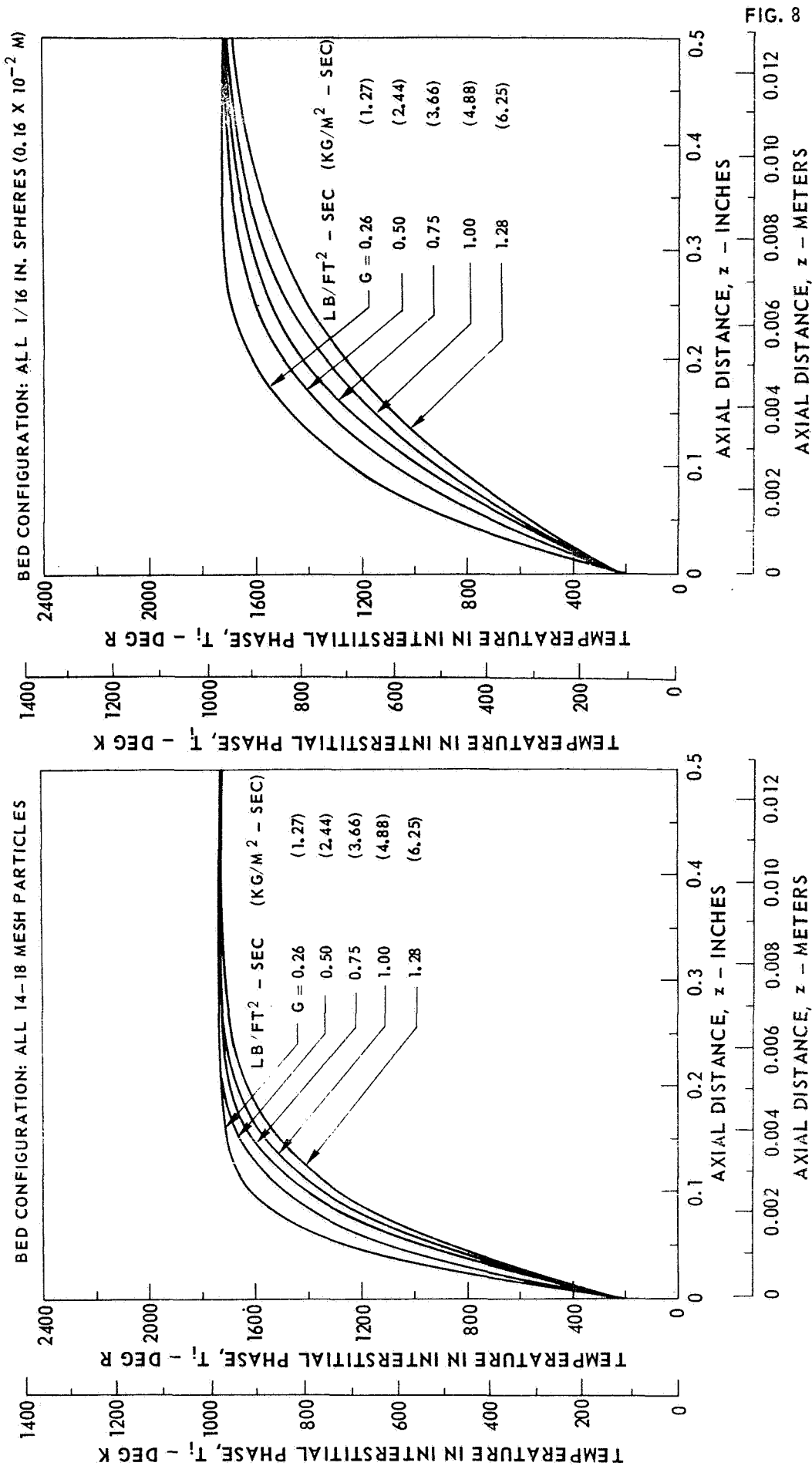
EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIUM WEIGHT-FRACTION = 0.25

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 X 10⁴ N/M²)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

FEED MIXTURE RATIO = 1.0 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)



EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIUM WEIGHT-FRACTION = 0.50

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

FEED TEMPERATURE = 210 DEG R (117 DEG K)

FEED MIXTURE RATIO = 1.0 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)

BED CONFIGURATION: ALL 14-18 MESH PARTICLES

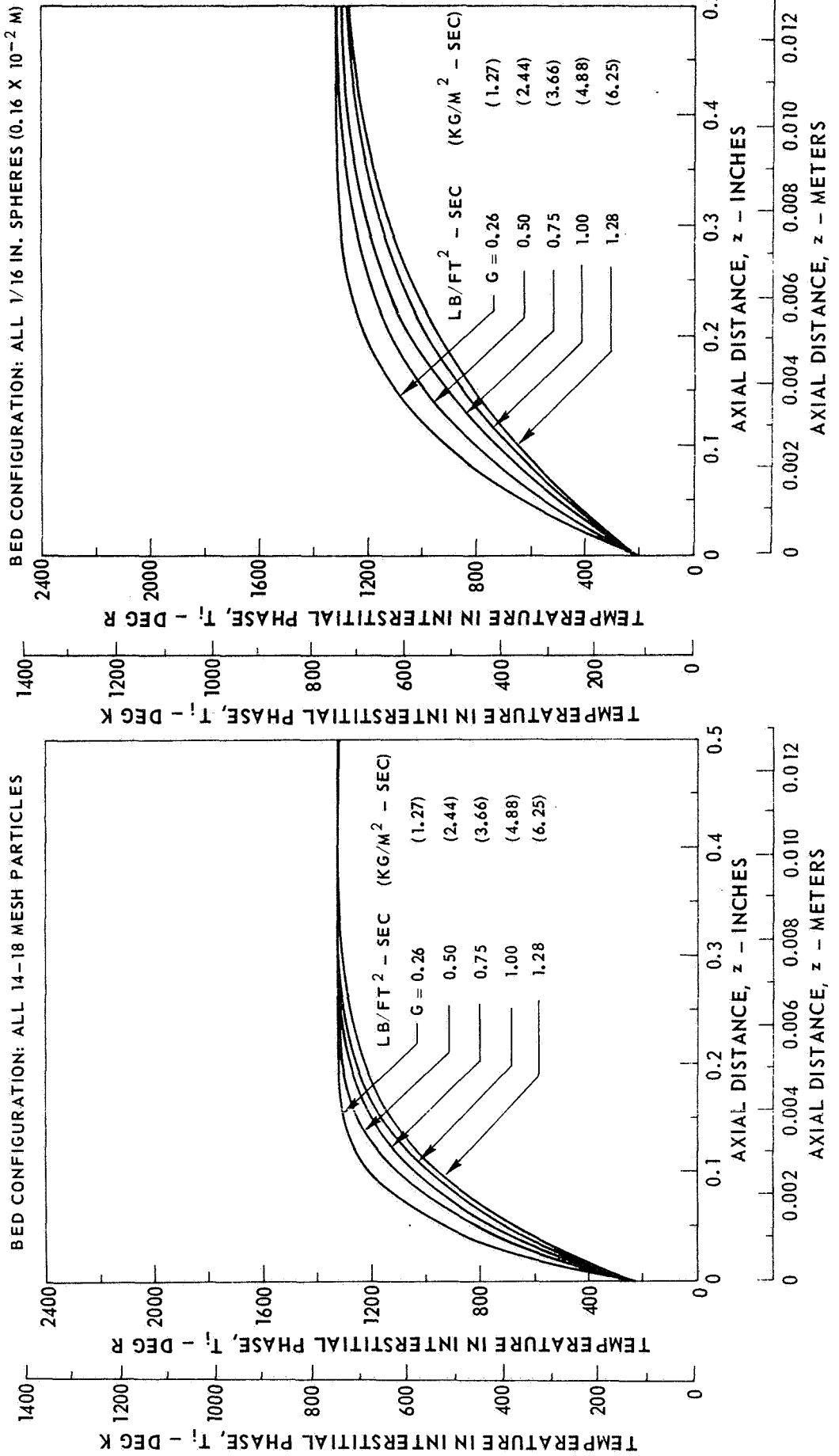


FIG. 9

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

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

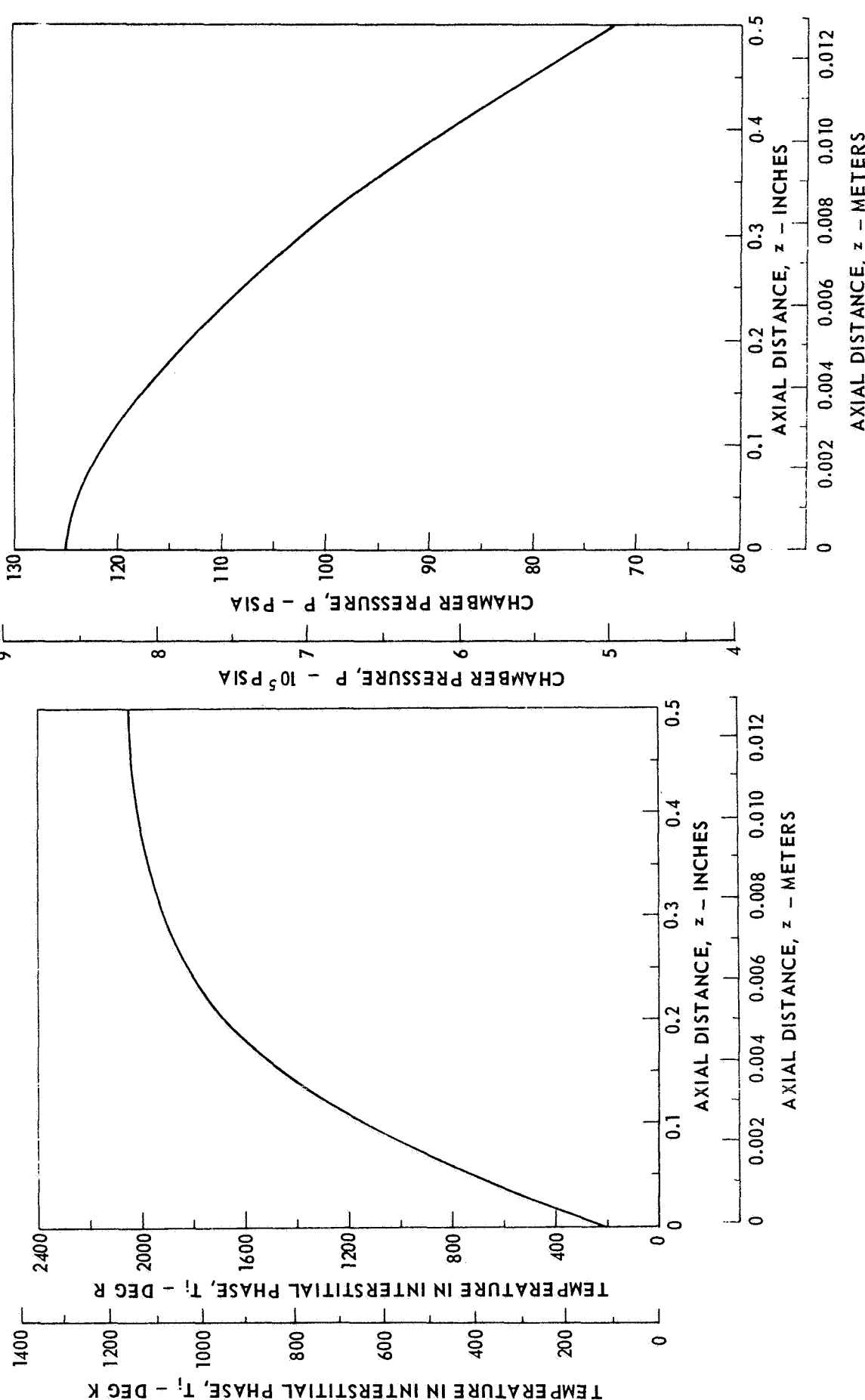
FEED MIXTURE RATIO = 1.0 LB O₂ / LB H₂ (1.0 KG O₂ / KG H₂)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

MASS FLOW RATE = 5.25 LB/FT² - SEC (25.6 KG/M² - SEC)

NO HELIUM DILUTION

BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES



AXIAL DISTANCE, z - METERS

AXIAL CONCENTRATION PROFILES FOR A HIGH NOMINAL CHAMBER PRESSURE

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

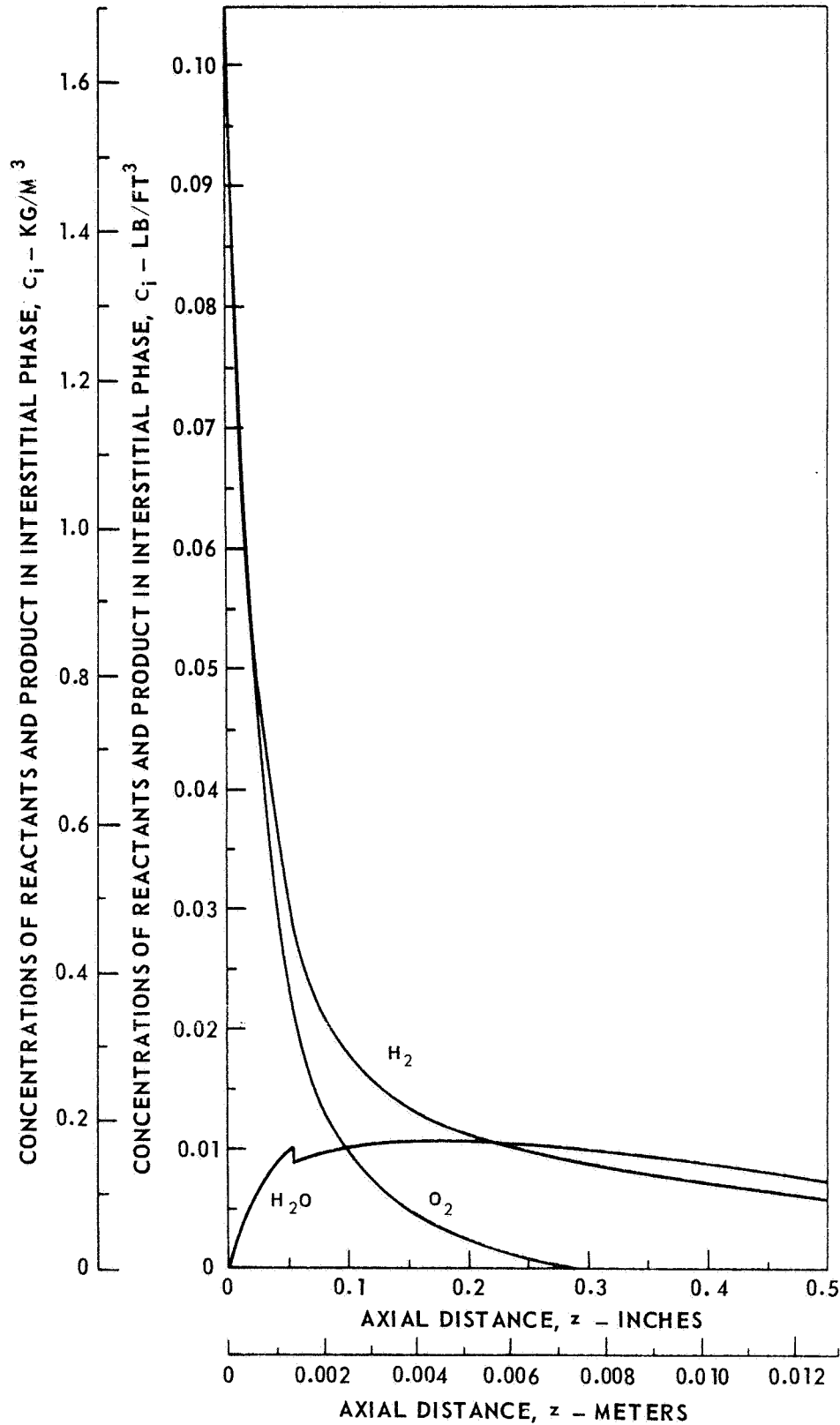
FEED TEMPERATURE = 210 DEG R (117 DEG K)

MASS FLOW RATE = 5.25 LB/FT² - SEC (25.6 KG/M² - SEC)

FEED MIXTURE RATIO = 1.0 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)

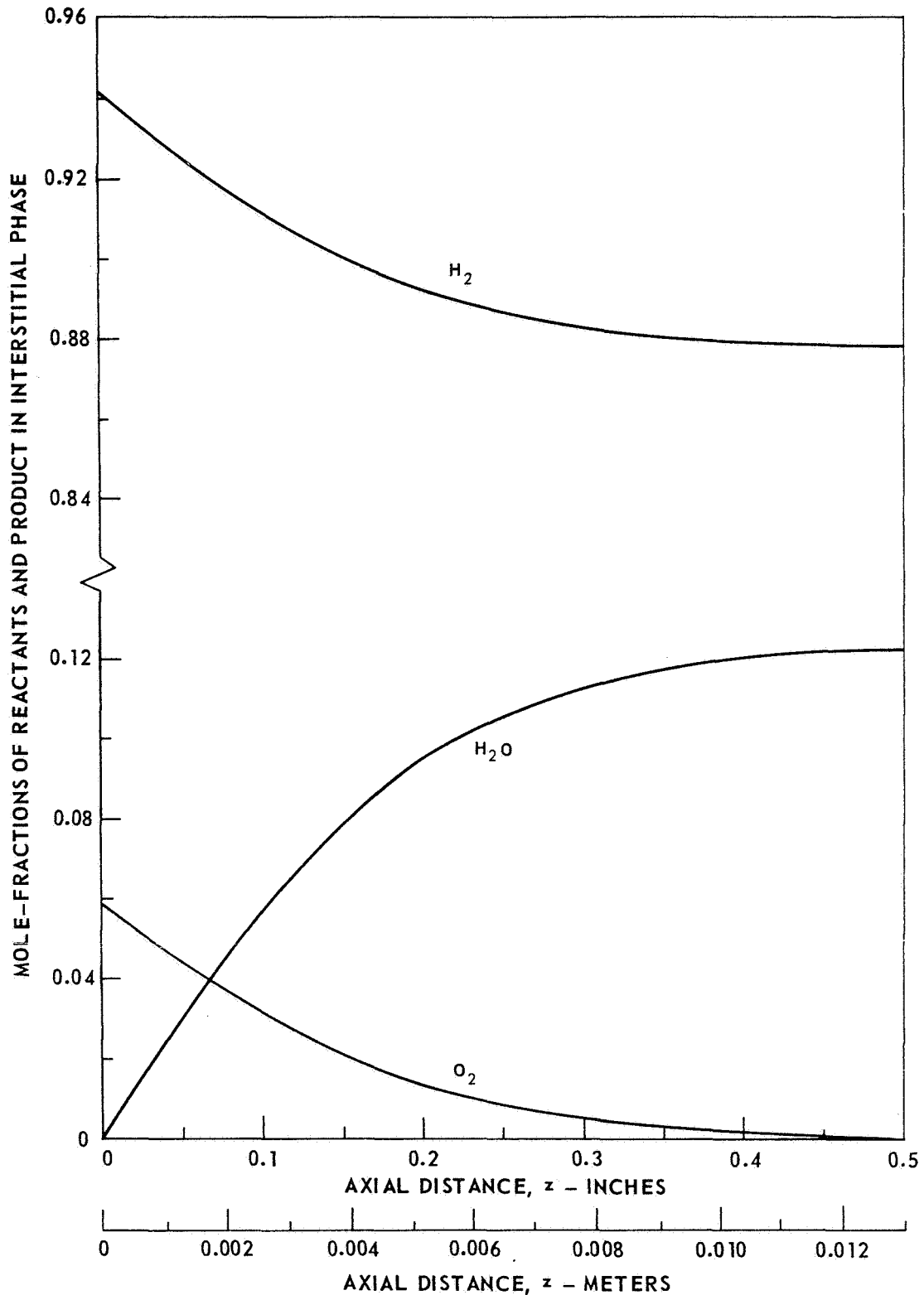
NO HELIUM DILUTION

BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES



AXIAL MOLE-FRACTION PROFILES FOR A HIGH NOMINAL CHAMBER PRESSURE

NOMINAL CHAMBER PRESSURE = 100 PSIA ($6.89 \times 10^5 \text{ N/M}^2$)
 FEED TEMPERATURE = 210 DEG R (117 DEG K)
 FEED MIXTURE RATIO = 1.0 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)
 NO HELIUM DILUTION
 MASS FLOW RATE = 5.25 LB/FT² - SEC. (25.6 KG/M² - SEC)
 BED CONFIGURATION: ALL 14-18 MESH CATALYST PARTICLES



EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

NO HELIUM DILUTION

NOMINAL CHAMBER PRESSURE = 100 PSIA (6.89 X 10⁵ N/M²)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

FEED MIXTURE RATIO = 1.0 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)

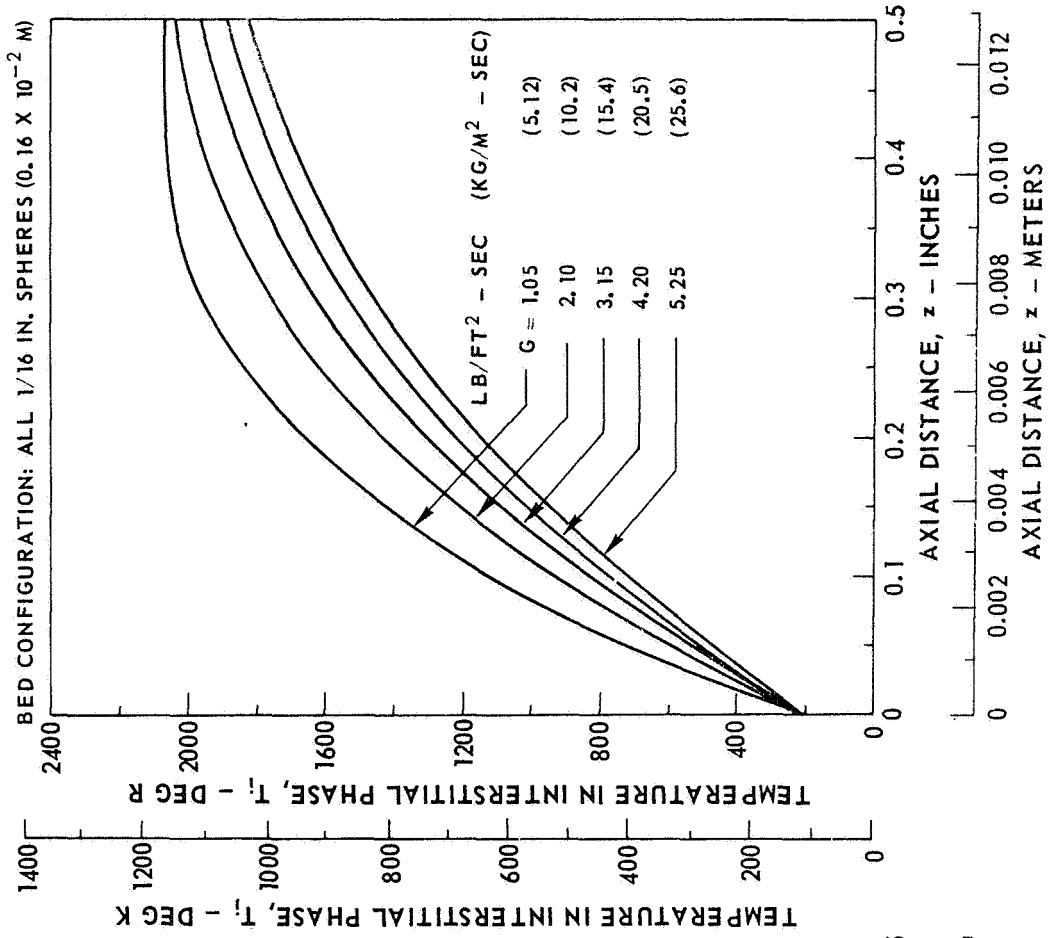
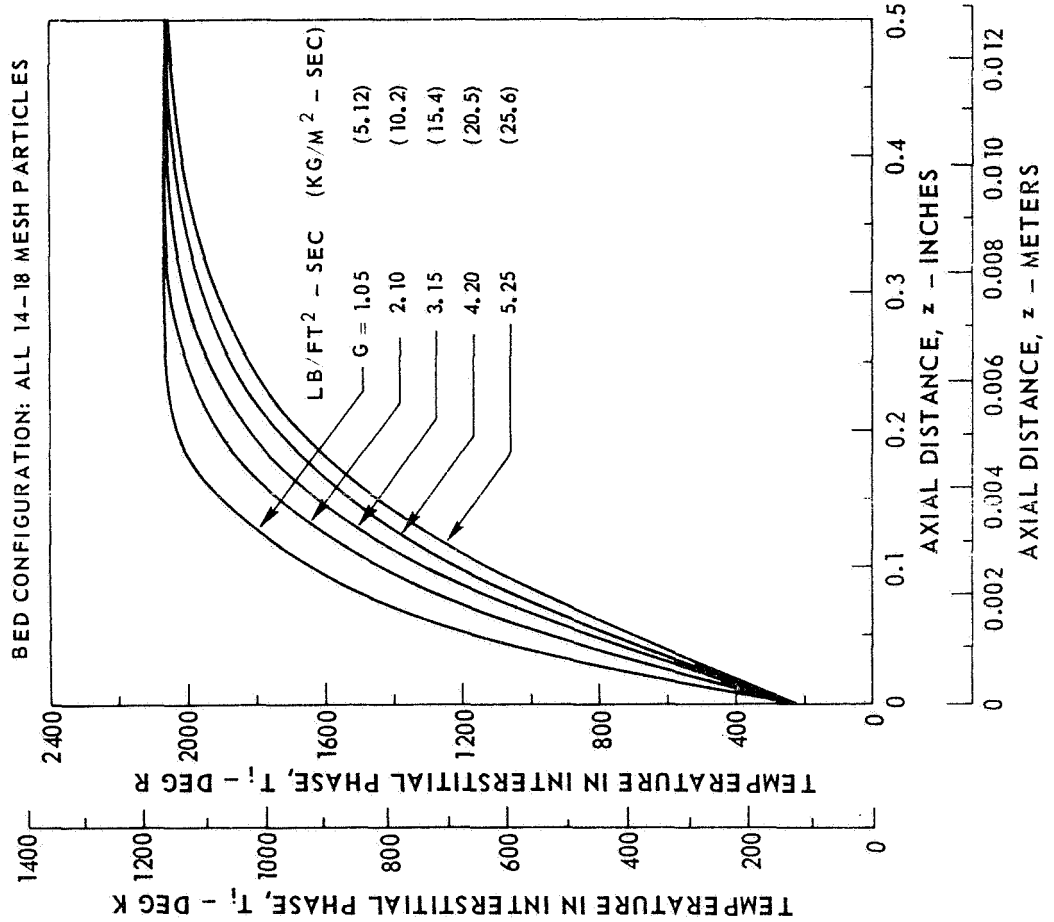


FIG. 13

EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

H910721

HELIUM WEIGHT - FRACTION = 0.25

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 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)

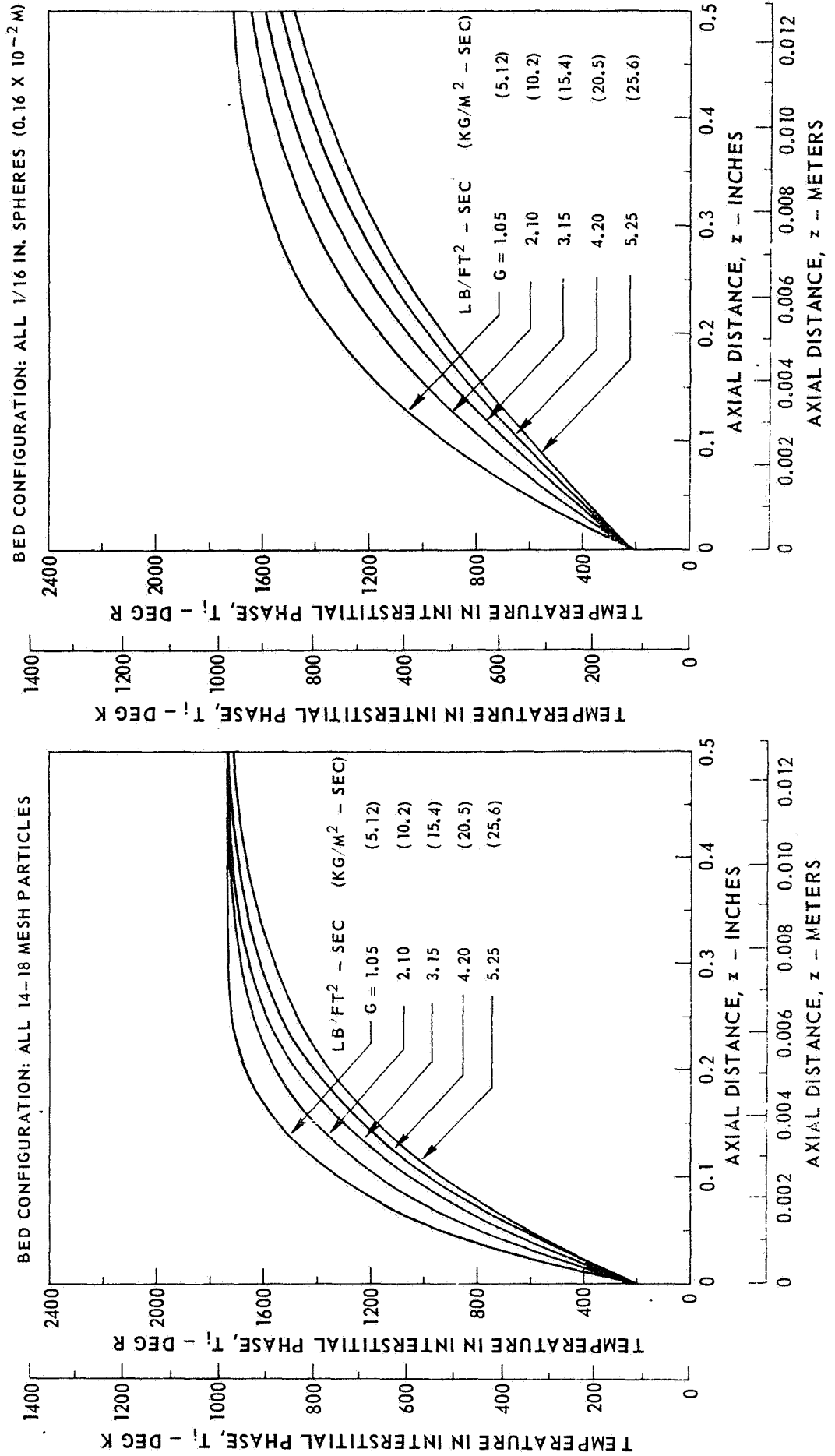


FIG. 14

EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

H9 10721

HELIUM WEIGHT-FRACTION = 0.50

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 LB O₂/LB H₂ (1.0 KG O₂/KG H₂)

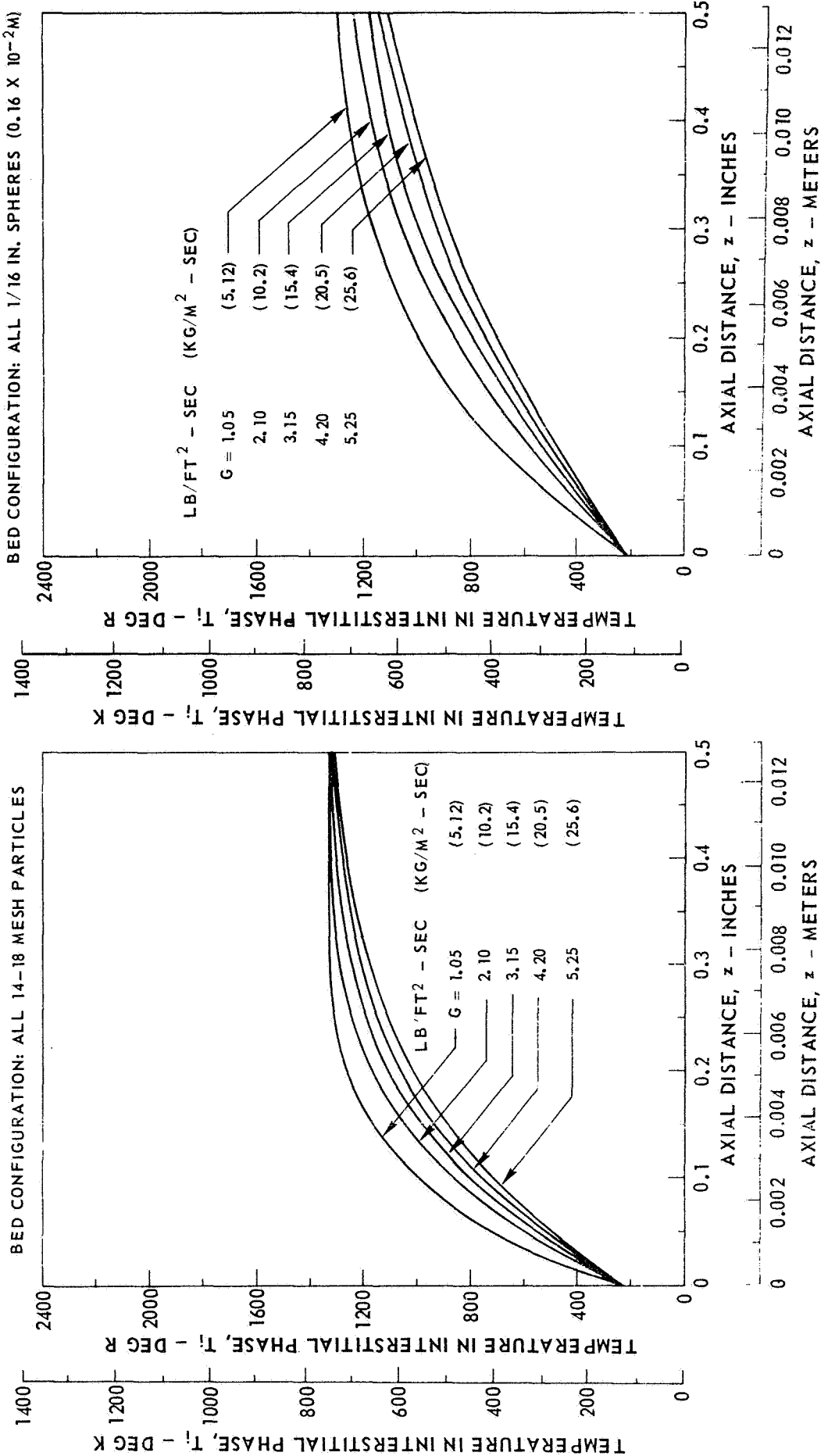


FIG. 15