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FINAL PROGRESS REPORT

STUDY OF CATALYTIC REACTORS FOR HYDROGEN-OXYGEN IGNITION

by

Arthur S. Kesten

prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

JULY, 1969

CONTRACT NASW-1795

United Aircraft Research Laboratories
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EAST HARTFORD, CONNECTICUT

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August 28, 1968 - May 28, 1969

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ABSTRACT

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

FOREWORD

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

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

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

Report H910721

Study of Catalytic Reactors for Hydrogen-Oxygen Ignition

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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 adequantely 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

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

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

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

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

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

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

where

$$\frac{1}{\rho_i} \frac{d\rho_i}{dz} \left[1 - w_i^{H_2O(s)} - w_i^{H_2O(\ell)} \right] = \frac{dw_i^{H_2O(s)}}{dz} + \frac{dw_i^{H_2O(\ell)}}{dz} + \frac{\rho_i^{(v)}}{\rho_i} \left[\frac{1}{P} \frac{dP}{dz} + \frac{1}{\overline{M}^{(v)}} \frac{d\overline{M}^{(v)}}{dz} - \frac{1}{T_i} \frac{dT_i}{dz} \right] \qquad (6)$$

and

$$\frac{1}{\overline{M}^{(v)}} \frac{d\overline{M}^{(v)}}{dz} = - \left[\frac{\sum\limits_{\substack{J \\ (vapor)}} \frac{dw_i^J}{dz} \Big/ M^J}{\sum\limits_{\substack{J \\ (vapor)}} \frac{w_i^J}{M^J}} \right] \qquad (7)$$

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

$$h_c = .74 \bar{c}_f^{(v)} G \left(\frac{G}{A_p \mu} \right)^{-.41} \qquad (8)$$

$$k_c^J = \frac{.61G}{\rho_i^{(v)}} \left(\frac{\mu}{\rho_i^{(v)} D_i^J} \right)^{-.667} \left(\frac{G}{A_p \mu} \right)^{-.41} \qquad (9)$$

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

$$\frac{dh_i}{dz} = -\frac{1}{G}\left\{ H r_{hom}\delta + \hbar_c A_p\left[T_i - (T_p)_s\right] + k_c^{H_2O(v)} A_p\left[c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)}\right]\left[\Delta H^f + \Delta H^c\right]\right\} \qquad (10)$$

In this "ice region"

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

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

$$\frac{dh_i}{dz} = -\frac{1}{G}\left\{ H r_{hom}\delta + \hbar_c A_p\left[T_i - (T_p)_s\right] + k_c^{H_2O(v)} A_p\left[c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)}\right]\left[\Delta H^c + \Delta H^f\left(\frac{h_i - h_i^{(s)}}{h_i^{(s-\ell)} - h_i^{(s)}}\right)\right]\right\} \qquad (12)$$

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

$$\frac{dw_i^{H_2O(s)}}{dz} = \frac{dw_i^{H_2O}}{dz}\left[\frac{h_i^{(s-\ell)} - h_i}{h_i^{(s-\ell)} - h_i^{(s)}}\right] - \frac{1}{(h_i^{(s-\ell)} - h_i^{(s)})}\frac{dh_i}{dz} \qquad (13)$$

$$\frac{dw_i^{H_2O(\ell)}}{dz} = \frac{dw_i^{H_2O}}{dz}\left[\frac{h_i - h_i^{(s)}}{h_i^{(s-\ell)} - h_i^{(s)}}\right] + \frac{1}{(h_i^{(s-\ell)} - h_i^{(s)})}\frac{dh_i}{dz} \qquad (14)$$

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

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

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

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

In this "liquid region"

$$\frac{dw_i^{H_2O}}{dz} = \frac{dw_i^{H_2O(\ell)}}{dz} \tag{17}$$

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

$$\frac{dh_i}{dz} = -\frac{1}{G}\Big\{H r_{hom}\delta + h_c A_p\left[T_i - (T_p)_s\right] + k_c^{H_2O(v)} A_p\left[c_i^{H_2O(v)} - (c_p)_s^{H_2O(v)}\right]\left[\Delta H^c\left(\frac{h_i - h_i^{(\ell)}}{h_i^{(\ell-v)} - h_i^{(\ell)}}\right)\right]\Big\} \tag{18}$$

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

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

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

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

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

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

$$\frac{dh_i}{dz} = -\frac{1}{G}\left\{Hr_{hom}\delta + \hbar_c A_p\left[T_i - (T_p)_s\right]\right\} \qquad (22)$$

and

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

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

$$r_{hom} = 0.16 \times 10^{14} \, {c_i}^{H_2} \, {c_i}^{O_2} \, e^{-35,800/T_i} \text{ lbs } H_2 \text{ reacted/ft}^3\text{-sec}$$

$$\left(= 0.10 \times 10^{13} \, {c_i}^{H_2} \, {c_i}^{O_2} \, e^{-19,889/T_i} \text{ kg } H_2 \text{ reacted/m}^3\text{-sec}\right) \qquad (24)$$

where the concentrations are in lb/ft^3 (kg/m^3) 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*:

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*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.

$$r_{het} = \alpha c_p^{H_2} (c_p^{O_2})^{0.8} e^{-5000/T_p} \quad \text{lbs } H_2 \text{ reacted / ft}^3\text{-sec}$$

$$(= 0.11 \alpha c_p^{H_2} (c_p^{O_2})^{0.8} e^{-2778/T_p} \quad \text{kg } H_2 \text{ reacted / m}^3\text{-sec} \tag{25}$$

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 instanteously 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 (6.89×10^4 N/m^2), a mixture ratio of 1.0 lb O_2/lb H_2, an inlet temperature of 210 deg R (117 deg K), and no helium dilution. The calculations were made for a reaction chamber 0.5 in. (0.013 m) long and 0.87 in. (0.022 m) in diameter, with a total propellant flow of 0.0053 lb/sec (0.0024 kg/sec); this corresponds to a mass flow rate of 1.28 lb/ft^2-sec (6.25 kg/m^2-sec). In order to accommodate this rather high flow rate in this low pressure system, the upstream chamber pressure was taken as 30 psia (2.07×10^5 N/m^2) (in subsequent calculations at lower flow rates the upstream chamber pressure was lowered correspondingly). The calculated axial temperature and chamber pressure profiles for this reference case are shown in Fig. 1. The axial concentration profiles for hydrogen, oxygen, and water (solid, liquid and vapor) are shown in Fig. 2 and the associated mole-fraction profiles are illustrated in Fig. 3.

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

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

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

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

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

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

Definition of Rate-Controlling Processes

As noted previously, preliminary indications (Ref. 13) are that, under steady-state conditions, diffusion of reactants from the free-gas phase to the surface of the catalyst particles may control the rate of the hydrogen-oxygen reaction throughout the reactor. Although the calculated results described in the preceding section were based on this assumption, further validation is required using detailed engine test data. If the assumption is valid, it implies that at steady-state, catalyst particle temperatures at an axial position near the inlet of the reactor are considerably higher than the bulk fluid temperature at the same axial position. It is apparent that this same condition cannot exist in the early stages of <u>transient</u> 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 <u>within</u> 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, ft^{-1}(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, Btu/lb-deg R (Cal/kg-deg K)
$\overline{C_f}$	Average specific heat of fluid in the interstitial phase, Btu/lb-deg R (Cal/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, lb/ft^2-sec (kg/m^2-sec)
h_i	Enthalpy, Btu/lb (Cal/kg)
$h_i^{(s)}$	Enthalpy at the Ice/Ice-Liquid interface, Btu/lb (Cal/kg)
$h_i^{(s-\ell)}$	Enthalpy at the Ice-Liquid/Liquid interface, Btu/lb (Cal/kg)
$h_i^{(\ell)}$	Enthalpy at the Liquid/Liquid-Vapor interface, Btu/lb (Cal/kg)
$h_i^{(\ell-v)}$	Enthalpy at the Liquid-Vapor/Vapor interface, Btu/lb (Cal/kg)
h_c	Heat transfer coefficient, Btu/ft^2-sec-deg R (Cal/m^2-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, Btu/ft-sec-deg R (Cal/m-sec-deg K)

M	Molecular weight, lb/lb mole (kg/kg mole)
$\overline{M}$	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

$H_2O(s)$	Refers to water in the solid phase
$H_2O(\ell)$	Refers to water in the liquid phase
$H_2O(v)$	Refers to water in the vapor phase
J	Refers to chemical species (e.g. H_2, O_2, H_2O, 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

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

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

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

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

$$H D_p \left(\frac{dc_p}{dx}\right)_s = \hbar_c \left[T_i - (T_p)_s\right] \tag{I-4}$$

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

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

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

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

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

$$aA + bB + \ldots \rightarrow tT + \ldots .$$

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

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

$$\begin{array}{ccc} D_p^B \nabla^2 c_p^B - \dfrac{b}{a}\dfrac{M^B}{M^A} r_{het}^A & (c_p^A, c_p^B, \ldots, c_p^T, \ldots, T_p) & = 0 \\ \vdots & \vdots & \vdots \end{array} \tag{I-8}$$

$$\begin{array}{ccc} D_p^T \nabla^2 c_p^T + \dfrac{t}{a}\dfrac{M^T}{M^A} r_{het}^A & (c_p^A, c_p^B, \ldots, c_p^T, \ldots, T_p) & = 0 \\ \vdots & \vdots & \vdots \end{array} \tag{I-9}$$

and

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

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

$$D_p^A \left(\frac{dc_p}{dx}\right)_s^A = k_c^A \left[c_i^A - (c_p)_s^A\right] \tag{I-11}$$

$$\begin{array}{ccccc} D_p^B \left(\dfrac{dc_p}{dx}\right)_s^B & = & \dfrac{bM^B}{aM^A} D_p^A \left(\dfrac{dc_p}{dx}\right)_s^A & = & k_c^B \left[c_i^B - (c_p)_s^B\right] \\ \vdots & & \vdots & & \vdots \end{array} \tag{I-12}$$

$$\begin{array}{ccccc} D_p^T \left(\dfrac{dc_p}{dx}\right)_s^T & = & -\dfrac{tM^T}{aM^A} D_p^A \left(\dfrac{dc_p}{dx}\right)_s^A & = & k_c^T \left[c_i^T - (c_p)_s^T\right] \\ \vdots & & \vdots & & \vdots \end{array} \tag{I-13}$$

and

$$H^A D_p^A \left(\frac{dc_p}{dx}\right)_s^A = \hbar_c \left[T_i - (T_p)_s\right] \tag{I-14}$$

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

$$\begin{aligned} c_p^B - (c_p)_s^B &= \frac{bM^B}{aM^A}\,\frac{D_p^A}{D_p^B}\left[c_p^A - (c_p)_s^A\right] \\ \vdots\qquad\qquad & \qquad\qquad\quad \vdots \end{aligned} \qquad \text{(I-15)}$$

$$\begin{aligned} c_p^T - (c_p)_s^T &= \frac{tM^T}{aM^A}\,\frac{D_p^A}{D_p^T}\left[(c_p)_s^A - c_p^A\right] \\ \vdots\qquad\qquad & \qquad\qquad\quad \vdots \end{aligned} \qquad \text{(I-16)}$$

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

$$\begin{aligned} c_i^B - (c_p)_s^B &= \frac{bM^B}{aM^A}\,\frac{k_c^A}{k_c^B}\left[c_i^A - (c_p)_s\right] \\ \vdots\qquad\qquad & \qquad\qquad\quad \vdots \end{aligned} \qquad \text{(I-17)}$$

$$\begin{aligned} c_i^T - (c_p)_s^T &= \frac{tM^T}{aM^A}\,\frac{k_c^A}{k_c^T}\left[(c_p)_s^A - c_i^A\right] \\ \vdots\qquad\qquad & \qquad\qquad\quad \vdots \end{aligned} \qquad \text{(I-18)}$$

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,CSV,KP,MU,PRIME,Z,NX0,ZETA,ZETAIN
      COMMON /BLOCK2/ CONST,PPP,POWERR(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),KCR(2),KCP(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         CF3VT(34),CF3ST(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 = 143.4
      CF3L  = 1.0
      R     = 10.73
 1    READ (5,100) TITLE
 100  FORMAT (14A6)
      IF (TITLE(1)-END) 26,10,26
 26   WRITE (6,200) TITLE
 200  FORMAT (1H1,14A6//)
      READ (5,250) PRIME
 250  FORMAT (A2)
 30   READ (5,300) T,P,G,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,
     X       ZCON,ZEND,ALPHA,AEXP,BEXP,AGM,ALPHAK,ZETAIN
 300  FORMAT (8E10.5)
      WRITE (6,400)
 400  FORMAT (/11X,'T',11X,'P',11X,'G',11X,'H',10X,'C1',10X,'C2',10X,'C3
     X',10X,'C4',10X,'M1',10X,'M2')
      WRITE (6,500) T,P,G,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,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
     XX,'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,E10.5,2X,
     XE10.5,2X,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) AEXP,BEXP,AGM,ALPHAK,ZETAIN
 900  FORMAT (/6X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5,2X,E10.5/)
      READ (5,950) NOFZ
 950  FORMAT (1I2)
      NZTBL = 2*NOFZ+4
      NOFZ4 = NOFZ+4
      NOFZ5 = NOFZ4+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(I),I=1,4)
      READ (5,21) (APVSZ(I),I=5,NOFZ4)
      READ (5,21) (APVSZ(I),I=NOFZ5,NZTBL)
      READ (5,20) (DELVSZ(I),I=1,4)
      ~~READ (5,21) (DELVSZ(I),I=5,NOFZ4)~~
      READ (5,21) (DELVSZ(I),I=NOFZ5,NZTBL)
      WRITE (6,999)
  999 FORMAT (///55X,13H A VS Z TABLE)
      WRITE (6,22) (AVSZ(I),I=1,4)
   22 FORMAT (40X,4E13.5)
      ~~WRITE (6,23) (AVSZ(I),I=5,NOFZ4)~~
   23 FORMAT (1X,10E13.5)
      WRITE (6,25)
   25 FORMAT ( / )
      WRITE (6,23) (AVSZ(I),I=NOFZ5,NZTBL)
      WRITE (6,24)
   ~~24 FORMAT ( // )~~
      WRITE (6,997)
  997 FORMAT (54X,14H AP VS Z TABLE)
      WRITE (6,22) (APVSZ(I),I=1,4)
      WRITE (6,23) (APVSZ(I),I=5,NOFZ4)
      WRITE (6,25)
      ~~WRITE (6,23) (APVSZ(I),I=NOFZ5,NZTBL)~~
      WRITE (6,24)
      WRITE (6,995)
  995 FORMAT (52X,17H DELTA VS Z TABLE)
      WRITE (6,22) (DELVSZ(I),I=1,4)
      WRITE (6,23) (DELVSZ(I),I=5,NOFZ4)
      ~~WRITE (6,25)~~
      WRITE (6,23) (DELVSZ(I),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 (////50X,'******** OPERATIONS COMPLETE ********')
      STOP
      END
```

```
WIPT   FOR ICE
       SUBROUTINE ICE (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/   T,P,H,C1,C2,C3,C4,M1,M2,M3,M4,D01,D02,D03,D04,TS,
      A        ZCON,ZEND,G,DHEZ,H3,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,
      A        A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETAIN
       COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
      A        ,MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
      A         CF3VT(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
      A        (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' 41X '*********************** ICE REGION ****************
      A***' ///)
       LFLAG = 0
       Z = 0.
       AP = 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 (6,300)
       WRITE (6,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
    1  CALL UNBAR (AVSZ,1,Z,0.,A,KK)
       CALL UNBAR (APVSZ,1,Z,0.,AP,KK)
       CALL UNBAR (DELVSZ,1,Z,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,T,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 SORAD (RHO,KC1,KC2,KC3V,HG,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,
      A                 CFBAR)
       IF (1165.-TPS) 11,33,33
   33  CALL UNBAR (VPVST,1,TPS,0.,VP,KK)
       TEST = CF53V*R*TPS/M3
       IF (VP-TEST) 12,11,11
   12  WRITE (6,200)
  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.,DELHC,KK)
       RHOM = 0.
```

```
      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 = -((HR*RHOM*DELTA+HC*AP*TITP)+(KC3V*AP*C1CP3V*(DELHF+DELHC))
     ∧        )/G
      DELTZ = ZCON/DHDZ
      ZTEST = ZEND/10.
      IF (DELTZ.GT.ZTEST) DELTZ = ZTEST
      DTDZ = DHDZ/CPBAR
      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./(64.4*A*RHO))
      DPDZ = DPDZ*AP/144.
      W1 = C1/RHO
      W2 = C2/RHO
      W3 = C3/RHO
      W4 = C4/RHO
      DRHODZ = (RHO/(1.-W3))*(DW3DZ+RHOV/RHO*(1./P*DPDZ+1./MBARV*DMBRDZ-
     ∧         1./T*DTDZ))
      RHOFAC = (-1./(1.-W3))*(DW3DZ+RHOV/RHO*(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)
      H = H+DHDZ*DELTZ
      MFRAC4 = C4/M4/(C1/M1+C2/M2+C3/M3+C4/M4)
      Z = Z+DELTZ
      P = P+DPDZ*DELTZ
      IF (P) 136,137,137
  137 IF (LFLAG.EQ.1) GO TO 50
      T = T+DTDZ*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) 60,50,40
   40 WRITE (6,300)
  300 FORMAT (///11X,'Z',9X,'TEMP',9X,'C1',10X,'C2',10X,'C3',10X,'C4',8X
     ∧,'MFRAC1',5X,'MFRAC2',6X,'MFRAC3',6X,'MFRAC4')
      WRITE (6,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
  400 FORMAT (/6X,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 (6,56)
   56 FORMAT (///58X,16HTHAT'S ALL FOLKS )
      CALL EXIT
   60 DELTZ = (TS-TT)/DTDZ
      C1 = C1P
      C2 = C2P
      C3 = C3P
      C4 = C4P
      T = TS
      H = HP
      Z = ZP
      P = PP
      LFLAG = 1
      GO TO 20
  136 PCHECK = -1.
      RETURN
   99 WRITE (6,90)
   90 FORMAT ('0' // 45X 'AXIAL INCREMENTS HAVE EXCEEDED BED LENGTH')
      CALL EXIT
      END
 WIPT 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/  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,ZETAIN
      COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
     X      ,MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
     X      CF3VT(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' 38X '********************** ICE-LIQUID REGION **********
     X*********** ///)
      LFLAG = 0
      HS = H
      C3S = C3
      W3S = W3
      C3L = 0.
      AP = 1.0
 1    CALL UNBAR (AVSZ,1,Z,0.,A,KK)
      CALL UNBAR (APVSZ,1,Z,0.,AP,KK)
      CALL UNBAR (DELVSZ,1,Z,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,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 SGRAD (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,
     X                CFBAR)
      IF (1165.-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
     XST 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 = DW3DZ*((HSL-H)/(HSL-HS)-(1./(HSL-HS)*DHDZ))
      DW3LDZ = DW3DZ*((H-HS)/(HSL-HS)+(1./(HSL-HS)*DHDZ))
      DHDZ = -((HR*RHOM*DELTA+HC*AP*T1TP)+(KC3V*AP*C1CP3V*(DELHC+DELHF*
     X       ((H-HS)/(HSL-HS)))))/G
      DELTZ = ZCON/DHDZ
      ZTEST = ZEND/10.
      IF (DELTZ.GT.ZTEST) DELTZ = ZTEST
      DMBRDZ = (-MBARV)*((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./(64.4*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./
     X         MBARV*DMBRDZ))
      RHOFAC = (-1./(1.-W3S-W3L))*(DW3SDZ+DW3LDZ+RHOV/RHO*(1./P*DPDZ+1./
     X         MBARV*DMBRDZ))
      DRHODZ = DRHODZ*((1.-EXP(-RHOFAC*DELTZ))/(RHOFAC*DELTZ))
      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*DELTZ
      C2 = C2+DC2DZ*DELTZ
      C3L = C3L+DC3LDZ*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)
      FRAC3L  = C3L/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
      MFRAC4 = C4/M4/(C1/M1+C2/M2+C3/M3+C4/M4)
      H = H+DHDZ*DELTZ
      Z = Z+DELTZ
      P = P+DPDZ*DELTZ
      IF (P) 136,137,137
 137  IF (LFLAG.EQ.1) GO TO 50
      C3S = C3S+DC3SDZ*DELTZ
      FRAC3S  = C3S/M3/(C1/M1+C2/M2+C3/M3+C4/M4)
      C3 = C3S+C3L
      IF (C1.LT.0..OR.C2.LT.0..OR.C4.LT.0.) GO TO 50
      IF (Z.GT.ZEND) GO TO 99
      IF (C3S) 60,50,40
 40   WRITE (6,300)
 300  FORMAT (///11X,'Z',9X,'TEMP',11X,'C1',10X,'C2',10X,'C3S',9X,'C3L',
     X9X,'C4')
      WRITE (6,400) Z,T,C1,C2,C3S,C3L,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,'MFRAC3S',5X,'MFRAC3L',5X,'MFR
     XAC4'/)
      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) 55,55,54
54    RETURN
55    WRITE (6,56)
56    FORMAT (//,58X,16HTHAT'S ALL FOLKS )
      CALL EXIT
60    DELTZ = -C3SP/DC3SDZ
      C3S = 0.
      C1 = C1P
      C2 = C2P
      C3L = C3LP
      C4 = C4P
      H = HP
      Z = ZP
      P = PP
      LFLAG = 1
      GO TO 20
156   PCHECK = -1.
      RETURN
99    WRITE (6,90)
90    FORMAT ('0' // 45X 'AXIAL INCREMENTS HAVE EXCEEDED BED LENGTH')
      CALL EXIT
      END
```

```
WIPT  FOR LIQUID
      SUBROUTINE LIQUID (PCHECK)
      REAL  KC1,KC2,KC3V,MBARV,M1,M2,M3,M4,MU1VST,MU1,MU2VST,MU2,MU3VST,
     ^      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,
     ^      ZCON,ZEND,G,DHDZ,W3,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,
     ^      A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETAIN
      COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
     ^      ,MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
     ^       CF3VT(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
     ^      (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 '******************** LIQUID REGION **************
     ^******' ///)
      LFLAG = 0
      AF = 1.0
      CALL UNBAR (TVSVP,1,P,0.,TL,KK)
 1    CALL UNBAR (AVSZ,1,Z,0.,A,KK)
      CALL UNBAR (APVSZ,1,Z,0.,AP,KK)
      CALL UNBAR (DELVSZ,1,Z,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 (CF4VST,1,T,0.,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 SGRAD (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,
     ^            CFBAR)
      IF (1165.-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
     ^ST PARTICLE .... PROGRAM STOP FOLLOWS   *****')
      CALL EXIT
 11   CONTINUE
      CALL UNBAR (DHCVST,1,T,0.,DELHC,KK)
      RHOM = 0.
      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 = -((HR*RHOM*DELTA+HC*AP*TITP)+(KC3V*AP*CICP3V*DELHC))/G
      DELTZ = ZCON/DHDZ
      ZTEST = ZEND/10.
```

```
      IF (DELTZ.GT.ZTEST) DELTZ = ZTEST
      DTDZ = DHDZ/CFBAR
      DMBRDZ = (-MBARV)*((DW1DZ/M1+DW2DZ/M2+DW4DZ/M4)/(W1/M1+W2/M2+W4/M4
     A))
      DPDZ = ((DELTA-1.)/DELTA**3)*(1.75+(75.*MU*(1.-DELTA))/(A*G))*(G**
     A        2./(64.4*A*RHO))
      DPDZ = DPDZ*AF/144.
      P = P+DPDZ*DELTZ
      IF (P) 136,137,137
137   W1 = C1/RHO
      W2 = C2/RHO
      W3 = C3/RHO
      W4 = C4/RHO
      DRHODZ = (RHO/(1.-W3))*(DW3DZ+RHOV/RHO*(1./P*DPDZ+1./MBARV*DMBRDZ-
     A        1./T*DTDZ))
      RHOFAC = (-1./(1.-W3))*(DW3DZ+RHOV/RHO*(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)
      H = H+DHDZ*DELTZ
      Z = Z+DELTZ
      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*DELTZ
      IF (Z.GT.ZEND) GO TO 99
      IF (TL-T) 60,50,40
40    WRITE (6,300)
300   FORMAT (///11X,'Z',9X,'TEMP',9X,'C1',10X,'C2',10X,'C3',10X,'C4',8X
     X,'MFRAC1',5X,'MFRAC2',6X,'MFRAC3',6X,'MFRAC4')
      WRITE (6,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
400   FORMAT (/6X,E10.5,2X,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 (6,1111) 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 (6,56)
56    FORMAT (///58X,16HTHAT'S ALL FOLKS )
      CALL EXIT
60    DELTZ = (TL-TT)/DTDZ
      T = TL
      C1 = C1P
      C2 = C2P
      C3 = C3P
      C4 = C4P
      H = HP
      Z = ZP
      P = PP
      LFLAG = 1
      GO TO 20
136   PCHECK = -1.
      RETURN
99    WRITE (6,90)
90    FORMAT ('0' // 45X 'AXIAL INCREMENTS HAVE EXCEEDED BED LENGTH')
      CALL EXIT
      END
```

```
@IPT   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/   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,ZETAIN
       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        CF3VT(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
 C
      X        (24)
       WRITE (6,100)
   100 FORMAT ('1' 37X '********************** LIQUID-VAPOR REGION ********
      X*************' ///)
       LFLAG = 0
       HL = H
       C3V = 0.
       C3L = C3
       W3L = W3
       AP = 1.0
   1   CALL UNBAR (AVSZ,1,Z,0.,A,KK)
       CALL UNBAR (APVSZ,1,Z,0.,AP,KK)
       CALL UNBAR (DELVSZ,1,Z,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 (CF3VT,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 SGRAD (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,
      X              CFBAR)
       IF (1165.-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
      XST 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 = -((HR*RHOM*DELTA+HC*AP*TITP)+(KC3V*AP*CICP3V*(DELHC*((H-HL)
     λ       /(HLV-HL)))))/G
      DELTZ = ZCON/DHDZ
      ZTEST = ZEND/10.
      IF (DELTZ.GT.ZTEST) DELTZ = ZTEST
      DMBRDZ = (-MBARV)*((Dw1DZ/M1+Dw2DZ/M2+Dw3VDZ/M3+Dw4DZ/M4)/(w1/M1+
     λ          w2/M2+w3V/M3+w4/M4))
      DPDZ = ((DELTA-1.)/DELTA**3)*(1.75+(75.*MU*(1.-DELTA))/(A*G))*(G**
     λ        2./(64.4*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+RHOV/RHO*(1./P*DPDZ+1./MBARV*
     λ          DMBRDZ))
      RHOFAC = (-1./(1.-w3L))*(Dw3LDZ+RHOV/RHO*(1./P*DPDZ+1./MBARV*
     λ           DMBRDZ))
      DRHODZ = DRHODZ*((1.-EXP(-RHOFAC*DELTZ))/(RHOFAC*DELTZ))
      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*DELTZ
      C2 = C2+DC2DZ*DELTZ
      C3V = C3V+DC3VDZ*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)
      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*DELTZ
      Z = Z+DELTZ
      P = P+DPDZ*DELTZ
      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*DELTZ
      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 (6,300)
300   FORMAT (///11X,'Z',9X,'TEMP',11X,'C1',10X,'C2',10X,'C3L',9X,'C3V',
     λ9X,'C4')
      WRITE (6,400) Z,T,C1,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
    XAC4'/)
     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 (6,56)
56   FORMAT (///58X,16HTHAT'S ALL FOLKS )
     CALL EXIT
60   DELTZ = -C3LP/DC3LDZ
     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,MBARV,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,ZETAIN
       COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
      X       ,MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
      X        CF3VT(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, 02, H20,
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,Z,0.,A,KK)
       CALL UNBAR (APVSZ,1,Z,0.,AP,KK)
       CALL UNBAR (DELVSZ,1,Z,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 (CF3VT,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 SGRAD (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,CPS3V,
      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 = -(HR*RHOM*DELTA+HC*AP*TITP)/G
       IF (NONE.EQ.1) GO TO 23
       DELTZ = ZCON/DHDZ
       ZTEST = ZEND/10.
       IF (DELTZ.GT.ZTEST) DELTZ = 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.)/DELTA**3)*(1.75+(75.*MU*(1.-DELTA))/(A*G))*(G**
```

```
     X         2./(64.4*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 (6,300)
 300  FORMAT (///11X,'Z',9X,'TEMP',9X,'C1',10X,'C2',10X,'C3',10X,'C4',8X
     X,'MFRAC1',6X,'MFRAC2',6X,'MFRAC3',6X,'MFRAC4')
      WRITE (6,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
 400  FORMAT (/6X,E10.5,2X,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 (6,1111) H,P
 1111 FORMAT(/10X,'H(ENTHALPY) = ',E10.5,5X,'PRESSURE = ',E10.5)
      IF (LFLAG.EQ.1) GO TO 54
      IF (ABS(ZEND-Z)-EPS) 54,54,1
 50   WRITE (6,300)
      WRITE (6,400) Z,T,C1,C2,C3,C4,MFRAC1,MFRAC2,MFRAC3,MFRAC4
```

```
      WRITE (6,1111) H,P
      NONE = 1
      CICP1 = 0.
      CICP2 = 0.
      CICP3V = 0.
      TITP = 0.
      DELTZ = (ZEND-Z)/10.
      GO TO 1
  60  DELTZ = ZEND-ZP
      Z = ZEND
      C1 = C1P
      C2 = C2P
      C3 = C3P
      C4 = C4P
      T = TI
      H = HP
      P = PP
      LFLAG = 1
      NONE = 1
      GO TO 20
 136  PCHECK = -1.
  54  RETURN
      END
```

```
@IPT   FOR SGRAD
        SUBROUTINE SGRAD (RHO,KC1,KC2,KC3V,HC,CICP1,CICP2,CICP3V,TITP,TPS,
      ^         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,
      ^         ZCON,ZEND,G,DHDZ,W3,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,
      ^         A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETAIN
        COMMON /BLOCK2/ CONST,PPP,POWERR(2),POWERP(1),RGM(2),PGM(1),
      ^          RALPH(2),PALPH(1),KGM,ALPHAK,NR,NP,DOR(2),DOP(1)
        COMMON /BLOCK3/ DPR(2),DPP(1),KCR(2),KCP(1),CPSR(2),CPSP(1),CIR(2)
      ^          ,CIP(1),MR(2),MP(1),FR(2),FP(1),CPXR(2,100),CPXP(1,100),K0,
      ^          XOA,GAMMA,BETA,NA1,COEFR(2),COEFP(1),HFACTR,RFACTR
        COMMON /TABLES/ AVSZ(99),APVSZ(99),DELVSZ(99),HRVST(36),MU1VST(34)
      ^         ,MU2VST(34),MU3VST(32),MU4VST(34),CF1VST(34),CF2VST(34),
      ^          CF3VT(34),CF3ST(20),CF4VST(20),VPVST(36),TVSVP(36),DHCVST
      ^          (24)
        COMMON /FLAGS/ MMM,JJJ
        DIMENSION  CPOX(100),PCPOX(100),DX(100),RHET(100),DIR(2),DIP(1),
      ^             TPX(100),RGAMMA(2),PGAMMA(1),REXP(2),
      ^             PEXP(1),RK0(2),PK0(1),RK0TRM(2),PK0TRM(1)
        DIMENSION  REACTN(2),PRODCT(1)
  C    DEFINE DP FUNCTION
        DPF(X,Y,Z) = 14.7*Y/Z*(X/492.)**1.823*(1.-EXP(-.0672*Z*492./
      ^                 (14.7*X)))
  C    DEFINE KC FUNCTION
        KCF(A,B,C,D,E) = .01*A/B*(C/(B*D))**-.667*(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
        JJJ = 1
        NR = 2
        NP = 1
        CONST = 1.
        PPP = 0.
        KGM = 5000.
        NX0 = 0
        ZETA = 1.0
  C  ..... SET INITIAL PRODUCT VALUES (H20) .....
        PRODCT(1) = 'H20'
        CIP(1) = C3V
        DOP(1) = D03
        MP(1) = M3
        FP(1) = 0.
        POWERP(1) = 0.
        PGM(1) = 0.
        PALPH(1) = 0.
        COEFP(1) = 1.
        IF (PRIME.NE.'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) = '02'
        CIR(1) = C1
        CIR(2) = C2
        DOR(1) = D01
        DOR(2) = D02
        MR(1) = M1
```

```
      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 216
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
      DOR(1) = DO2
      DOR(2) = DO1
      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 = 0.126
      RFACTR = 7.936
 216  CONTINUE
C    SET INITIAL WEIGHTED AVERAGE FRACTIONS
      WAF1 = .8
      WAF2 = .2
      JWAF = 0
      XO = 0.
      JXO = 0
C    SET UP INITIALIZATION FOR EACH ENTRY TO 'SGRAD'
 1    LTFLG = 0
      NPART = 50
      LP1 = 1
      IPSP = 0.
C    INITIALIZE REACTANT PARAMETERS
      DO 110 I=1,NR
      DIR(I) = DOR(I)*14.7/P*(T/492.)**1.823
 110  CONTINUE
C    INITIALIZE PRODUCT PARAMETERS
      DIP(1) = DOP(1)*14.7/P*(T/492.)**1.823
 112  DO 114 I=1,NR
 114  KCR(I) = KCF(G,RHO,MU,DIR(I),AP)
      DO 115 I=1,NP
 115  KCP(I) = KCF(G,RHO,MU,DIP(I),AP)
      HC = .74*G*CPBAR*(G/(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(I) = DPF(T,DOR(I),P)
        DPRP = DPR(1)
        IF (I.EQ.1) GO TO 151
        QUOA = KCR(I)/KCR(1)
~~      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.
  151   CONTINUE
        DO 152 I=1,NP
        DPP(I) = DPF(T,DOP(I),P)
~~      QUOC = KCR(1)/KCP(I)~~
        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.
  152   CONTINUE
        CMCPN = CIR(1)-CPSR(1)
~~      CALL UNBAR (HRVST,1,T,0.,HR1,KK)~~
        HR1 = HR1*HFACTR
        SUM = 0.
  680   IF (LP1.EQ.1) GO TO 6
  40    TPSPP = 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,1,TPS,0.,HR1,KK)
        HR1 = HR1*HFACTR
        DPR(1) = DPF(TPS,DOR(1),P)
~~      DPR(2) = DPF(TPS,DOR(2),P)~~
        DPP(1) = DPF(TPS,DOP(1),P)
        DPRP = DPR(1)
        HRP = HR1
        TMTPN = 1-TPS
        DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
~~C   RETURN POINT IN ITERATION SCHEME TO OBTAIN X0~~
  61    GAMMA = KGM/TPS
        BETA = -CPSR(1)*HR1*DPR(1)/(KP*TPS)
        K0 = ALPHAR*EXP(-GAMMA)
C    CALCULATE X0
        X0P = X0
~~      X0 = A-ZETA*CPSR(1)/DCPDX~~
        X0A = X0/A
        IF (X0) 11,12,12
  11    X0 = 0.
        X0A = 0.
        X0P = 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
~~      QUOA = KCR(I)/KCR(1)~~
```

```
      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,NP~~
      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
~~      DCPDX = CIR(1)/A~~
      TPS = T-(SUM+HR1*DPR(1)*DCPDX)/HC
      IF (TPS.LT.0.) TPS = 1.
      CALL UNBAR (HRVST,1,TPS,0.,HR1,KK)
      HR1 = HR1*HFACTR
      DPR(1) = DPF(TPS,DOR(1),P)
~~      DPR(2) = DPF(TPS,DOR(2),P)~~
      DPP(1) = DPF(TPS,DOP(1),P)
      DPA = DPR(1)
      DPRP = DPR(1)
      HRP = HR1
      TMTPN = T-TPS
~~     GAMMA = KGM/TPS~~
      BETA = -CPSR(1)*HR1*DPR(1)/(KP*TPS)
      K0 = ALPHAK*EXP(-GAMMA)
      WRITE (6,132) EP1,TPS
  132 FORMAT (///37X,'WE HAVE CALCULATED A NEGATIVE X0 DURING ITERATION
     XNO',I3, /,39X,'SET X0 = 0. , CALCULATE TPS =',E11.5,' , AND CONTIN
~~     XUE ')~~
      GO TO 131
C     INTEGRATE FOR CP EQUATION
   12 CONTINUE
      CALL TRAP2 (X0A,1.,NPART,RIESUM)
C     MMM IS KHET INDICATOR FOR CALCULATING CP(X) PROFILE
~~C       MMM=0 IMPLIES CURRENT CP(X) PROFILE O.K.~~
C       MMM=1 IMPLIES CONCENTRATION HAS PENETRATED VERY RAPIDLY THRU CATALYST
C             PARTICLES (X0 = 0.)
C       MMM=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 (MMM.EQ.0) GO TO 15~~
      GO TO (11,14), MMM
   14 NPART = 100
      X0 = 0.
      X0A = 0.
      GO TO 12
~~C     CALCULATE NEW CPS~~
   15 CPS0 = CPSR(1)
      CMCPO = CMCPN
      CPSRPP = 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 = DCPDX*DPR(1)
~~      TGRAD =HC*(T-TPS)~~
```

```
      TPSPP = TPSP
      TPSP = TPS
      TMTPO = TMTPN
   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*HFACTR
      DPR(1) = DPF(TPS,DOR(1),P)
      DPR(2) = DPF(TPS,DOR(2),P)
      DPP(1) = DPF(TPS,DOP(1),P)
      DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
      TMTPN = T-TPS
      GAMMA = KGM/TPS
      BETA = -CPSR(1)*HR1*EPR(1)/(KP*TPS)
      KO = ALPHAK*EXP(-GAMMA)
C     TEST TEMPERATURE,CONCENTRATION FOR 5% LIMIT
      IF (ABS((TMTPO-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 (AMIN1(CPSR(1),CPSRP,CPSRPP)-CPSRP) 818,820,818
  818 IF (AMAX1(CPSR(1),CPSRP,CPSRPP)-CPSRP) 46,820,46
  820 IF (NXO.EQ.1) GO TO 826
      NXO = 1
      ZETA = ZETAIN
      WRITE (6,825)
  825 FORMAT (//5X,'CPSCAL CHANGED DIRECTION -- NEW EQ. FOR CPXF USED')
      GO TO 216
   46 CPSR(1) = (CPSR(1)*WAF2+CPSO*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(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.
  139 CONTINUE
C     CALCULATE CPS'S FOR PRODUCTS
  157 DO 140 I=1,NP
      QUOC = KCR(1)/KCP(I)
      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.
  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
```

```
      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 (6,98)
 98   FORMAT (//15X,'UNABLE TO FIND SUITABLE X0 AFTER  3  TRIES OF 25  I
     XTERATIONS EACH ... SET CPS = 0. AND CONTINUE')
      CPSR(1) = 0.
      CPSR(2) = CIR(2)-(GOOA*GOOB*(CIR(1)-CPSR(1)))
~~      IF (CPSR(2).LT.0.) CPSR(2) = 0.~~
      CPSP(1) = CIP(1)-(GOOC*GOOD*(CPSR(1)-CIR(1)))
      IF (CPSP(1).LT.0.) CPSP(1) = 0.
      TPS = T-(SUM+HR1*KCR(1)*(CIR(1)-CPSR(1)))/HC
      CALL UNBAR (HRVST,1,TPS,0.,HR1,KK)
      HR1 = HR1*HFACTR
~~      DPR(1) = DPF(TPS,DOR(1),P)~~
      DPR(2) = DPF(TPS,DOR(2),P)
      DPP(1) = DPF(TPS,DOP(1),P)
      DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
      GO TO 134
C     SATISFACTORY X0 HAS BEEN FOUND
~~ 828  NX0 = 2~~
 70   WRITE (6,16) LP1,X0
 16   FORMAT (////46X,'SATISFACTORY X0 FOUND AFTER',I3,' TRIES' /
     X          57X,'X0 =',E12.5)
      IF (NX0.NE.2) GO TO 827
      WRITE (6,826)
~~ 826  FORMAT (/5X,'CPSCAL CHANGED DIRECTION USING NEW CPXF EQ.  ---  USE~~
     X X0 FOUND AT THIS POINT')
 827  IF (X0A.LT..9995) GO TO 131
      CPSR(1) = 0.
      CPSR(2) = CIR(2)-(GOOA*GOOB*(CIR(1)-CPSR(1)))
      IF (CPSR(2).LT.0.) CPSR(2) = 0.
~~      CPOX(NX1) = 0.~~
      CPSP(1) = CIP(1)-(GOOC*GOOD*(CPSR(1)-CIR(1)))
      IF (CPSP(1).LT.0.) CPSP(1) = 0.
      TPS = T-(SUM+HR1*KCR(1)*(CIR(1)-CPSR(1)))/HC
      CALL UNBAR (HRVST,1,TPS,0.,HR1,KK)
      HR1 = HR1*HFACTR
~~      DPR(1) = DPF(TPS,DOR(1),P)~~
      DPR(2) = DPF(TPS,DOR(2),P)
      DPP(1) = DPF(TPS,DOP(1),P)
      DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
      WRITE (6,193)
 193  FORMAT (// 50X 'X0/A GREATER THAN .9995 .. SET CPS = 0. AND CONTIN
     XUE' )
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 136
 135  CICP1 = CIR(2) -CPSR(2)
~~      CICP2 = CIR(1)~~
```

```
      KC1 = KCR(2)
      KC2 = KCR(1)
  136 CONTINUE
      CICP3V = CIP(1)-CPSP(1)
      ~~KC3V = KCP(1)~~
      TITP = T-TPS
      WRITE (6,610) CICP1,CICP2,CICP3V,TITP
      RETURN
  133 LP2 = 1
      NX = 24
      ~~NX1 = NX+1~~
      NXM1 = NX-1
      DPA = DPR(1)
      CPXR(1,NX1) = CPSR(1)
  291 X0A = X0/A
      V = -KCR(1)/DPR(1)
      ~~IHT1 = 1~~
      K = 2
      R1 = 0.
      R2 = 0.
      PS1 = 0.
      PS2 = 0.
      ~~DELX0A = (1.-X0A)/FLOAT(NX)~~
C    CALCULATE PROFILE CURVES FOR INTEGRAND FUNCTIONS
      XA = X0A
      DO 770 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-X0A)/(1.-X0A))**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
      ~~QU01 = DPR(1)/DPR(I)~~
      QU02 = COEFR(I)*MR(I)/(COEFR(1)*MR(1))
      CPXR(I,J)=CPSR(I)     +QU01*QU02*(CPXR(1,J)-CPXR(1,NX1))
      IF (CPXR(I,J).LT.0.) CPXR(I,J)=0.
  141 CONTINUE
C  CALCULATE CPS'S FOR PRODUCTS
  ~~158 DO 142 I=1,NP~~
      QU03 = DPR(1)/DPP(I)
      QU04 = COEFP(I)*MP(I)/(COEFR(1)*MR(1))
      CPXP(I,J)=CPSP(I)     +QU03*QU04*(CPXR(1,NX1)-CPXR(1,J))
      IF (CPXP(I,J).LT.0.) CPXP(I,J)=0.
  142 CONTINUE
      ~~QUOTA = 1.~~
      QUOTB = 1.
      DO 143 I=1,NR
      POWA = CPXR(I,J)**PR(I)
      QUOTA = QUOTA*POWA
  143 CONTINUE
      ~~DO 144 I=1,NP~~
      IF (PP(I)) 1000,1001,1000
 1000 POWB = CPXP(I,J)**PP(I)
      GO TO 1002
 1001 POWB = 1.
 1002 QUOTB = QUOTB*POWB
  ~~144 CONTINUE~~
```

```
C     CALCULATE GENERALIZING TERM   (ADSORPTION)
      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
      RK0(I) = RALPH(I)*EXP(-RGAMMA(I))
      IF (RK0(I)) 1003,1004,1003
 1003 RK0TRM(I) = RK0(I)*CPXR(I,J)**POWERR(I)*EXP(REXP(I))
      GO TO 1007
 1004 RK0TRM(I) = 0.
 1007 SUMTRM = SUMTRM+RK0TRM(I)
  606 CONTINUE
      DO 607 I=1,NP
      PGAMMA(I) = PGM(I)/T
      PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
      PK0(I) = PALPH(I)*EXP(-PGAMMA(I))
      IF (PK0(I)) 1005,1006,1005
 1005 PK0TRM(I) = PK0(I)*CPXP(I,J)**POWERP(I)*EXP(PEXP(I))
      GO TO 1008
 1006 PK0TRM(I) = 0.
 1008 SMTERM = SMTERM+PK0TRM(I)
  607 CONTINUE
      ADSORB = (CONST+SUMTRM+SMTERM)**PPP
      GENERL = 1./ADSORB
      RHET(J) = K0*QUOTA*QUOTB*EXP(GAMMA*BETA*(1.-CPXR(1,J)/CPXR(1,NX1))
     A   /(1.+BETA*(1.-CPXR(1,J)/CPXR(1,NX1))))
      RHET(J) = RHET(J)*GENERL
      RHET(J) = RHET(J)*RFACTR
      DX(J) = XA
      XA = XA+DELXOA
  770 CONTINUE
C     TAKE INTERVAL FUNCTN 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 = XOA+DELXOA
      CTRM = (A*V+1.)/(A*V)
C     INTEGRAL EQUATION FOLLOWS
C     CPOX(1) IS SPECIAL CASE ... X=X0
      DXL = XOA
      DXU = DXL+DELXOA
      RR1 = 0.
      DO 577 I=1,NX
      RR1 = RR1+RHET(I)*(EVAL2(DXL,DXU)-CTRM*EVAL1(DXL,DXU))
      DXL = DXU
      DXU = DXU+DELXOA
  577 CONTINUE
      CPOX(1) = CIR(1)-A*A/DPR(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,INT1
      R1 = R1+RHET(I)*EVAL1(XOA,XA)
      XOA = XA
      XA = XA+DELXOA
  772 CONTINUE
```

```
      R1 = R1*(1./XOA-CTRM)
      XAD = XA
      XA = XA-DELXOA
      DO 773 I=INT1,NXM1
      PS1 = PS1+RHET(I+1)*EVAL2(XA,XAD)
      PS2 = PS2+RHET(I+1)*EVAL1(XA,XAD)
      XA = XAD
      XAD = XAD+DELXOA
  773 CONTINUE
      R2 = PS1-CTRM*PS2
      INT1 = INT1+1
      CPOX(K) = CIR(1)-A*A/DPR(1)*(R1+R2)
      IF (CPOX(K).LT.0.) CPOX(K)=0.
      XOA = XO/A
      XA = XOA+DELXOA
      K = K+1
      R1 = 0.
      R2 = 0.
      PS1 = 0.
      PS2 = 0.
      IF (K.LE.NX) GO TO 769
C    CPOX(NX1) IS SPECIAL CASE ... X=A
      DXL = XOA
      DXU = DXL+DELXOA
      RR2 = 0.
      DO 578 I=1,NX
      RR2 = RR2+RHET(I)*EVAL1(DXL,DXU)
      DXL = DXU
      DXU = DXU+DELXOA
  578 CONTINUE
      CPOX(NX1) = CIR(1)-A*A/DPR(1)*(1.-CTRM)*RR2
      IF (CPOX(NX1)) 190,190,191
  190 CPOX(NX1) = 0.
      CPSR(1) = 0.
      CPSR(2) = CIR(2)-(QUCA*QUOB*(CIR(1)-CPSR(1)))
      IF (CPSR(2).LT.0.) CPSR(2) = 0.
      CPSP(1) = CIP(1)-(QUCC*QUOD*(CPSR(1)-CIR(1)))
      IF (CPSP(1).LT.0.) CPSP(1) = 0.
      TPS = T-(SUM+HR1*KCR(1)*(CIR(1)-CPSR(1)))/HC
      CALL UNBAR (HRVST,1,TPS,0.,HR1,KK)
      HR1 = HR1*HFACTR
      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 (6,192)
  192 FORMAT (//10X'CONCENTRATIONS CALCULATED FROM INTEGRATION SECTION N
     XEGATIVE OR ZERO ... SET CPS = 0. AND CONTINUE')
      GO TO 154
C    CALCULATE A NEW TPS
  191 CONTINUE
      HRP = HR1
      DPRP = DPR(1)
      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*HFACTR
      DPR(1) = DPF(TPS,DUR(1),P)
      DPR(2) = DPF(TPS,DUR(2),P)
```

```
      DPP(1) = DPF(TPS,DOP(1),P)
      DCPDX = KCR(1)/DPR(1)*(CIR(1)-CPSR(1))
      TMTPO = TMTPN
      TMTPN = T-TPS
C     TWO PASSES NEEDED BEFORE CHECK ON TEMP,CONC CAN BE MADE
   33 IF (LP2.EQ.1) GO TO 27
      CMCPO = CMCPN
      CMCPN = CIR(1)-CPOX(NX1)
      IF (ABS(TMTPO-TMTPN)/TMTPN - .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 56
C  AVERAGE PRESENT AND PAST CALCULATED PROFILES EVERY 5TH PASS TO SMOOTH
   57 CPXR(1,I) = (CPOX(I)+PCPOX(I))/2.
C  STORE PRESENT CALCULATED PROFILE
   56 PCPOX(I) = CPOX(I)
   55 CONTINUE
      CMCPN = CIR(1)-CPXR(1,NX1)
      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*HFACTR
      DPR(1) = DPF(TPS,DOR(1),P)
      DPR(2) = DPF(TPS,DOR(2),P)
      DPP(1) = DPF(TPS,DOP(1),P)
      DCPDX = KCR(1)/DPRP*(CIR(1)-CPXR(1,NX1))
      TMTPO = TMTPN
      TMTPN = T-TPS
      LP2 = LP2+1
      IF (LP2-50) 29,29,30
   30 WRITE (6,16) CPOX(NX1)
   16 FORMAT (///31X,52HUNABLE TO CONVERGE ON CPS IN  50 TRIES ... CP(X/
     XA) =,E12.5)
      WRITE (6,83) GRAD,TGRAD
      GO TO 26
   29 GAMMA = KGA/TPS
      BETA = -CPXR(1,NX1)*HR1*DPR(1)/(KP*TPS)
      KO = ALPHAK*EXP(-GAMMA)
      DO 752 I=2,NR
      QUOA = KCR(1)/KCR(I)
      QUOB = COEFR(I)*MR(I)/(COEFR(1)*MR(1))
      CPSR(I) = CIR(I)-(QUOA*QUOB*(CIR(1)-CPXR(1,NX1)))
      IF (CPSR(I).LT.0.) CPSR(I)=0.
  752 CONTINUE
      DO 753 I=1,NP
      QUOC = KCR(1)/KCP(I)
      QUOD = COEFP(I)*MP(I)/(COEFR(1)*MR(1))
      CPSP(I) = CIP(I)-(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(I))
      CPXR(1,I) = CPOX(I)
```

```
180   CONTINUE
      WRITE (6,779)
779   FORMAT ( ////34X,'REACTANT AND PRODUCT CONCENTRATION PROFILES FOR
     XFINAL ITERATION')
      DO 777 I=1,1
      WRITE (6,23) REACTN(I),REACTN(I),REACTN(I),REACTN(I),REACTN(I),
     X        (DX(J),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,I3,6H TRIES /
     X          45X,27HCP(X) AT PARTICLE SURFACE =,E12.5 )
      DCPJDX = DCPDX*DPR(1)
      TGRAD = HC*(T-TPS)
      WRITE (6,83) DCPJDX,TGRAD
83    FORMAT (46X,'KCR(1)*(CIR(1)-CPSR(1)) =',E12.5 / 54X,'HC*(T-TPS) ='
     X,E12.5)
      WRITE (6,185) DCPDX
185   FORMAT (56X,'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 = CIP(1) - CPXP(1,NX1)
      KC3V = KCP(1)
      CPS3V = CPXP(1,NX1)
      TITP = T - TPS
      WRITE (6,610) CICP1,CICP2,CICP3V,TITP
610   FORMAT (/5X,'C1-CPS1 = ',E10.5,10X,'C2-CPS2 = ',E10.5,10X,'C3V-CPS
     X3V = ',E10.5,10X,'T-TPS = ',E10.5/)
26    RETURN
      END
```

```
WIPT  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,K0,KP,KCR,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,CF3L,R,DELHF,ALPHA,AGM,AEXP,BEXP,
     X      A,AP,DELTA,C3V,KP,MU,PRIME,Z,NX0,ZETA,ZETAIN
      COMMON /BLOCK2/ CONST,PPP,POWERR(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),KCR(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),K0,
     X       X0A,GAMMA,BETA,NX1,COEFR(2),COEFP(1),HFACTR,RFACTR
      COMMON /FLAGS/ MMM,JJJ
      DIMENSION  RGAMMA(2),PGAMMA(1),REXP(2),
     X            PEXP(1),RK0(2),PK0(1),RK0TRM(2),PK0TRM(1),
     X            CPXR1(2),CPXR2(2),CPXP1(1),CPXP2(1),CPXRR(2),CPXPP(1)
C     DEFINE RHET FUNCTION
      RHETF(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.EQ.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,X0A,CPSR(1))
      CPXR2(1) = CPXF(XUPPER,X0A,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
 22   DO 11 I=1,NP
      QUO3 = DPR(1)/DPP(I)
      QUO4 = COEFP(I)*MP(I)/(COEFR(1)*MR(1))
      CPXP1(I) = CPSP(I)+QUO3*QUO4*(CPSR(1)-CPXR1(1))
      CPXP2(I) = CPSP(I)+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
```

```
      DO 13 I=1,NP
      POWBA = CPXP1(I)**PP(I)
      POWBB = CPXP2(I)**PP(I)
      IF (PP(I)) 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
      RK0(I) = RALPH(I)*EXP(-RGAMMA(I))
      IF (CPXR1(I)) 608,608,609
  609 RK0TRM(I) = RK0(I)*CPXR1(I)**POWERR(I)*EXP(REXP(I))
      GO TO 610
  608 RK0TRM(I) = 0.
  610 SUMTRM = SUMTRM+RK0TRM(I)
  606 CONTINUE
      DO 607 I=1,NP
      PGAMMA(I) = PGM(I)/T
      PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
      PK0(I) = PALPH(I)*EXP(-PGAMMA(I))
      PK0TRM(I) = PK0(I)*CPXP1(I)**POWERP(I)*EXP(PEXP(I))
      SMTERM = SMTERM+PK0TRM(I)
  607 CONTINUE
      ADSORB = (CONST+SUMTRM+SMTERM)**PPP
      GENERL = 1./ADSORB
      RHET1 = RHETF(K0,QUOTAA,QUOTBA,GAMMA,BETA,CPXR1(1),CPXR2(1))*
     A        GENERL
      RHET1 = RHET1*RFACTR
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
      RK0(I) = RALPH(I)*EXP(-RGAMMA(I))
      IF (RK0(I)*CPXR2(I)) 614,614,416
  416 RK0TRM(I) = RK0(I)*CPXR2(I)**POWERR(I)*EXP(REXP(I))
      SUMTRM = SUMTRM+RK0TRM(I)
  614 CONTINUE
      DO 615 I=1,NP
      PGAMMA(I) = PGM(I)/T
      PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
      PK0(I) = PALPH(I)*EXP(-PGAMMA(I))
      PK0TRM(I) = PK0(I)*CPXP2(I)**POWERP(I)*EXP(PEXP(I))
      SMTERM = SMTERM+PK0TRM(I)
  615 CONTINUE
      ADSORB = (CONST+SUMTRM+SMTERM)**PPP
```

```
      GENERL = 1./ADSORB
      RHET2 = RHETF(K0,QUOTAB,QUOTBB,GAMMA,BETA,CPXR2(1),CPXR2(1))*
     A   GENERL
      RHET2 = RHET2*RFACTR
      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 6 J=1,N
C    CALCULATE CP(X) FOR KEY PARTICLE REACTANTS (TO USE IN RHET TERM)
      CPXRR(1) = CPXF(XPH,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(I) = CPSP(I)+QUO3*QUO4*(CPSR(1)-CPXRR(1))
 15   CONTINUE
C    CALCULATE RHET EXPRESSION
      QUOTA = 1.
      QUOTB = 1.
      DO 16 I=1,NR
      POWA = CPXRR(I)**PR(I)
      QUOTA = QUOTA*POWA
 16   CONTINUE
      DO 17 I=1,NP
      POWB = CPXPP(I)**PP(I)
      IF (PP(I)) 1005,1006,1005
 1006 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,NR
      RGAMMA(I) = RGM(I)/T
      REXP(I) = RGAMMA(I)*CONNUM/CONDEN
      RK0(I) = RALPH(I)*EXP(-RGAMMA(I))
      RK0TRM(I) = RK0(I)*CPXRR(I)**POWERR(I)*EXP(REXP(I))
      SUMTRM = SUMTRM+RK0TRM(I)
 622  CONTINUE
      DO 623 I=1,NP
      PGAMMA(I) = PGM(I)/T
      PEXP(I) = PGAMMA(I)*CONNUM/CONDEN
      PK0(I) = PALPH(I)*EXP(-PGAMMA(I))
      PK0TRM(I) = PK0(I)*CPXPP(I)**POWERP(I)*EXP(PEXP(I))
      SMTERM = SMTERM+PK0TRM(I)
 623  CONTINUE
      ADSORB = (CONST+SUMTRM+SMTERM)**PPP
      GENERL = 1./ADSORB
      RHET = RHETF(K0,QUOTA,QUOTB,GAMMA,BETA,CPXRR(1),CPXR2(1))*GENERL
      RHET = RHET*RFACTR
      IF (J.EQ.NM.AND.RHET.LE.0.) MMM=2
```

```
      IF (MMM.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
8     CONTINUE
      RIESUM = HH*(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         CF3VT(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 -5.290E+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
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
C  TABLE OF O2 VISCOSITY (LB/FT-SEC)  VS  TEMPERATURE (DEG R)
      DATA (MU2VST(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
C  TABLE OF H2O (VAPOR) VISCOSITY (LB/FT-SEC)  VS  TEMPERATURE (DEG R)
      DATA (MU3VST(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
C  TABLE OF HE VISCOSITY (LB/FT-SEC)  VS  TEMPERATURE (DEG R)
      DATA (MU4VST(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/
C
C
C                 ..... FIVE SPECIFIC HEAT TABLES FOLLOW .....
C
C  TABLE OF H2 SPECIFIC HEAT (BTU/LB-DEG R)  VS  TEMPERATURE (DEG R)
      DATA (CP1VST(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
C  TABLE OF O2 SPECIFIC HEAT (BTU/LB-DEG R)  VS  TEMPERATURE (DEG R)
      DATA (CP2VST(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 (CF3V(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     .4406   ,     .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
C     ------------------  MARCH 4, 1961 ------------                    UNBAR004
C     ------------------  MODIFIED 7/62 -----------------               UNBAR005
~~C     ------------------     TO DO QUADRATIC AND LINEAR INTERPOLATION ALSO~~ UNBAR006
C                                                                       UNBAR007
      II = IK+1                                                         UNBAR008
      N = 3                                                             UNBAR009
      N2= 2                                                             UNBAR010
            IF (T(II)-3.) 700,701,702                                   UNBAR011
~~700         IF (T(II)+0.) 60,701,704~~                                    UNBAR012
704         IF (T(II)-2.) 705,706,701                                   UNBAR013
705   N = 1                                                             UNBAR014
            GO TO 707                                                   UNBAR015
706   N = 2                                                             UNBAR016
707   N2= 1                                                             UNBAR017
~~701   II = II+1~~                                                         UNBAR018
702   N1 = N +1                                                         UNBAR019
            DO 50 L = II,II                                             UNBAR020
            IF ( T(L) + 0. ) 60,60,51                                   UNBAR021
60     KK = -1                                                          UNBAR022
       ZZ = 0.                                                          UNBAR023
        ~~GO TO 9999~~                                                      UNBAR024
51    NX = T(L)                                                         UNBAR025
            IF (T(L+1) + 0. ) 60,52,50                                  UNBAR026
52    NY = 0                                                            UNBAR027
            GO TO 53                                                    UNBAR028
50    NY = T(L+1)                                                       UNBAR029
~~53        CONTINUE~~                                                      UNBAR030
      KK   = 0                                                          UNBAR031
      KY   = 0                                                          UNBAR032
      XX   = XIN                                                        UNBAR033
      YY   = YIN                                                        UNBAR034
      J1   = II+2                                                       UNBAR035
      ~~J2   = NX+II+1~~                                                    UNBAR036
      IF(XX-T(J1))301,306,400                                           UNBAR037
400         DO 302 J=J1,J2                                              UNBAR038
            IF (XX-T(J)) 304,304,302                                    UNBAR039
302   CONTINUE                                                          UNBAR040
309   KK   = 2                                                          UNBAR041
      ~~XX   = T(J2)~~                                                      UNBAR042
308   JX1 = J2-N                                                        UNBAR043
            GO TO 305                                                   UNBAR044
301   KK   = 1                                                          UNBAR045
      XX   = T(J1)                                                      UNBAR046
306   JX1 = J1                                                          UNBAR047
            ~~GO TO 305~~                                                   UNBAR048
304         IF (J-J1-1) 301,306,307                                     UNBAR049
307         IF (J-J2)   303,308,309                                     UNBAR050
303   JX1 = J-N2                                                        UNBAR051
305   CONTINUE                                                          UNBAR052
      XINT   = XX                                                       UNBAR053
      ~~IF (NY) 1500, 1500, 3000~~                                          UNBAR054
1500        DO 1599 L=1,N1                                              UNBAR055
             X(L) = T(JX1)                                              UNBAR056
             LY = JX1 + NX                                              UNBAR057
             Y(L) = T(LY)                                               UNBAR058
1599   JX1 = JX1+1                                                      UNBAR059
      ~~I = 1~~                                                             UNBAR060
```

```
      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   = 6                                                          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 4050 MM=1,N1                                           UNBAR094
~~    Y(I+1) = Y(I+1) + T(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 = YY~~                                                       UNBAR101
      I=  1                                                             UNBAR102
 54   D  = 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 ) 57,58,57                                            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  D = D * TPAL1                                                     UNBAR117
              GO TO (711,712,713) ,N                                    UNBAR118
~~ 711 X(J)   = TPAL1/A(J+1)~~                                          ~~UNBAR119~~
```

```
          GO TO 55                                                      UNBAR120
  712  X(J)   = -TPAL1                                                  UNBAR121
          GO TO 55                                                      UNBAR122
  713  X(J)   = (X(J+2)-X(J))*TPAL1                                     UNBAR123
   55     CONTINUE                                                      UNBAR124
       A(1) = A(N+2)                                                    UNBAR125
       ZZ = 0.                                                          UNBAR126
         DO 56 J=1,N1                                                   UNBAR127
         X(J) = D/(A(J)*A(J+1)*   X(J))                                 UNBAR128
       ZZ = ZZ + Y(J)*   X(J)                                           UNBAR129
   56     CONTINUE                                                      UNBAR130
   59     IF (I) 5098,5098,9999                                         UNBAR131
 9999  KK   = KK+KY                                                     UNBAR132
          RETURN                                                        UNBAR133
       END
```

APPENDIX III

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

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 X 10^4 N/M^2)

FEED MIXTURE RATIO 1.0 LB O_2/LB H_2 (1.0 KG O_2/KG H_2) FEED TEMPERATURE = 210 DEG R (117 DEG K)

MASS FLOW RATE = 1.28 LB/FT^2 – SEC (6.25 KG/M^2 – SEC) NO HELIUM DILUTION

BED CONFIGURATION: ALL 14–18 MESH CATALYST PARTICLES

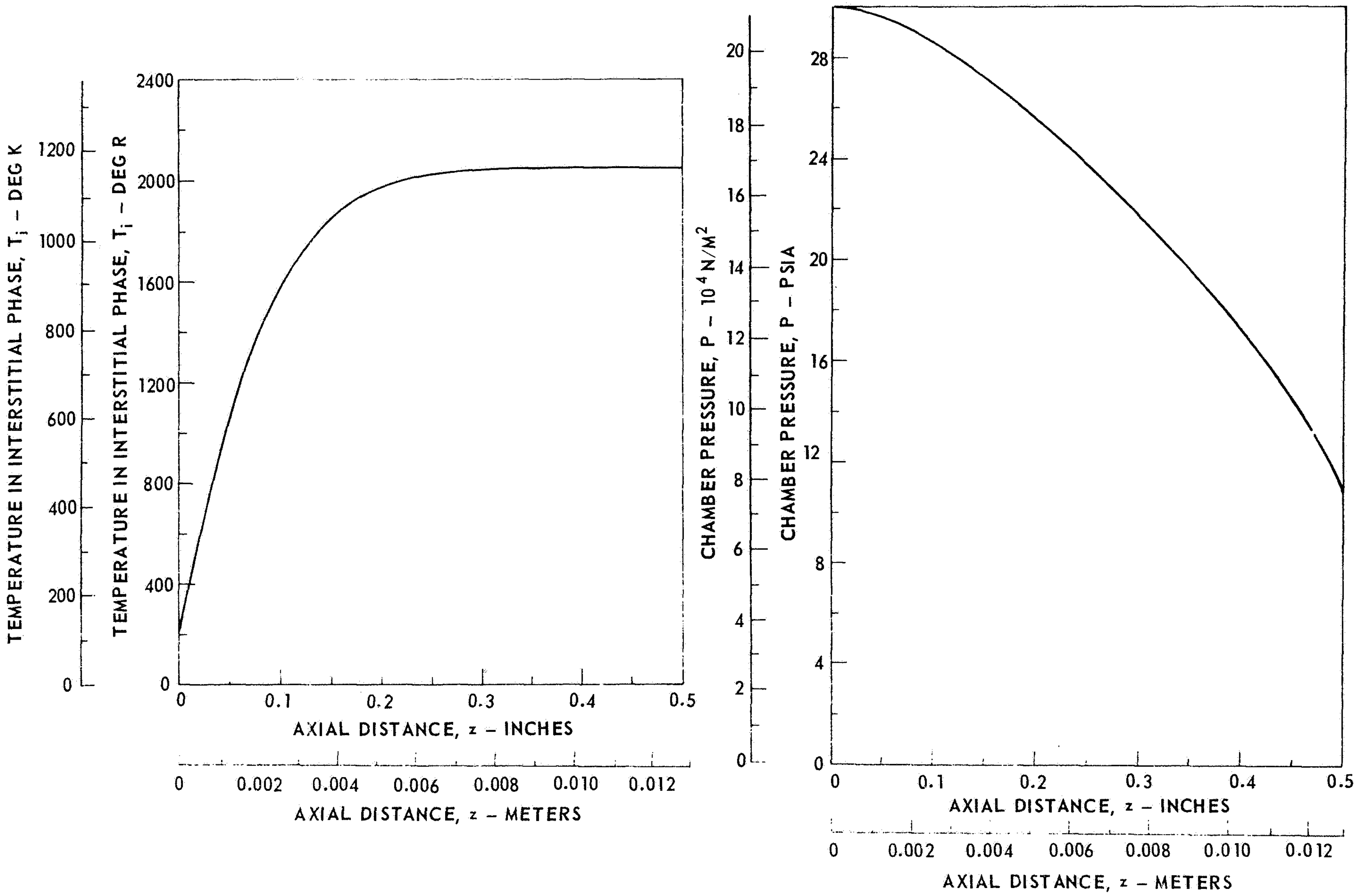


FIG. 1

FIG. 2

AXIAL CONCENTRATION PROFILES FOR A LOW NOMINAL CHAMBER PRESSURE

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

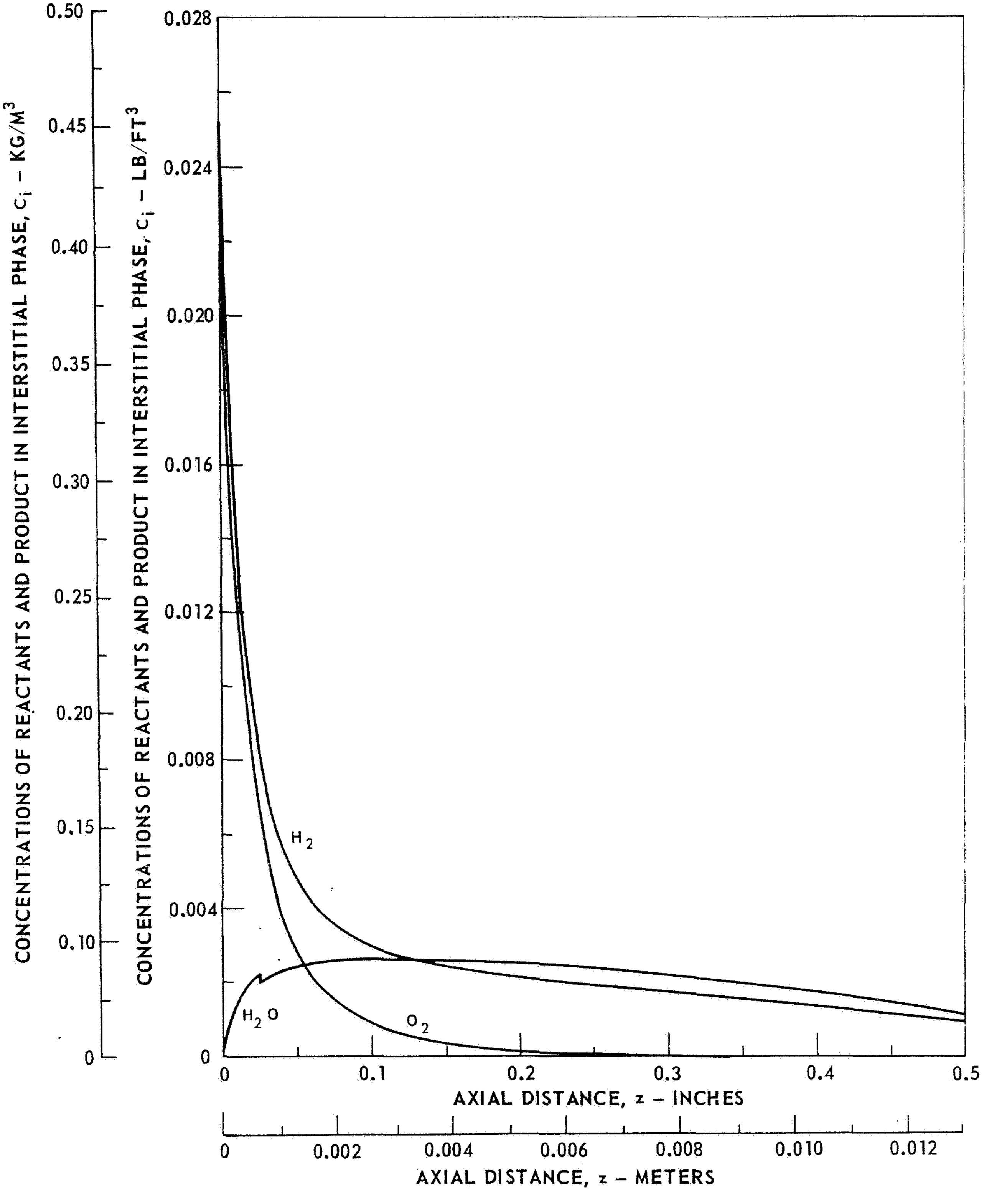
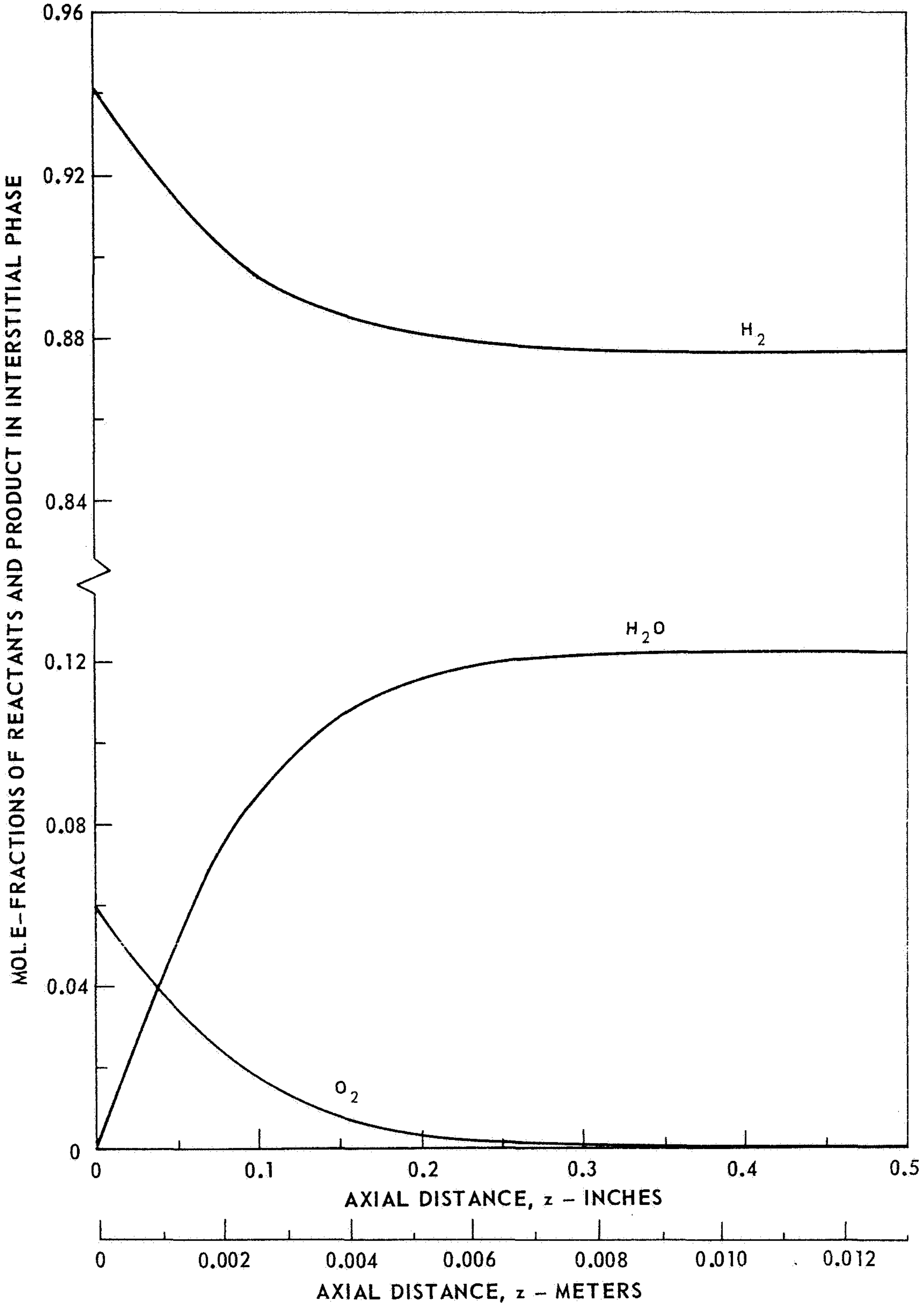


FIG. 3

AXIAL MOLE-FRACTION PROFILES FOR A LOW NOMINAL CHAMBER PRESSURE

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



EFFECT OF PROPELLANT FEED TEMPERATURE ON AXIAL TEMPERATURE PROFILES

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 X 10^4 N/M^2)

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

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

NO HELIUM DILUTION

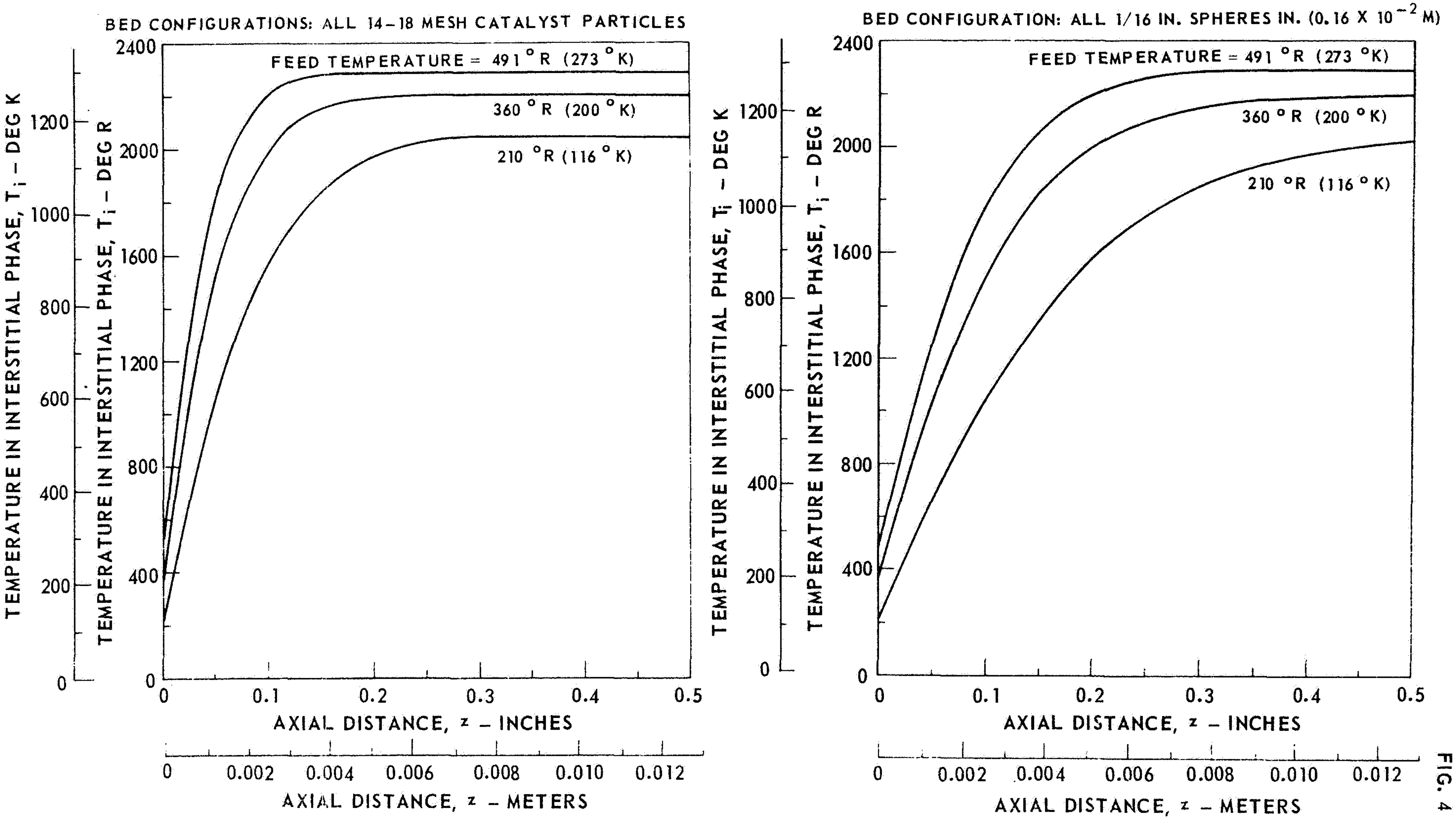


FIG. 4

EFFECT OF STOICHIOMETRY ON AXIAL TEMPERATURE PROFILES

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89×10^4 N/M^2)
FEED TEMPERATURE = 210 DEG R (117 DEG K)
MASS FLOW RATE = 1.28 LB/FT^2 – SEC (6.25 KG/M^2 – SEC)

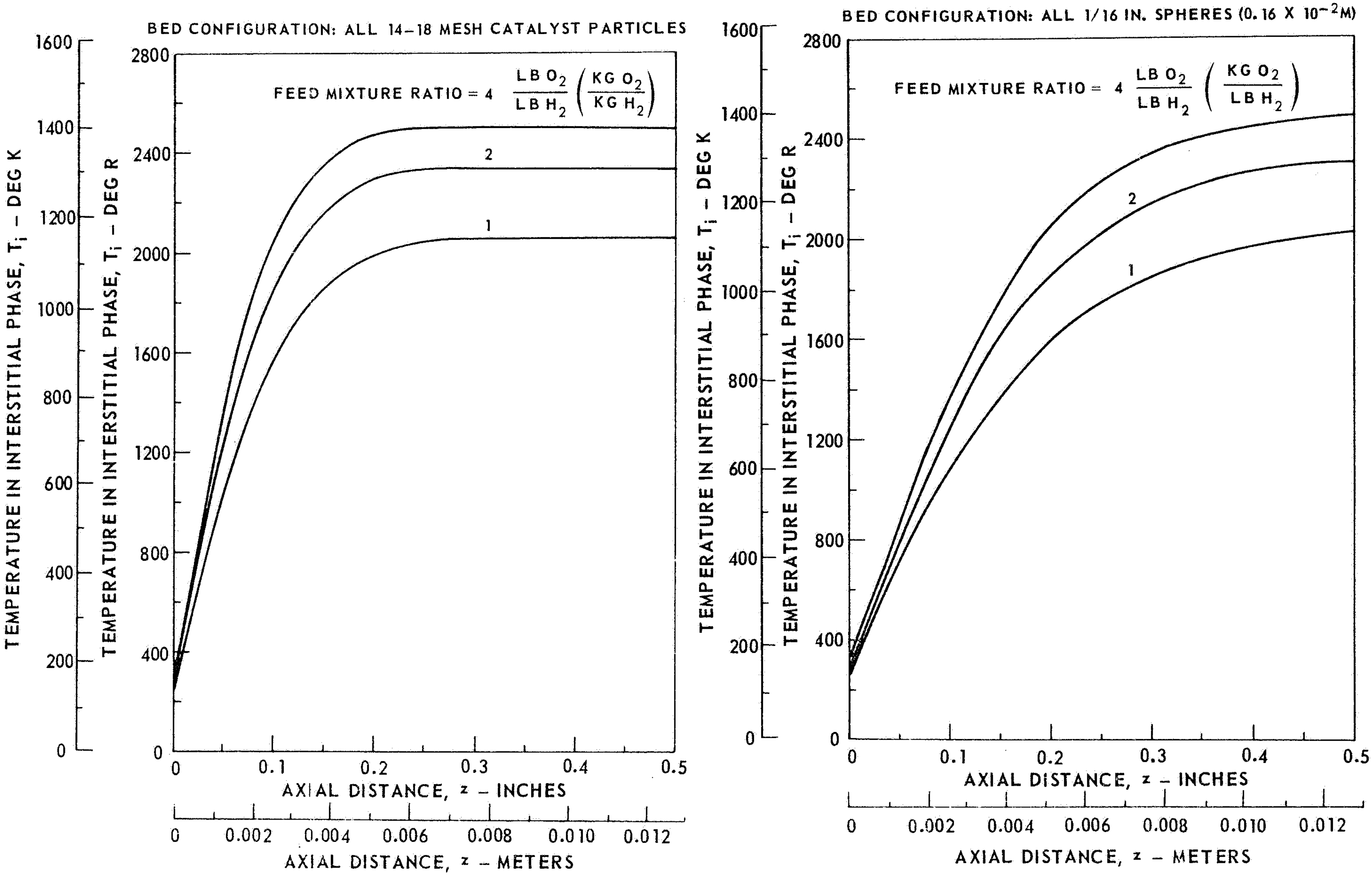


FIG. 5

EFFECT OF HELIUM DILUTION ON AXIAL TEMPERATURE PROFILES

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89 X 10^4 N/M^2)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

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

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

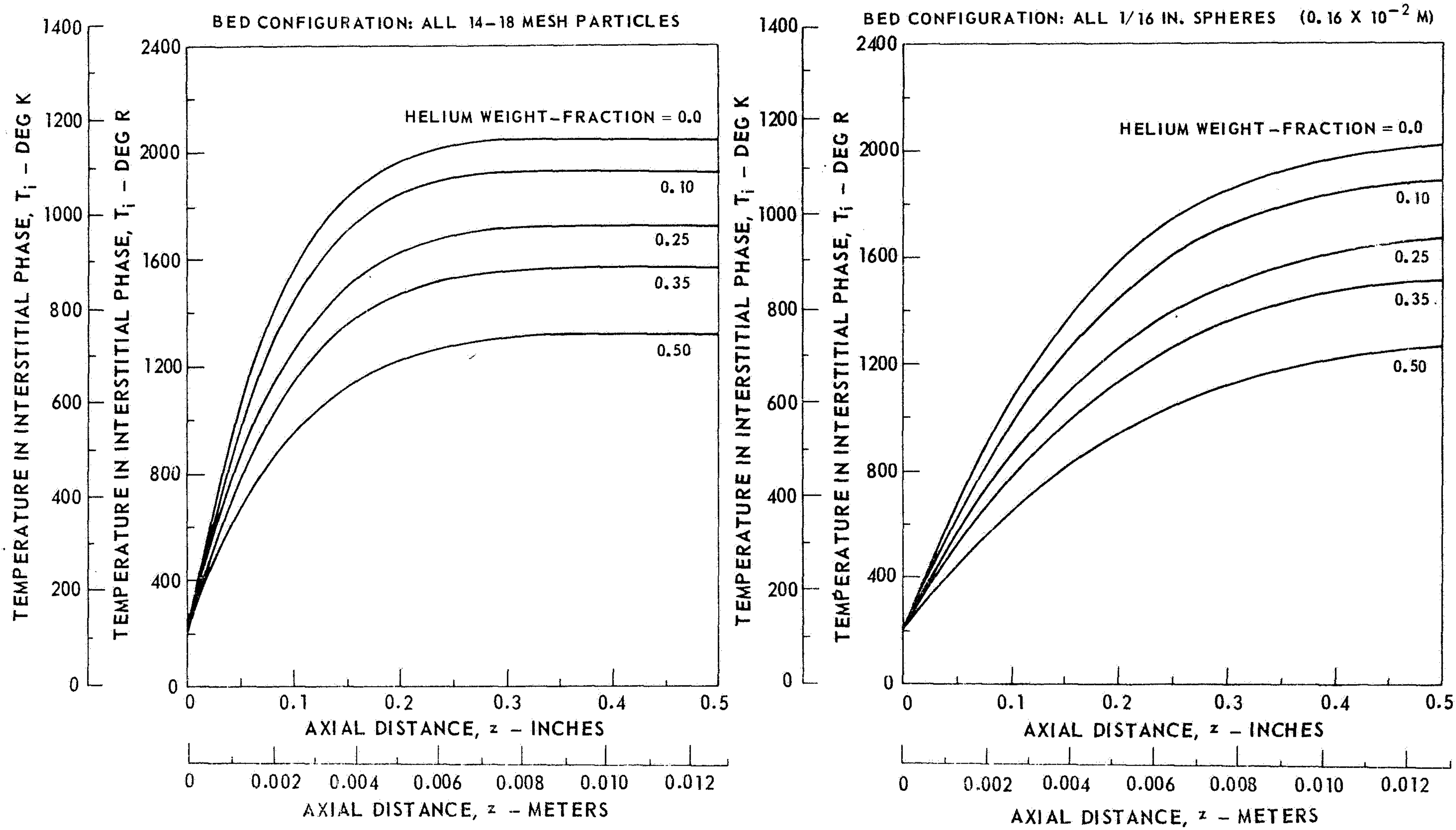


FIG. 6

EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

NO HELIUM DILUTION

NOMINAL CHAMBER PRESSURE = 10 PSIA (6.89×10^4 N/M^2)

FEED TEMPERATURE = 210 DEG R (117 DEG K)

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

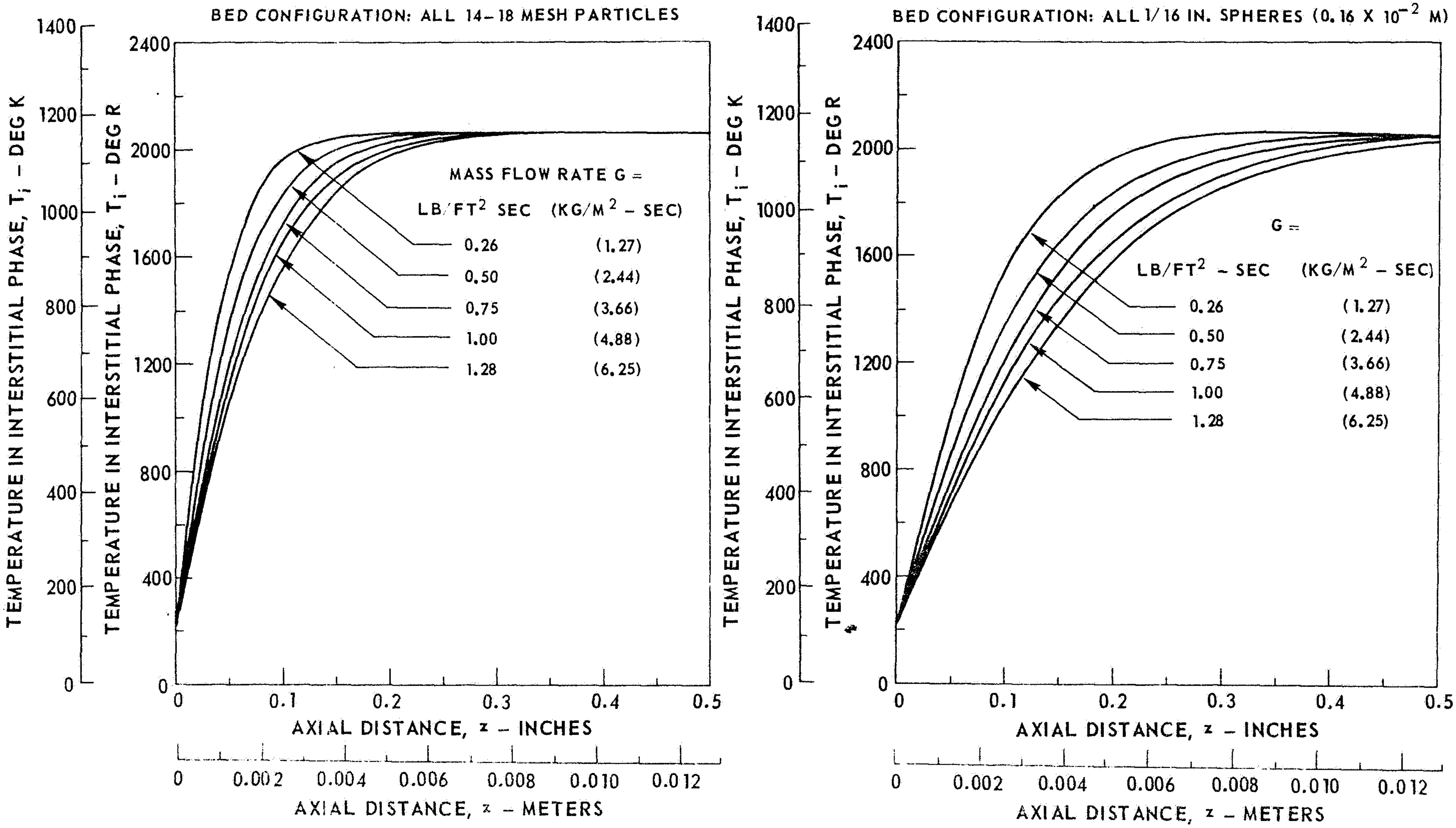


FIG. 7

EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIUM WEIGHT–FRACTION = 0.25

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

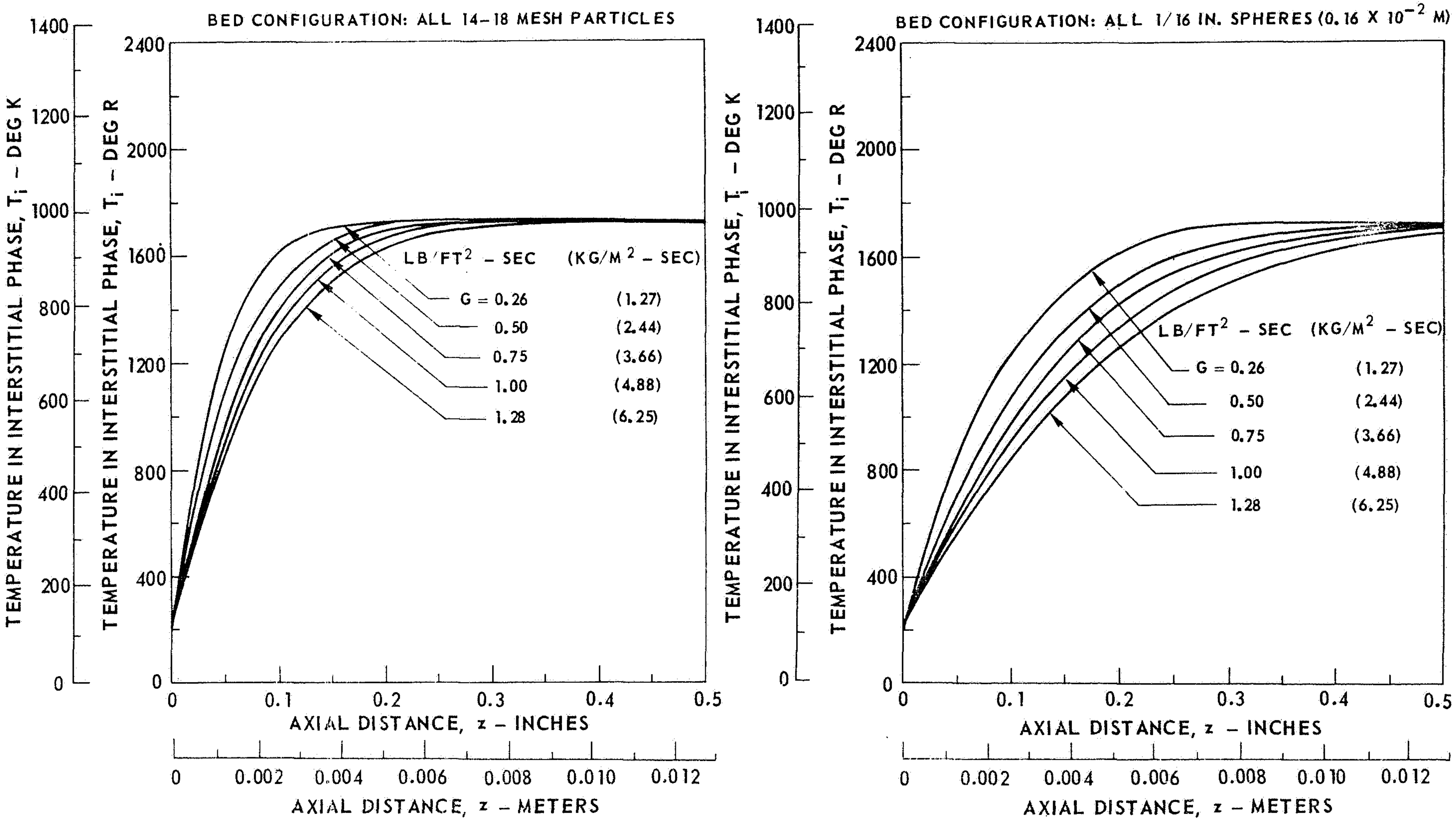


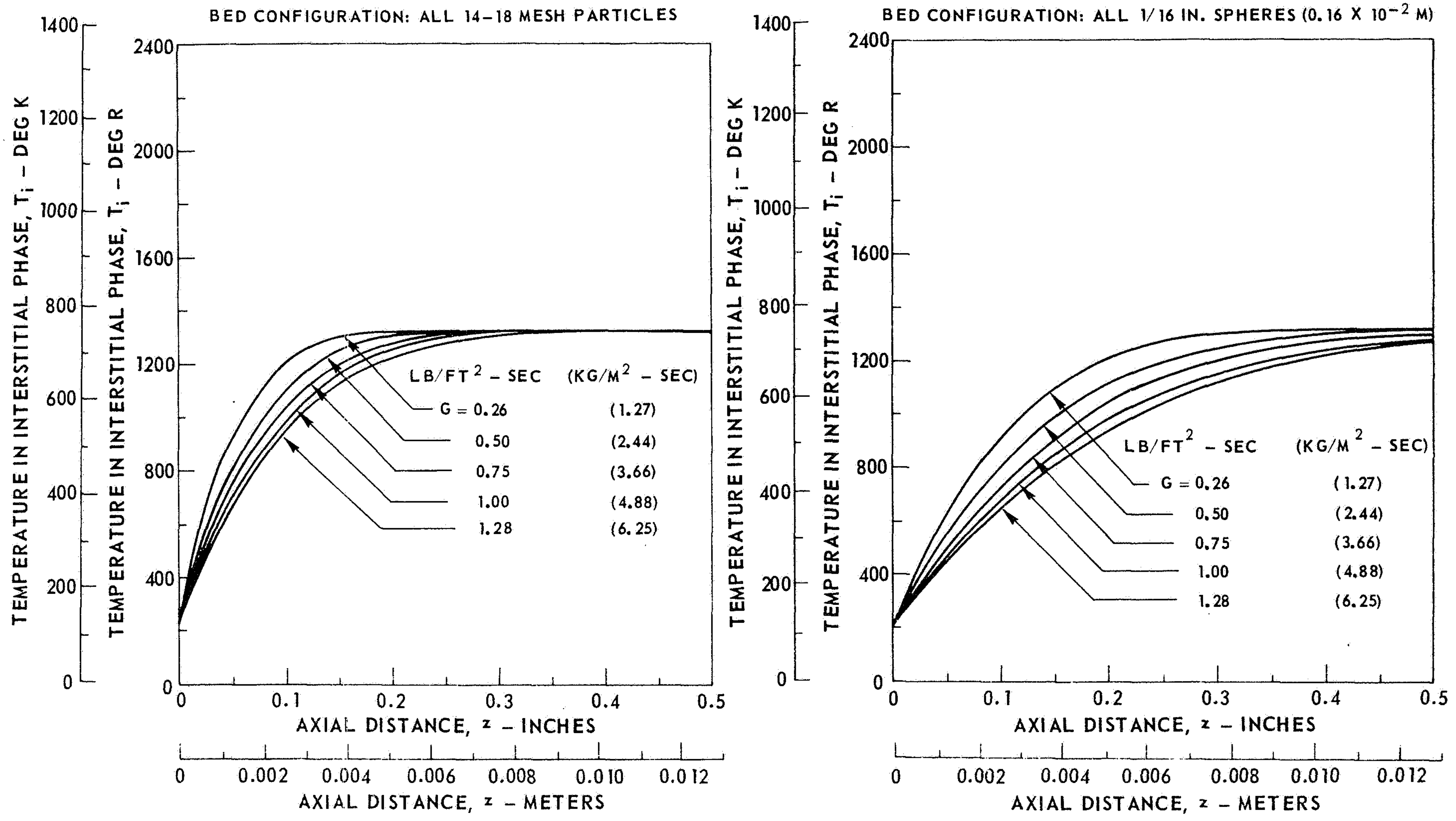
FIG. 8

FIG. 9

EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIUM WEIGHT-FRACTION = 0.50

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



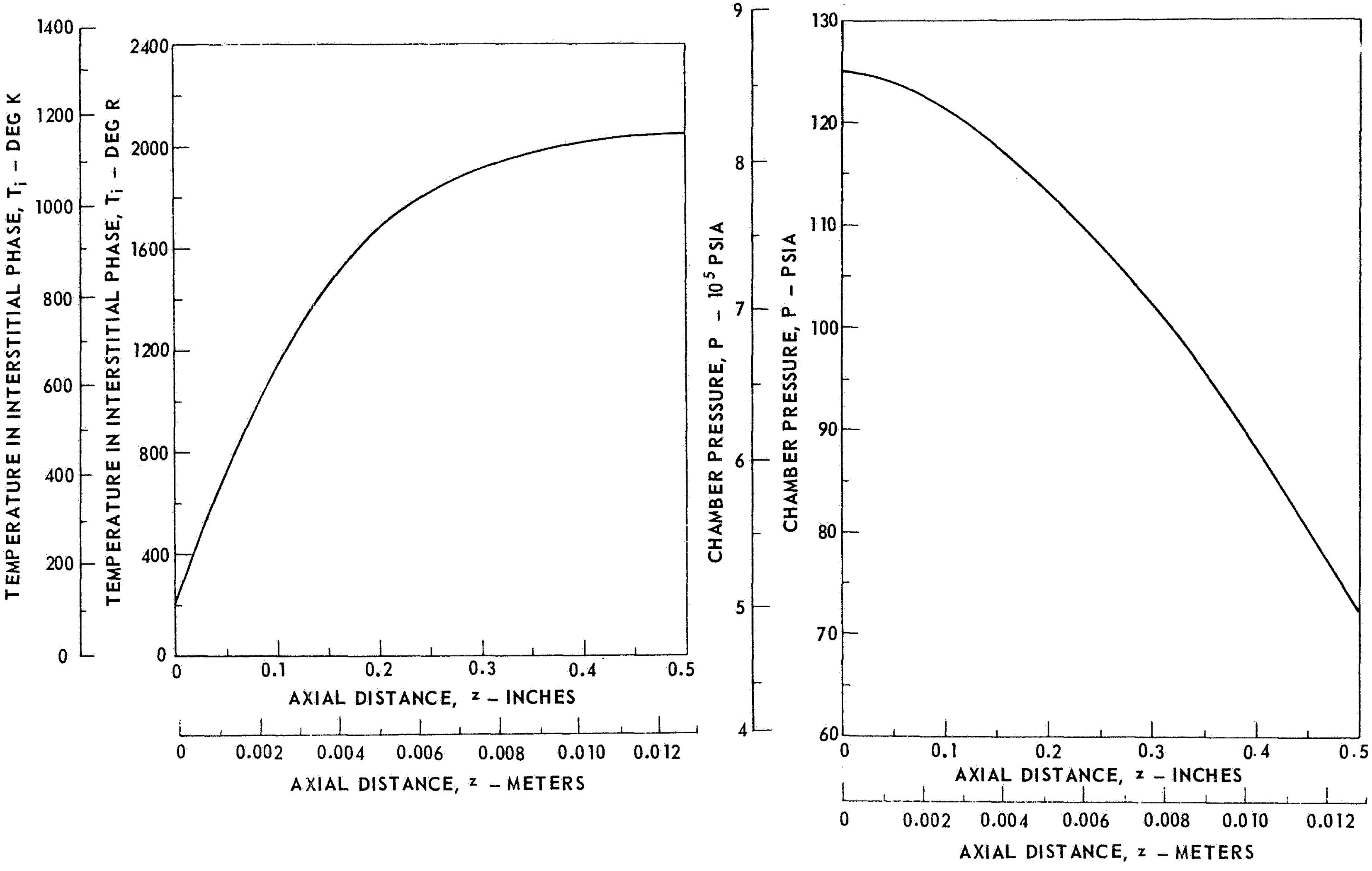
BED CONFIGURATION: ALL 14-18 MESH PARTICLES

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

FIG. 10

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

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



AXIAL CONCENTRATION PROFILES FOR A HIGH NOMINAL CHAMBER PRESSURE

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

FEED TEMPERATURE = 210 DEG R (117 DEG K)

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

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

NO HELIUM DILUTION

BED CONFIGURATION: ALL 14–18 MESH CATALYST PARTICLES

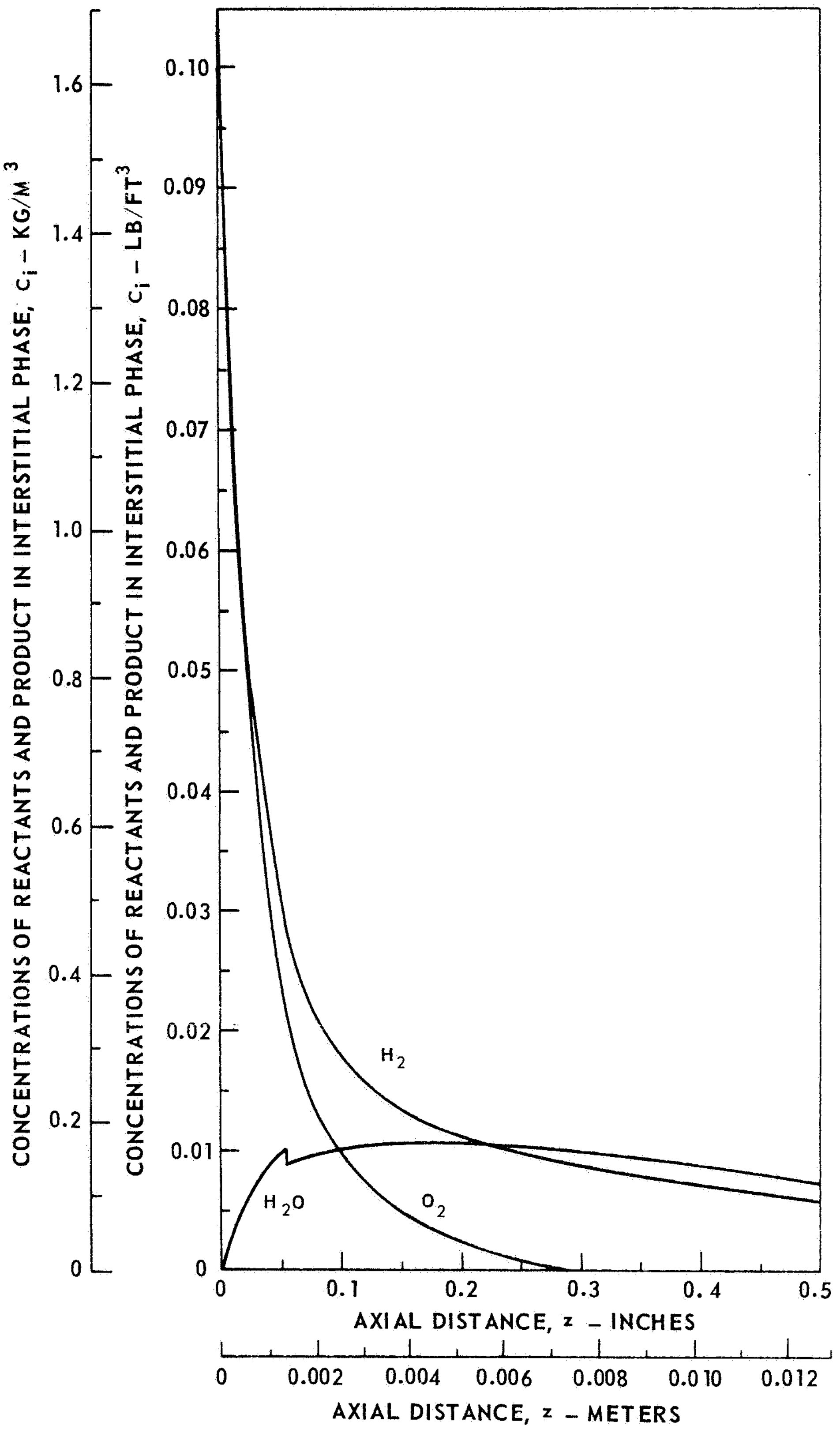


FIG. 12

AXIAL MOLE-FRACTION PROFILES FOR A HIGH NOMINAL CHAMBER PRESSURE

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

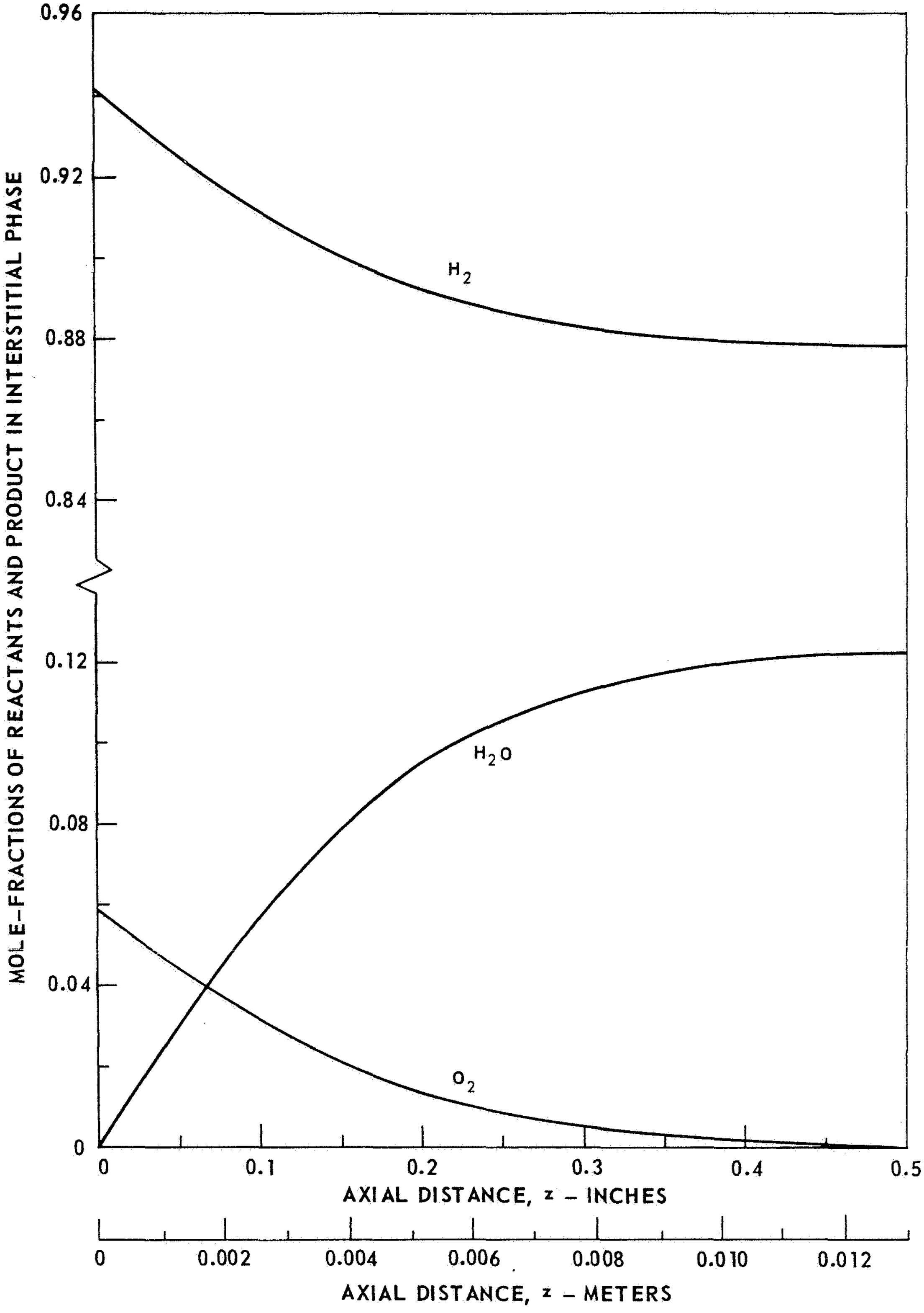


FIG. 13

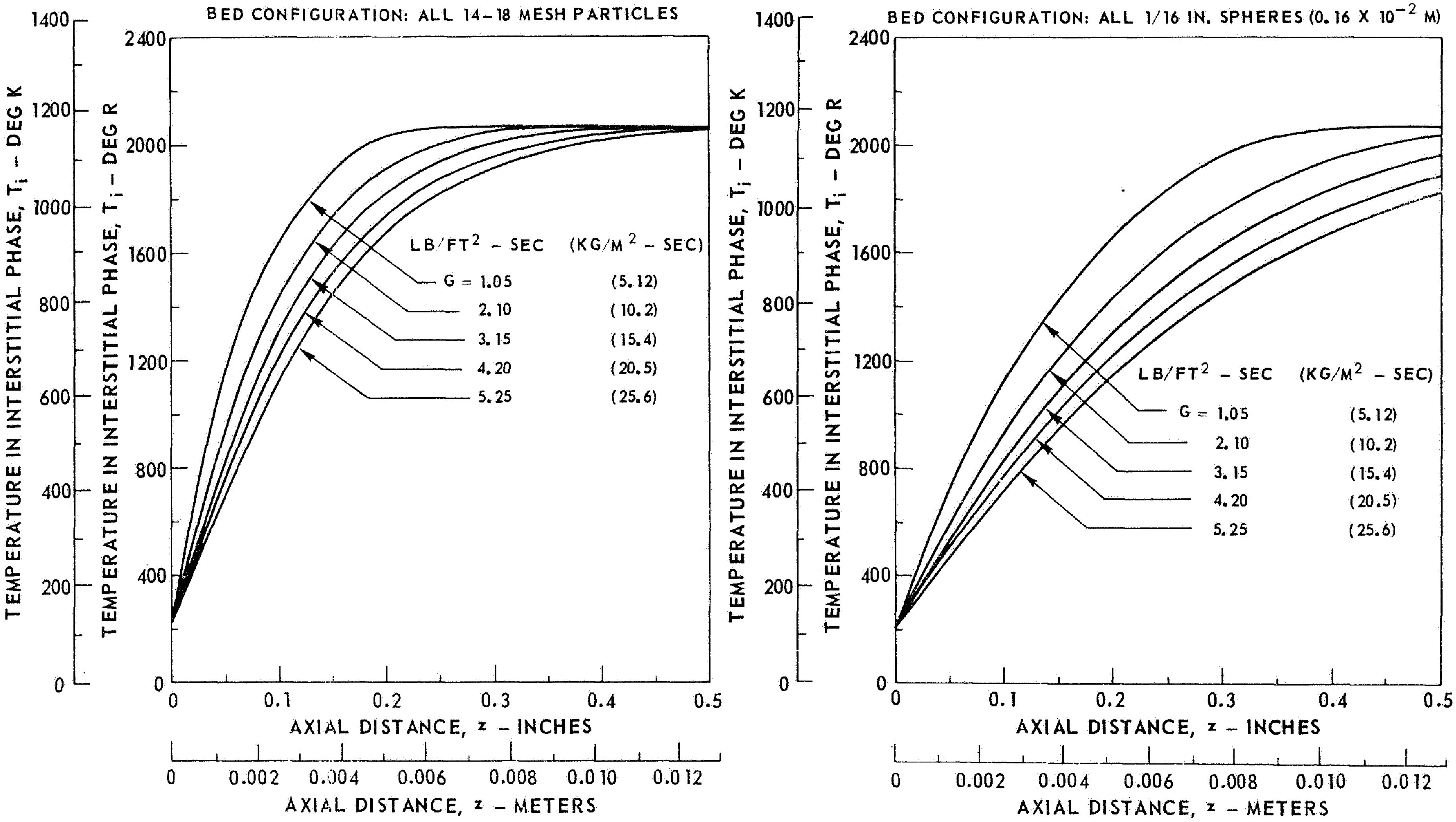
EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

NO HELIUM DILUTION

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

FEED TEMPERATURE = 210 DEG R (117 DEG K)

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



EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIUM WEIGHT-FRACTION = 0.25

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

FEED TEMPERATURE = 210 DEG R (117 DEG K)

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

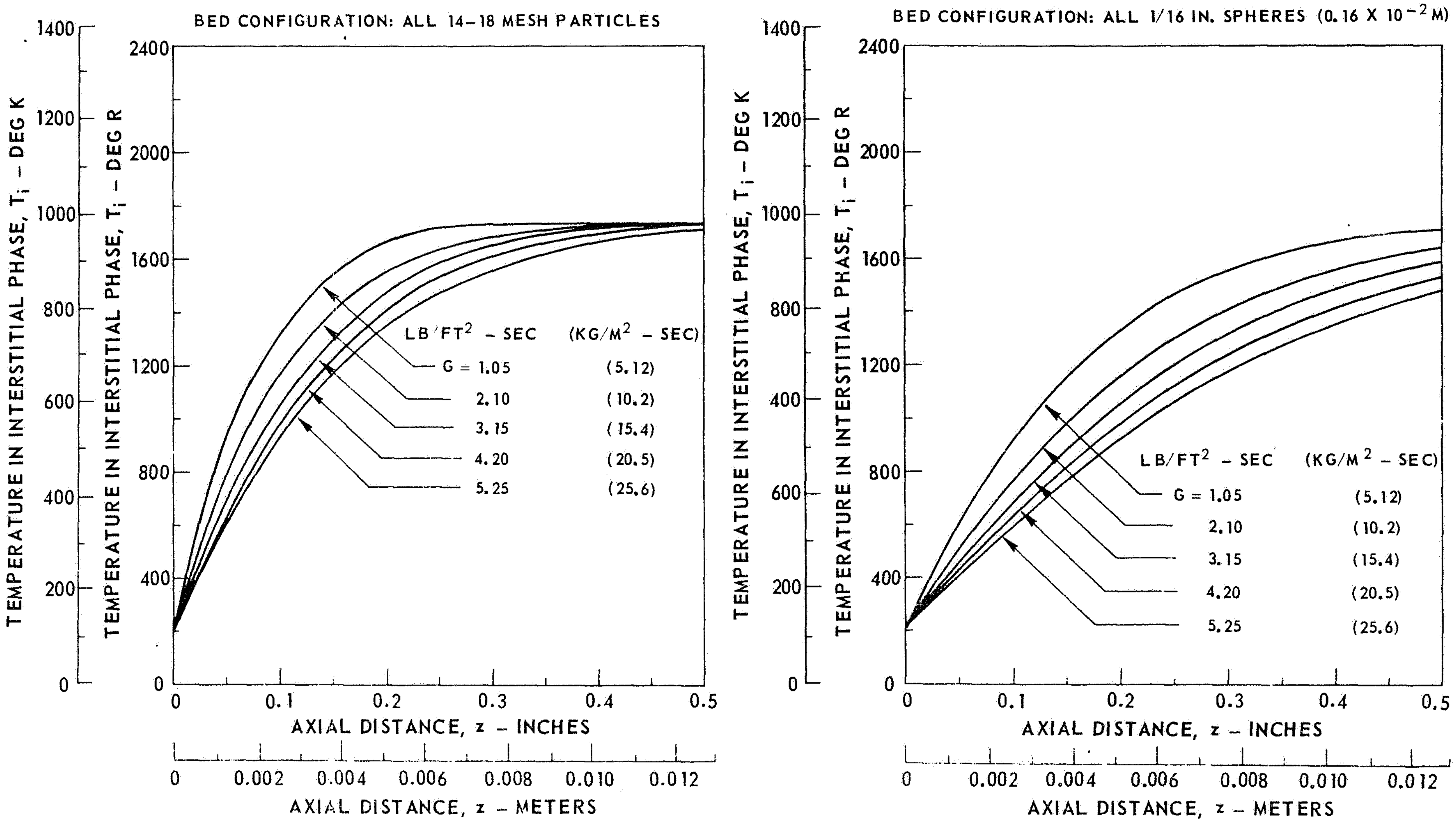


FIG. 14

EFFECT OF MASS FLOW RATE ON AXIAL TEMPERATURE PROFILES

HELIUM WEIGHT-FRACTION = 0.50

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

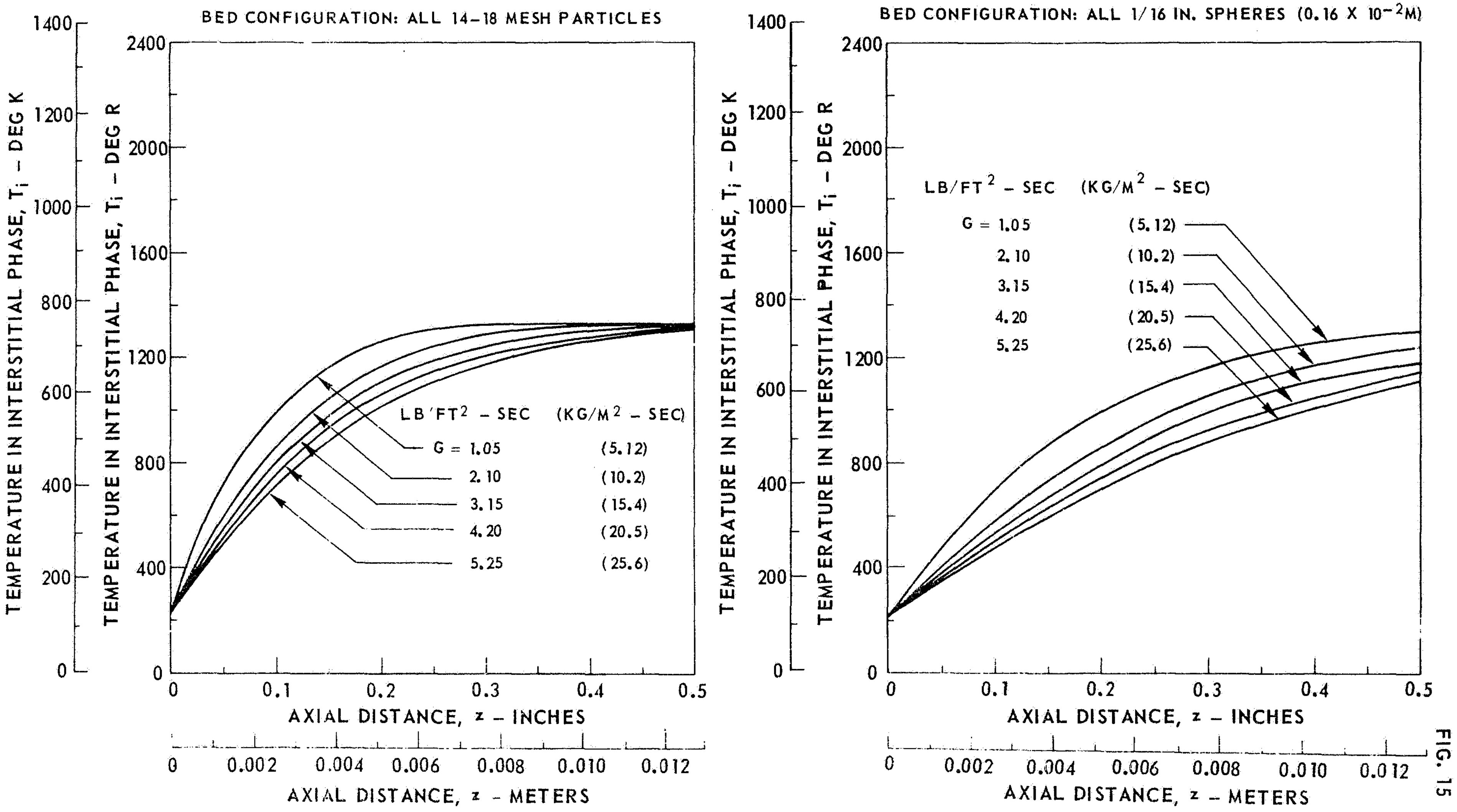


FIG. 15