NASA
UACRL G910461-30

COMPUTER PROGRAMS MANUAL

ANALYTICAL STUDY OF CATALYTIC REACTORS FOR HYDRAZINE DECOMPOSITION

ONE-AND TWO-DIMENSIONAL STEADY-STATE PROGRAMS

by
E.J. SMITH, D.B. SMITH and A.S. KESTEN

prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

AUGUST, 1968

CONTRACT NAS 7-458

United Aircraft Research Laboratories

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ABSTRACT

Two machine computational programs have been developed under NASA Contract NAS 7-458 to calculate the steady-state temperature and reactant concentration distributions in typical catalyzed hydrazine decomposition reaction chambers. One program is based upon a one-dimensional model of the reactor system which describes the behavior of reactors having radially uniform injection profiles and catalyst bed configurations, while the other program is based upon a two-dimensional model which permits consideration of nonuniform radial injection and of catalyst bed configurations exhibiting both radial and axial nonuniformities.

The one- and two-dimensional models and the computer programs developed from these models are described in detail in this computer manual. The manual contains operating instructions for these programs as well as descriptions of input and output formats, including all output messages. Also included is a discussion of possible operational problems which might arise together with appropriate means for solving these problems.

FOREWORD

This work was performed by United Aircraft Research Laboratories for the National Aeronautics and Space Administration under Contract NAS 7-458 initiated April 15, 1966.

Included among those who cooperated in performance of the work under NAS 7-458 were Dr. A. S. Kesten, Program Manager, Dr. W. G. Burwell, Chief, Kinetics and Thermal Sciences Section, Mr. D. B. Smith, Project Analyst, and Mrs. E. J. Smith, Applied Mathematician.

This work was conducted under program management of the NASA Chief, Liquid Propulsion Experimental Engineering Systems, NASA Headquarters, Washington, D. C., and the Technical Manager was Mr. T. W. Price, Jet Propulsion Laboratory, Pasadena, California.

Report G910461-30

Analytical Study of Catalytic Reactors

for Hydrazine Decomposition

Computer Programs Manual

One- and Two-Dimensional Steady-State Models

Contract NAS 7-458

SUMMARY

A description is contained herein of two machine computational programs developed under Contract NAS 7-458 with the National Aeronautics and Space Administration. These programs represent one- and two-dimensional steady-state models of catalyzed hydrazine decomposition reaction chambers. Both of these models consider both thermal and catalytic decomposition of reactants, along with simultaneous heat and mass transfer between the free-gas phase and the gas within the pores of the catalyst pellets. The one-dimensional model of the reactor system describes the behavior of reactors having radially uniform injection profiles and catalyst bed configurations, while the two-dimensional model permits consideration of nonuniform radial injection and of catalyst bed configurations exhibiting both radial and axial nonuniformities.

A general description of the one and two-dimensional models and a discussion of the machine programs developed from these models are contained in this manual. A description of input and output for both the one- and two-dimensional steady-state programs are included in the discussion together with examples of typical data cases. Also included is a description of several operational problems which might be encountered while using the programs along with appropriate means for solving these problems. In addition, a short write-up of the subroutines contained in each deck is included along with general flow charts of the major routines.

INTRODUCTION

Under Contract NAS 7-458, the Research Laboratories of United Aircraft Corporation are performing analytical studies of the behavior of distributed-feed catalytic reactors for hydrazine decomposition. The specific objectives of this program are (a) to develop computer programs for predicting the temperature and concentration distributions in monopropellant hydrazine catalytic reactors in which hydrazine can be injected at arbitrary locations in the reaction chamber and (b) to perform calculations using these computer programs to demonstrate the effects of various system parameters on the performance of the reactor.

Progress previously reported in the first annual report (Ref. 1) included the development of a computer program which describes the steady-state behavior of a continuous flow type reactor system in which complete radial mixing in the free-gas (or liquid) phase was assumed. Progress previously reported in the second annual report (Ref. 2) included an extension of the steady-state program to include radial as well as axial variations in temperature and concentrations in order to permit an analysis of various injection schemes and catalyst bed configurations which exhibit radial nonuniformities. These programs had been used to calculate temperature and reactant concentration distributions as functions of feed temperature, chamber pressure, mass flow rate distribution, catalyst size distribution, and embedded injector locations. As part of the third year of contract effort attention has been directed toward preparing a manual describing to potential users the operation of these computer programs. The manual includes a general description of the one- and two-dimensional models as well as a detailed discussion of the machine programs representing these models.

DESCRIPTION OF ANALYSES

The analysis of a hydrazine engine reaction system carried out to date pertains to a reaction chamber of arbitrary cross section packed with catalyst particles into which liquid hydrazine is injected at arbitrarily selected locations. Catalyst particles are represented as "equivalent" spheres with a diameter taken as a function of the particle size and shape. Both thermal and catalytic vapor phase decomposition of hydrazine and ammonia are considered in developing equations describing the concentration distributions of these reactants. Diffusion of reactants from the 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 taken into account since the decomposition reactions are accompanied by the evolution or absorption of heat.

One-Dimensional Steady-State Model

In developing the one-dimensional steady-state model, the temperature and reactant concentrations in the interstitial phase (i.e., the free-fluid phase as distinguished from the gas phase within the porous particles) are assumed to vary only with axial distance along the bed. In the entrance region of the reaction chamber, where the temperature is low enough to permit the existence of liquid hydrazine, vaporization of liquid is assumed to occur as a result of decomposition of vapor hydrazine within the pores of the catalyst particles. That is, catalytic reaction is assumed to be fast enough to keep liquid hydrazine from wetting the pores of the particles; the hydrazine concentration at the surface of the catalyst particles at any axial location in the entrance region is then computed from the vapor pressure of liquid hydrazine in the interstitial phase at the same axial location. Neglecting axial diffusion of heat or mass, the change in enthalpy of the interstitial phase in the region where liquid hydrazine is present (i.e., where $h_i \leq h_i^V$) is related to the concentration gradient at the surface of the porous catalyst particles by

$$G \frac{dh}{dz} + H^{N_2H_4} D_p A_p \left(\frac{dc_p^{N_2H_4}}{dx} \right)_s + F(h_i - h_F) = 0 \quad \text{for } h_i \leq h_i^V \qquad (1)$$

The variation of mass flow rate, G, with axial distance is easily computed from the rate of feed of liquid hydrazine from the distributed injectors into the system. In the region where liquid hydrazine exists at temperatures below the vaporization temperature, the temperature may be obtained from

$$T_i = T_F + \frac{h_i - h_F}{C_F} \qquad \text{for } h_i < h_i^L \qquad (2)$$

In the two-phase region, where $T_i = T_{vap}$, the weight-fraction of vapor may be computed from

$$\text{WEIGHT - FRACTION VAPOR} = \frac{h_i - h_i^L}{h_i^V - h_i^L} \qquad \text{for } h_i^L \leq h_i \leq h_i^V \qquad (3)$$

At the axial position at which the enthalpy of the interstitial phase is just equal to the enthalpy of vapor hydrazine at the boiling point ($h_i = h_i^V$), the fraction of hydrazine injected upstream of that point which has been decomposed is easily calculated from an overall heat balance. The associated amounts of ammonia, nitrogen, and hydrazine formed from decomposition of hydrazine can then be calculated taking the decomposition reaction as

$$2N_2H_4 \longrightarrow 2NH_3 + N_2 + H_2$$

It should be noted that this is the overall reaction scheme determined experimentally for both homogeneous decomposition of hydrazine (Refs. 3 , 4 , 5) and low pressure heterogeneous decomposition of hydrazine on platinum surfaces (Ref. 6).*

In the remainder of the reaction chamber, where $h_i > h_i^V$, heat is being supplied to the system by homogeneous as well as heterogeneous decomposition of hydrazine. In addition, at sufficiently high temperature, heat is removed from the system by the endothermic decomposition of ammonia. For $h_i > h_i^V$ then, the change in enthalpy with axial distance is related to the reactant concentrations in the interstitial phase and at the surface of the porous catalyst particles by

$$\frac{dh_i}{dz} = -\frac{1}{G}\left\{F(h_i-h_F) + A_p h_c\left[T_i - (T_p)_s\right] + H^{N_2H_4} r_{hom}^{N_2H_4}\delta\right\} \tag{4}$$

The changes in reactant weight fractions in the interstitial phase with axial distance are related to the reactant concentrations in the interstitial phase and at the surface of the porous catalyst particles by

$$\frac{dw_i^{N_2H_4}}{dz} = \frac{1}{G}\left\{F - r_{hom}^{N_2H_4}\delta - A_p\,(k_C\,c_i)^{N_2H_4} - F\left(\frac{c_i}{\rho_i}\right)^{N_2H_4}\right\} \tag{5}$$

*It is more commonly assumed, without benefit of experimental evidence, that the decomposition reaction is $3\,N_2H_4 \longrightarrow 4\,NH_3 + N_2$, followed by dissociation of one of the four ammonia molecules to nitrogen and hydrogen. This two-step process leads to the same overall reaction cited above but assumes that a minimum of 25 percent of the ammonia produced by hydrazine decomposition also decomposes. The fractional ammonia dissociation, f, calculated assuming the validity of the two-step process is related by the fractional ammonia dissociation calculated in the present report by

$$(f)_{\text{two-step process}} = \frac{3\,(f)_{\text{present report}} + 1}{4}$$

$$\frac{dw_i^{NH_3}}{dz} = \frac{1}{G}\left\{ r_{hom}^{N_2H_4}\,\delta\,\frac{M^{NH_3}}{M^{N_2H_4}} + A_p\,(k_C c_i)^{N_2H_4}\,\frac{M^{NH_3}}{M^{N_2H_4}} - A_p\left(k_C\left[c_i - (c_P)_S\right]\right)^{NH_3} - F\left(\frac{c_i}{\rho_i}\right)^{NH_3} \right\} \tag{6}$$

$$\frac{dw_i^{N_2}}{dz} = \frac{1}{G}\left\{ \frac{1}{2}\, r_{hom}^{N_2H_4}\,\delta\,\frac{M^{N_2}}{M^{N_2H_4}} + \frac{A_p}{2}\,(k_C c_i)^{N_2H_4}\,\frac{M^{N_2}}{M^{N_2H_4}} + \frac{A_p}{2}\left(k_C\left[c_i - (c_P)_S\right]\right)^{NH_3}\frac{M^{N_2}}{M^{NH_3}} - F\left(\frac{c_i}{\rho_i}\right)^{N_2} \right\} \tag{7}$$

$$\frac{dw_i^{H_2}}{dz} = \frac{1}{G}\left\{ \frac{1}{2}\, r_{hom}^{N_2H_4}\,\delta\,\frac{M^{H_2}}{M^{N_2H_4}} + \frac{A_p}{2}\,(k_C c_i)^{N_2H_4}\,\frac{M^{H_2}}{M^{N_2H_4}} + \frac{3A_p}{2}\left(k_C\left[c_i - (c_P)_S\right]\right)^{NH_3}\frac{M^{H_2}}{M^{NH_3}} - F\left(\frac{c_i}{\rho_i}\right)^{H_2} \right\} \tag{8}$$

where the film coefficients, h_c and k_c, may be estimated from (Ref. 7)

$$h_C = 0.74\left(\frac{G}{A_p\mu}\right)^{-0.41}(\bar{C}_F G) \tag{9}$$

and

$$k_C^J = \left(\frac{0.61\,G}{\rho_i}\right)\left(\frac{\mu}{\rho_i D_i^J}\right)^{-0.667}\left(\frac{G}{A_p\mu}\right)^{-0.41} \tag{10}$$

The changes in reactant concentrations with axial distance are then given by

$$\frac{dc_i^J}{dz} = \rho_i\,\frac{dw_i^J}{dz}\;[illegible]\;\rho_i\;\frac{[illegible]}{dz} \tag{11}$$

where

$$\frac{d\rho_1}{dz} = \rho_1 \left[\frac{1}{\bar{M}}\frac{d\bar{M}}{dz} - \frac{1}{T_1}\frac{dT_1}{dz} + \frac{1}{P}\frac{dP}{dz}\right] \tag{12}$$

and

$$\frac{1}{\bar{M}}\frac{d\bar{M}}{dz} = -\frac{1}{\sum_J \frac{w_1^J}{M^J}} \sum_J \frac{1}{M^J}\frac{dw_1^J}{dz} \tag{13}$$

and

$$\frac{dP}{dz} = -\left(\frac{1-\delta}{\delta^3}\right)\left(1.75 + \frac{150(1-\delta)}{2aG/\mu}\right)\left(\frac{G^2}{2a\rho_1 g_c}\right) \tag{14}$$

The temperature of the interstitial phase in this region is related to the enthalpy by

$$h_1 - h_1^V = \int_{T_{vap}}^{T_1} C_F \, dT_1 \tag{15}$$

It should be noted that the hydrazine concentration at the surface of a catalyst particle in the vapor region, $(c_p)_s^{N_2H_4}$, is taken as zero. This reflects the fact that the catalytic reaction is so fast that the rate of decomposition is controlled by the rate of diffusion of hydrazine from the bulk vapor, through a stagnant gas film surrounding the catalyst particles, to the outside surface of the particles. In the case of ammonia, film diffusion is rapid relative to the rate of dissociation of ammonia within the particles. The concentration of ammonia at the surface of the catalyst particles, $(c_p)_s^{NH_3}$, is therefore fairly close to the ammonia concentrations in the bulk vapor phase, $c_1^{NH_3}$. The surface concentration can be calculated, along with the concentration profile in the porous particles, at any axial location by solving simultaneously the equations representing film and pore diffusion of heat and mass. In describing the diffusion of mass within a porous pellet, it is assumed that changes in the mass density of fluid within the particle are negligible relative to changes in concentration of the reacting species. In addition, pressure changes within the particle resulting from nonequimolar diffusion are neglected, as is heat transported by pore diffusion of mass. Assuming constant diffusion coefficients, D_p, and thermal conductivities, K_p, the equations describing heat and mass transfer within a catalyst particle may be written as

$$D_P^{NH_3} \nabla^2 c_P^{NH_3} - r_{het}^{NH_3} = 0 \qquad (16)$$

$$K_P \nabla^2 T_P - H^{NH_3} r_{het}^{NH_3} = 0 \qquad (17)$$

The boundary conditions which consider diffusion of heat and mass through a film surrounding a spherical particle are

$$D_P^{NH_3} \left(\frac{dc_P}{dx}\right)_S^{NH_3} = k_C^{NH_3} \left[c_i^{NH_3} - (c_P)_S^{NH_3} \right] \qquad (18)$$

and

$$\left(H k_C c_i\right)^{N_2H_4} + H^{NH_3} D_P^{NH_3} \left(\frac{dc_P}{dx}\right)_S^{NH_3} = h_C \left[T_i - (T_P)_S \right] \qquad (19)$$

Using Eqs. (16) and (17), Prater (Ref. 8) has pointed out that temperature and concentration are related quite simply by

$$T_P - (T_P)_S = \frac{HD_P}{K_P} \left[(c_P)_S - c_P \right] \qquad (20)$$

The use of this relationship enables the reaction rate, $r_{het}^{NH_3}$, to be written as a function of concentration alone instead of concentration and temperature. In this case, however, the reaction rate is a function of two parameters, $(T_p)_s$ and $(c_p)_s^{NH_3}$, which are yet to be determined. Equation 16 can be solved for the concentration at any point in the porous particle in terms of the reaction rate, $r_{het}^{NH_3}$, and the interstitial concentration, $c_i^{NH_3}$. The solution is derived in Refs. 2 and 9 as an implicit integral equation given by

$$c_P(x)^{NH_3} = c_i^{NH_3} - \left[\frac{1}{x} - \frac{a k_C^{NH_3} - D_P^{NH_3}}{a^2 k_C^{NH_3}}\right] \int_0^x \xi^2 \frac{r_{het}^{NH_3}(c_P)}{D_P^{NH_3}} d\xi$$
$$- \int_x^a \left[\frac{1}{\xi} - \frac{a k_C^{NH_3} - D_P^{NH_3}}{a^2 k_C^{NH_3}}\right] \xi^2 \frac{r_{het}^{NH_3}(c_P)}{D_P^{NH_3}} d\xi \qquad (21)$$

In order to determine the particle ammonia concentration profile directly in terms of the interstitial temperature and reactant concentrations it is necessary to solve Eqs. 18, 19 and 21 simultaneously.

In the special case of negligible film resistance to heat and mass transfer (i.e. $(T_p)_s = T_i$ and $(c_p)_s = c_i$), Eq. (21) can be written, for any reacting species, as

$$c_p(x) = c_i - \left[\frac{1}{x} - \frac{1}{a}\right] \int_0^x \xi^2 \frac{r_{het}(C_p)}{D_p} d\xi - \int_x^a \left[\frac{1}{\xi} - \frac{1}{a}\right] \xi^2 \frac{r_{het}(C_p)}{D_p} d\xi \qquad (22)$$

It is Eq. (22) which is used to describe the hydrazine concentration profiles within the catalyst particles located in the liquid region of the reaction chamber. In this liquid region it is assumed that liquid hydrazine wets the outside surface of the catalyst particles so that $(c_p)_s^{N_2H_4} = c_i^{N_2H_4}$, where $c_i^{N_2H_4}$ is the vapor concentration in equilibrium with liquid hydrazine at temperature T_i. In the liquid-vapor region the situation is somewhat more complicated since it is difficult to predict whether liquid or a combination of liquid and vapor wets the outside surface of the catalyst particles. Both of these options are presently in the computer program representing the steady-state model. In the case in which both the liquid and vapor are taken to wet the particle surface, it is assumed that, at a given axial location, the fraction of the surface covered by vapor is equal to the weight-fraction of vapor present. Decomposition rates, computed assuming pure liquid surface coverage and then pure vapor coverage, are weighted accordingly. Fortuitously, for the system considered here, the liquid-vapor region is so narrow that the choice of either of these options has negligible effect on the resulting temperature distributions (Ref. 1).

Finite difference methods have been used to program for digital computation the ordinary differential equations describing the changes in enthalpy and reactant concentrations in the interstitial phase. No iteration is necessary to solve these equations numerically when the incremental axial distances are sufficiently small. The size of a succeeding increment is calculated at each axial position as a function of the rates of change of temperature and fractional ammonia dissociation with axial distance. However, Eqs. (21) and (22), which must be solved simultaneously with the differential equations, are implicit integral equations which require iterative procedures for solution. Hand calculations have indicated that convergence to solutions for $c_p(x)$ are difficult to achieve unless the initial estimates of the concentration distributions are fairly accurate. Methods have been developed for generating these estimates and iterative procedures have been devised which effect rapid convergence over a fairly wide range of conditions. These procedures are presently used as subroutines in the main program representing the steady-state model.

Two-Dimensional Steady-State Model

In developing the two-dimensional steady-state model of a hydrazine reactor system the temperature and reactant concentrations in the bulk fluid phase are permitted to vary with radial and axial position in the reaction chamber. In the entrance region of the reactor, where the temperature is low enough to permit the existence of liquid hydrazine, radial mixing between adjacent layers of liquid is neglected. The equations representing the change in liquid enthalpy and temperature with axial distance at any radial position are the same as those developed for the one-dimensional model described previously. As in the one-dimensional model, catalytic reaction is assumed to be fast enough to keep liquid hydrazine from wetting the pores of the particles; the hydrazine concentration at the surface of the catalyst particles at any location in the entrance region is then computed from the vapor pressure of liquid hydrazine in the interstitial phase at the same location.

In the vapor regions of the reaction chamber, turbulent diffusion of heat and mass is considered as a mechanism for radial mixing. Radial heat and mass fluxes are computed as functions of temperature and reactant concentration gradients. Heat is being supplied to the system by homogeneous as well as heterogeneous decomposition of hydrazine, and is being removed from the system by the catalytic decomposition of ammonia. The change in enthalpy with axial distance at any radial location is related to the reactant concentrations in the interstitial phase and at the surface of the porous catalyst particles by

$$\frac{\partial h_i}{\partial z} = -\frac{1}{G}\left\{F\,(h_i - h_F) + A_P h_C\left[T_1 - (T_P)_S\right] + H^{N_2H_4}\, r_{hom}^{N_2H_4}\,\delta + \frac{\partial q_r}{\partial r}\,\delta + \frac{q_r}{r}\,\delta + \frac{\partial T_1}{\partial r}\,\delta \sum_j N_r^{\,j}\, C_F^{\,j}\right\} \qquad (23)^*$$

The changes in reactant weight fractions in the interstitial phase with axial distance at any radial location are related to the reactant concentrations in the interstitial phase and at the surface of the porous catalyst particles by

*Equations of this type are presented in somewhat different form in Ref. 7. The last term on the right-hand side of the equation reflects the heat transferred by the radial diffusion of mass.

$$\frac{\partial w_i^{N_2H_4}}{\partial z} = \frac{1}{G}\left\{F - r_{hom}^{N_2H_4}\,\delta - A_p\,(k_c c_i)^{N_2H_4} - \frac{\partial N_r^{N_2H_4}}{\partial r}\,\delta - \frac{N_r^{N_2H_4}}{r}\,\delta - F\left(\frac{c_i}{\rho_i}\right)^{N_2H_4}\right\} \tag{24}$$

$$\frac{\partial w_i^{NH_3}}{\partial z} = \frac{1}{G}\left\{r_{hom}^{N_2H_4}\,\delta\,\frac{M^{NH_3}}{M^{N_2H_4}} + A_p\,(k_c c_i)^{N_2H_4}\frac{M^{NH_3}}{M^{N_2H_4}} - A_p\left(k_c\left[c_i - (c_p)_S\right]\right)^{NH_3} - \frac{\partial N_r^{NH_3}}{\partial r}\,\delta - \frac{N_r^{NH_3}}{r}\,\delta - F\left(\frac{c_i}{\rho_i}\right)^{NH_3}\right\} \tag{25}$$

$$\frac{\partial w_i^{N_2}}{\partial z} = \frac{1}{G}\left\{\frac{1}{2}\,r_{hom}^{N_2H_4}\,\delta\,\frac{M^{N_2}}{M^{N_2H_4}} + \frac{A_p}{2}\,(k_c c_i)^{N_2H_4}\frac{M^{N_2}}{M^{N_2H_4}} + \frac{A_p}{2}\left(k_c\left[c_i - (c_p)_S\right]\right)^{NH_3}\frac{M^{N_2}}{M^{NH_3}} - \frac{\partial N_r^{N_2}}{\partial r}\,\delta - \frac{N_r^{N_2}}{r}\,\delta - F\left(\frac{c_i}{\rho_i}\right)^{N_2}\right\} \tag{26}$$

$$\frac{\partial w_i^{H_2}}{\partial z} = \frac{1}{G}\left\{\frac{1}{2}\,r_{hom}^{N_2H_4}\,\delta\,\frac{M^{H_2}}{M^{N_2H_4}} + \frac{A_p}{2}\,(k_c c_i)^{N_2H_4}\frac{M^{H_2}}{M^{N_2H_4}} + \frac{3A_p}{2}\left(k_c\left[c_i - (c_p)_S\right]\right)^{NH_3}\frac{M^{H_2}}{M^{NH_3}} - \frac{\partial N_r^{H_2}}{\partial r}\,\delta - \frac{N_r^{H_2}}{r}\,\delta - F\left(\frac{c_i}{\rho_i}\right)^{H_2}\right\} \tag{27}$$

where

$$q_r = -\lambda\,(\partial T_i / \partial r) \tag{28}$$

$$N_r^J = -\epsilon\,(\partial c_i^J / \partial r)_r \tag{29}$$

$$h_c = 0.74 \left[\frac{G}{A_p \mu}\right]^{-0.41} [\bar{C}_F G] \tag{30}$$

$$k_c^J = \left[\frac{0.61G}{\rho_i}\right] \left[\frac{\mu}{\rho D_i^J}\right]^{-0.657} \left[\frac{G}{A_p \mu}\right]^{-0.41} \tag{31}$$

The eddy conductivity and diffusivity may be estimated from (Ref. 11)

$$\lambda = \frac{a \bar{C}_F G}{5\delta} \quad \text{and} \quad \epsilon = \frac{aG}{5\rho_i} \tag{32}$$

The changes in reactant concentrations with axial distance are then given by

$$\frac{\partial c_i^J}{\partial z} = \rho_i \frac{\partial w_i^J}{\partial z} + \frac{c_i^J}{\rho_i} \frac{\partial \rho_i}{\partial z} \tag{33}$$

where

$$\frac{\partial \rho_i}{\partial z} = \rho_i \left[\frac{1}{\bar{M}} \frac{\partial \bar{M}}{\partial z} - \frac{1}{T_i} \frac{\partial T_i}{\partial z} + \frac{1}{P} \frac{dP}{dz}\right] \tag{34}$$

$$\frac{1}{\bar{M}} \frac{\partial \bar{M}}{\partial z} = - \frac{1}{\sum_J (w_i^J / M^J)} \sum_J \frac{1}{M^J} \frac{\partial w_i^J}{\partial z} \tag{35}$$

and the pressure drop may be estimated from the Ergun equation (Ref. 7) as

$$\frac{dp}{dz} = - \left(\frac{1-\delta}{\delta^3}\right) \left(1.75 + \frac{150(1-\delta)}{2aG/\mu}\right) \left(\frac{G^2}{2a\rho_i g_c}\right) \tag{36}$$

The mass flow rate, G, is computed as a function of the rate of feed of liquid hydrazine from the distributed injectors into the system. Bulk radial flow, caused by particle-fluid viscous interaction, is neglected. It is assumed, therefore, that downstream of the injectors the mass flow rate profile remains unchanged.

DISCUSSION OF ONE- AND TWO-DIMENSIONAL STEADY-STATE COMPUTER PROGRAMS

The equations representing the one- and two-dimensional steady-state models have been programmed for the UNIVAC 1108 digital computer. These computer programs are discussed below. Included in this discussion are input and output descriptions and descriptions of common operational problems associated with the programs.

One-Dimensional Steady-State Model

Input Description

The following is a listing of the necessary input for the one-dimensional steady-state computer program. The input format is given in Table I. The coding of a sample data case is shown in Fig. 1 and a listing of the input data punch cards corresponding to this sample data case is shown in Fig. 2. The card numbers in the text below correspond to the card numbers (first column) of Table I. For each run there will be only <u>one</u> card number one. Cards 2 through 16 should be repeated for each data case to be run.

1. The first card contains the number NCASE. This number indicates the number of data cases with each run. $1 \le$ NCASE ≤ 999.

2. The second card is the title card used for individual data case identification. The title may be any alpha numeric information desired.

3. The third card contains the indicators ØPTIØN and PRINT and the number NØFZ. ØPTIØN is used to indicate which method of analyzing the liquid-vapor region is desired. If ØPTIØN = 2, the program will use the method in subroutine LQV2. If ØPTIØN $\neq$ 2, the program will use the method in subroutine LQVP. These two methods are described in Appendix I. PRINT is used to indicate which type of printout is desired. If PRINT = 0 or is blank, the "standard output" described in the section on output is printed. If PRINT = 1, both the "standard" and "nonstandard output" are printed. "Nonstandard output" is also described in the section on output. NØFZ is the number of axial stations (Z's) to be used in the three tables input on cards 8 through 16.

4. The fourth card contains the eight constants ZO, GO, FC, ALPHA3, HF, R, WM4, and WM3.

ZO	is the axial distance to the end of a buried injector in ft. (Ref. 1).

GO is the inlet mass flow rate in lb/ft^2-sec. It must be greater than zero.

FC is the rate of feed of hydrazine from buried injectors (Ref. 1) into the system in lb/ft^3-sec.

ALPHA3 is the preexponential factor in the rate equation for the thermal decomposition of hydrazine (See Ref. 1). It equals $2.14 \times 10^{10} sec^{-1}$.

HF is the enthalpy of liquid hydrazine entering the bed in Btu/lb.

R is a gas constant. It equals 10.73 (psia-ft^3)/(lb mole-deg R).

WM4 is the molecular weight of hydrazine. It equals 32.048 lb/lb mole.

WM3 is the molecular weight of ammonia. It equals 17.032 lb/lb mole.

5. The fifth card contains the eight constants WM2, WM1, ALPHA1, ALPHA2, AGM, BGM, KP, and CGM.

WM2 is the molecular weight of nitrogen. It equals 28.016 lb/lb mole.

WM1 is the molecular weight of hydrogen. It equals 2.016 lb/lb mole.

ALPHA1 is the preexponential factor in the rate equation for the catalytic decomposition of hydrazine (See Ref. 1). For the Shell 405 catalyst it equals $10^{10} sec^{-1}$.

ALPHA2 is the preexponential factor in the rate equation for the catalytic decomposition of ammonia (See Ref. 1). For the Shell 405 catalyst it equals $10^{11}(lb/ft^3)^{1.6}(sec)^{-1}$.

AGM is the activation energy for the catalytic decomposition of hydrazine, divided by the gas constant. For the Shell 405 catalyst it equals 2500 deg R.

BGM is the activation energy for the catalytic decomposition of ammonia, divided by the gas constant. For the Shell 405 catalyst it equals 50,000 deg R.

KP is the thermal conductivity of the porous catalyst particle. For the Shell 405 catalyst it equals 0.4×10^{-4} Btu/ft-sec-deg R.

CGM is the activation energy for the thermal decomposition of hydrazine, divided by the gas constant. It equals 33,000 deg R.

6. The sixth card contains the seven constants TF, CFL, ENMX1, ENMX2, ENMX3, DIF3, DIF4, and the inlet value of PRES.

TF is the temperature of liquid hydrazine entering the bed in deg R.

CFL is the specific heat of liquid hydrazine. It equals 0.7332 Btu/lb-deg R.

ENMX1 is the constant used to determine the size of axial station increments in the liquid region. It equals 200. Increasing this number would result in a decrease in size of axial station increments (and an increase in computer run time).

ENMX2 is the constant used to determine the size of axial station increments in the liquid-vapor region. It equals 40. Increasing this number would result in a decrease in size of axial station increments (and an increase in computer run time).

ENMX3 is the constant used to determine the size of axial station increments in the vapor region. It equals 80. Increasing this number would result in a decrease in size of axial station increments (and an increase in computer run time).

DIF3 is the diffusion coefficient of ammonia in the gas phase at STP. It equals $0.17 \times 10^{-3} ft^2/sec$.

DIF4 is the diffusion coefficient of hydrazine in the gas phase at STP. It equals $0.95 \times 10^{-4} ft^2/sec$.

PRES is the inlet chamber pressure in psia.

7. The seventh card contains the four constants ZEND, EN1, EN2, and EN3.

ZEND is the catalytic bed length in ft.

EN1 is the order of hydrazine catalytic decomposition reaction with respect to hydrazine. For the Shell 405 catalyst it equals 1.0.

EN2 is the order of ammonia catalytic decomposition reaction with respect to ammonia. For the Shell 405 catalyst it equals 1.0.

EN3 is the order of ammonia catalytic decomposition reaction with respect to hydrogen. For the Shell 405 catalyst it equals -1.6.

8. Cards 8 through 10 contain ZTBLA(I), the interpolation table used to obtain the catalyst particle radius at any point along the reactor bed. Subroutine UNBAR, an interpolation routine developed at the United Aircraft Research Laboratories, is used to obtain an appropriate particle radius, A, for a given axial station, Z(I), along the bed. For this table there should be a total of (NØFZ) Z's and (NØFZ) A's. The table is set up as follows.

CARD NO.

8 This card contains the four table descriptors used by UNBAR. The first descriptor signifies the table number. For this program it equals 0.0. The second descriptor tells at what location in the array the table starts; the tables in this program are read in such that this number equals 1.0. The third descriptor is the number of independent variables in the table (in this case, the number of Z's). This number equals NØFZ. The fourth descriptor for a univariate table such as this one should equal 0.0.

9 These cards contain the monatonically increasing Z values. Enough cards should be used to contain NØFZ values of Z at the rate of ten per card. For example, if NØFZ = 12, 12 values of Z should be input using two cards with ten values on the first card and the 2 remaining values on the second card.

10 These cards contain the A's which correspond to the Z's listed on cards 9. Enough cards should be used to contain NØFZ values of A at the rate of ten per card.

9. Cards 11 through 13 contain ZTBLAP(I), the interpolation table used to obtain the total external catalyst particle surface area per unit volume of bed (AP). These AP values are obtained from UNBAR as func-

tic.s of axial distance (Z) as in the ZTBLA table discussed above. For this table there should be a total of (NØFZ) Z's and (NØFZ) AP's. The table is set up as follows:

CARD NO.

11 This card is exactly the same as card 8.

12 These cards are exactly the same as cards 9.

13 These cards contain the AP values which correspond to the Z's listed on cards 12. Enough cards should be used to contain NØFZ values of AP at the rate of ten per card.

10. Cards 14 through 16 contain ZTBLD(I), the interpolation table used to obtain the interparticle void fraction (DELA). These DELA values are obtained from UNBAR as functions of axial distance (Z) as in the ZTBLA table discussed above. For this table there should be a total of (NØFZ) Z's and (NØFZ) DELA's. The table is set up as follows:

CARD NO.

14 This card is exactly the same as card 8.

15 These cards are exactly the same as cards 9.

16 These cards contain the DELA values which correspond to the Z's listed on cards 15. Enough cards should be used to contain NØFZ values of DELA at the rate of ten per card.

TABLE I
One-Dimensional Steady-State Computer Program
Input Format

CARD NUMBER	NUMBER OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
1	1	I3*	1-3	NCASE	-	No. of cases
2	1	14A6	1-80	Title	-	-
3	1	2I2, I3 *	1-2	ØPTIØN	-	Liq.-Vap. Indicator
				PRINT	-	Print Indicator
				NØFZ	-	No. of Z's in Input Tables
4	1	8E10.5	1-10	ZO	Z_o	Axial distance to injector end
			11-20	GO	G_o	Inlet mass flow rate
			21-30	FC	F	Distributed feed rate
			31-40	ALPHA3	α_{hom}	Preexponential factor
			41-50	HF	h_F	Enthalpy of feed
			51-60	R	R	Gas constant
			61-70	WM4	$M^{N_2H_4}$	Molecular wt. of N_2H_4
			71-80	WM3	M^{NH_3}	Molecular wt. of NH_3
5	1	8E10.5	1-10	WM2	M^{N_2}	Molecular wt. of N_2
			11-20	WM1	M^{H_2}	Molecular wt. of H_2
			21-30	ALPHA1	$\alpha^{N_2H_4}$	Preexponential factor
			31-40	ALPHA2	α^{NH_3}	Preexponential factor
			41-50	AGM	$Q_{het}^{N_2H_4}/R$	Activation energy, deg R
			51-60	BGM	$Q_{het}^{NH_3}/R$	Activation energy, deg R
			61-70	KP	K_T	Thermal conductivity
			71-80	CGM	$Q_{hom}^{N_2H_4}/R$	Activation energy, deg R
6	1	8E10.5	1-10	TF	T_F	Feed temperature
			11-20	CFL	C_f	Specific heat of liquid N_2H_4
			21-30	ENMX1	-	Determines step size in liquid region
			31-40	ENMX2	-	Determines step size in liq-vapor region
			41-50	ENMX3	-	Determines step size in vapor region
			51-60	DIF3	$D_o^{NH_3}$	Diffusion coef. of NH_3
			61-70	DIF4	$D_o^{N_2H_4}$	Diffusion coef. of N_2H_4
			71-80	PRES	P	Inlet chamber pressure

*All I format numbers should be right adjusted

CARD NUMBER	NUMBER OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
7	1	8E10.5	1-10	ZEND	-	Bed length
			11-20	EN1	n	Order of decomposition reaction
			21-30	EN2	n	Order of decomposition reaction
			31-40	EN3	n	Order of decomposition reaction
8	1	4E8.5	1-8	0.		Table descriptor
			9-16	1.		Table descriptor
			17-24	NØFZ.		Table descriptor
			25-32	0.		Table descriptor
9*	*	10E8.5	1-18	Z(I)	z	Axial station
			9-16			
			17-24			
			↓			
			73-80			
10**	**	10E8.5	1-8	A(I)	a	Catalyst Particle Radius
			9-16			
			17-24			
			↓			
			73-80			
11	1	4E8.5	1-8	0.		Table descriptor
			9-16	1.		Table descriptor
			17-24	NØFZ.		Table descriptor
			25-32	0.		Table descriptor

*Enough cards should be used to contain NØFZ values of z at the rate of ten per card.

**Enough cards should be used to contain NØFZ values of A at the rate of ten per card.

TABLE I
(Continued)

CARD NUMBER	NUMBER OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
12*	*	10E8.5	1-8 9-16 17-24 ↓ 73-80	Z(I)	z	Axial station
13**	**	10E8.5	1-8 9-16 17-24 ↓ 73-80	AP(I)	A_p	Total external catalyst particle surface area per unit vol. of bed
14	1	4E8.5	1-8 9-16 17-24 25-32	0. 1. NØFZ. 0.		Table descriptor Table descriptor Table descriptor Table descriptor
15*	*	10E8.5	1-8 9-16 17-24 ↓ 73-80	Z(I)	z	Axial station
16**	**	10E8.5	1-8 9-16 ↓ 73-80	DELA(I)	δ	Interparticle void fraction

*Enough cards should be used to contain NØFZ values of z at the rate of ten per card.

**[illegible] to contain NØFZ values of A at the rate of ten per card

CODING OF A SAMPLE DATA CASE

One-Dimensional Steady-State Model

Card No.	1–8	9–16	17–24	25–32	33–40	41–48	49–56	57–64	65–72	73–80
1	1									
2	**SAMPLE DATA CASE (1-DIM SS)** IXED BED * 60 * 5.0 * P = 100									
3	1 0 20									
4	0.	5.0		0.	.214 E+11	0.	10.75	32.048		17.332
5	28.016	2.016		.1 E+11	1. E+11	2500.	50[illegible]2.	.40 E-4		33000.
6	530.	.7332		200.	4.	80.	.47 E-5	.95 E-4		100.
7	.25	1.		1.	-1.6					
8	0.	1.	50.							
9a	0.	.0055	.0111	.0167	.0168	.0439	.0575	.0711	.0847	.0983
9b	.1119	.1255	.1391	.1527	.1763	.1799	.1935	.2207	.2343	.2500
10a	.001	.001	.001	.001	.0064	.0064	[illegible]	.0064	.0064	.0064
10b	.0064	.0064	.0064	.0064	.0064	.0064	[illegible]	.0064	.0064	.0064
11	0.	1.	20.	0.						
12a	0.	.0055	.0111	.0167	.0168	.0439	.0575	.0711	.0847	.0983
12b	.1119	.1255	.1391	.1527	.1663	.1799	.1935	.2207	.2343	.2500
13a	2100.	2100.	2100.	2100.	330.	330.	330.	330.	330.	330.
13b	330.	330.	330.	330.	330.	330.	330.	330.	330.	330.
14	0.	1.	20.	0.						
15a	0.	.0055	.0111	.0167	.0168	.0439	.0575	.0711	.0847	.0983
15b	.1119	.1255	.1391	.1527	.1663	.1799	.1935	.2207	.2343	.2500
16a	.34	.34	.34	.34	.34	.34	.34	.34	.34	.34
16b	.34	.34	.34	.34	.34	.34	.34	.34	.34	.34

LISTING OF INPUT DATA PUNCH CARDS: SAMPLE CASE
One-Dimensional Steady-State Model

```
                                                                                                   Card No.
 1                                                                                                    1
**SAMPLE DATA CASE (1-DIM SS)**     MIXED BED * G0 = 3.0 * P = 100.                                   2
 1 0 20                                                                                               3
   0.        3.0       0.      .214 E+11   0.      10.73     32.048    17.032                         4
 28.016    2.016     .1 E+11   1. E+11   2500.     50000.    .40 E-4   33000.                         5
 530.      .7332     200.      40.       80.       .17 E-3   .95 E-4   100.                           6
  .25      1.        1.        -1.6                                                                   7
  0.       1.        20.       0.                                                                     8
  0.       .0055     .0111     .0167     .0168     .0439     .0575     .0711     .0847     .0983      9a
 .1119     .1255     .1391     .1527     .1663     .1799     .1935     .2207     .2343     .2500      9b
 .001      .001      .001      .001      .0064     .0064     .0064     .0064     .0064     .0064      10a
 .0064     .0064     .0064     .0064     .0064     .0064     .0064     .0064     .0064     .0064      10b
  0.       1.        20.       0.                                                                     11
  0.       .0055     .0111     .0167     .0168     .0439     .0575     .0711     .0847     .0983      12a
 .1119     .1255     .1391     .1527     .1663     .1799     .1935     .2207     .2343     .2500      12b
 2100.     2100.     2100.     2100.     330.      330.      330.      330.      330.      330.       13a
 330.      330.      330.      330.      330.      330.      330.      330.      330.      330.       13b
  0.       1.        20.       0.                                                                     14
  0.       .0055     .0111     .0167     .0168     .0439     .0575     .0711     .0847     .0983      15a
 .1119     .1255     .1391     .1527     .1663     .1799     .1935     .2207     .2343     .2500      15b
 .34       .34       .34       .34       .34       .34       .34       .34       .34       .34        16a
 .34       .34       .34       .34       .34       .34       .34       .34       .34       .34        16b
```

FIG. 2

Output Description

Output from the one-dimensional steady-state program is entirely in printout form. Standard output, which is printed out when input option PRINT = 0, includes all printing normally done during execution of any representative data case, three messages which pertain to calculations which do not follow the normal pattern in a typical run, and one error message which is followed by program termination. Non-standard output is printed in addition to the standard output when PRINT = 1. This non-standard output includes additional calculated values and comments which pertain to intermediate calculations. The print statements associated with each routine in which output is generated are described below.

Standard Output

MAIN program

1. A complete listing of all program input including FØRTRAN variable titles for all input variables.

2. Axial position, (Z), temperature, (TEMP), enthalpy, (H), and rate of change of enthalpy with axial distance, (DHDZ), for each axial position in the liquid region.

Subroutine LQVP or LQV2

1. Axial position, (Z), temperature, (TEMP), enthalpy, (H), and weight fraction of vapor, (WFV), for each axial position in the liquid-vapor region.

Subroutine VAPØR

1. Axial position, (Z), temperature, (TEMP), pressure (PRES), enthalpy, (H), and concentrations of hydrogen, (C1), nitrogen, (C2), ammonia, (C3), and hydrazine, (C4), at each axial position in the vapor region.

2. Mole fractions of hydrogen, (MFRAC1), nitrogen, (MFRAC2), ammonia, (MFRAC3), and hydrazine, (MFRAC4), and the fractional dissociation of ammonia, (FRAC3D), at each axial position in the vapor region.

3. All axial positions, (Z values), in the vapor region listed consecutively and MBAR and G values at the end of the reactor for use in preparing input to the transient model computer program.

4. "KOUNT = XX --- THIS INTERVAL HAS BEEN REDIVIDED XXXX TIMES"

For all cases involving a non-zero embedded injector feed rate, a check is made on the Z step size after each calculation. If the increment proves too large to yield satisfactory results, it is halved and re-checked. The procedure continues until a satisfactory interval size is found, and the above message is then printed.

5. "THERE IS A PUDDLE ØF CØLD HYDRAZINE AT THE LIQUID-VAPOR/VAPOR INTERFACE --- TRY USING A LARGER VALUE FØR GO"

When using a buried injector scheme it is possible to "flood" the region surrounding the injector tip with cold, liquid hydrazine. A sudden drop in axial temperatures at the liquid-vapor/vapor interface indicates that this has occurred, and in such cases the above message is printed and no further calculations are made.

Subroutine SGRAD

1. "WE HAVE CALCULATED A NEGATIVE XO DURING ITERATIØN NØ. XX. SET XO = 0, CALCULATE TPS = .XXXXX ± XX, AND CØNTINUE"

XO represents an approximation of the radial distance to which hydrazine penetrates the catalyst particle before being dissipated. It is determined through an iterative procedure, and in some instances initial guesses do not yield satisfactory results. In this case, corrective measures to yield a better approximation to XO are instituted and the procedure repeated. This message indicates only that corrective calculations to improve on the accuracy of XO are being initiated.

2. "UNABLE TØ CØNVERGE ØN CPS IN 50 TRIES --- CP(X/A) = .XXXXX ± XX"

If subroutine SGRAD cannot calculate a "converged"value for CPS after 50 iterations, the final value for CP at the particle surface is used to approximate CPS. This is a good approximation to CPS, however, and program calculations continue with the above message being printed.

3. "UNABLE TØ FIND SUITABLE XO AFTER FØUR TRIES ØF 25 ITERATIØNS EACH --- PRØGRAM STØP FØLLØWS"

If after four corrective attempts to approximate XO the procedure still does not yield satisfactory results, this message along with all unacceptable values for XO is printed and further calculations are stopped. An octal dump of core accompanies the program stop.

Non-Standard Output

Subroutine SLØPE

1. "INITIAL CHØICE THRØUGH ØRIGIN IS TØØ LARGE"

   When iterating to find a satisfactory approximation to the radial depth of penetration of hydrazine in a catalyst particle (XO calculation), an initial guess is the particle radius itself. If this proves to be an unsatisfactory choice, the above message is printed and a different initial guess is used.

2. "SATISFACTØRY STARTING CURVE FØUND AFTER XX TRAILS. THE VALUE ØF B (XO) IS .XXXXXX ± XX"

   This message indicates that a satisfactory approximation to the radial depth of penetration of hydrazine in a catalyst particle has been found, and appears frequently in calculations involving the liquid region of the reactor.

3. "INITIAL CHØICE THRU ØRIGIN SEEMINGLY ØK, BUT RESULTS RØTTEN AFTER 99 ITERATIONS --- SET XO = .000001* A AND USE MØRE REFINED TECHNIQUE"

   When calculating a concentration vs radial position profile within the catalyst particle, an initial guess at the profile is used assuming a linear profile from the center of the particle to the surface. It can happen that this appears to be a satisfactory first guess, but ultimately yields unsatisfactory results for the final "converged" values of CPA. In such instances the above message is printed and the iteration procedure is repeated using a new initial guess.

4. "ITERATIØN = XX

X/A	CPA	X/A	CPA	X/A	CPA	X/A	CPA
XXXX	XXXX	XXXX	XXXX	XXXX	XXXX	XXXX	XXXX
XXXX	XXXX	XXXX	XXXX	XXXX	XXXX	XXXX	XXXX
:	:	:	:	:	:	:	:
XXXX	XXXX	XXXX	XXXX	XXXX	XXXX	XXXX	XXXX

   THE SLØPE CØNVERGES TØ .XXXXXXX ± XX"

   When a converged value for the slope of the concentration profile curve at the catalyst particle surface has been calculated, the above "concentration profile" will be printed. The word "ITERATIØN" refers to the iteration count at the time of convergence. X/A is the normalized distance from the center of the catalyst particle of radius A to the surface. CPA is the concentration of hydrazine within the particle at the corresponding normalized radial distance. The final message indicates the final converged value of the slope. This block will be printed for each axial station of the liquid region.

5. "THE SLØPE CØNVERGES TØ .XXXXXX ± XX"

   This message indicates that the iterative procedure has achieved convergence on a value of the hydrazine concentration gradient at the catalyst particle surface, and appears frequently in calculations involving the liquid region of the reactor.

Subroutine SGRAD

1. A listing of converged reactant concentration (CP(X/A)) versus normalized radial distance within the catalyst particle (X/A) at each axial position in the vapor region.

2. (a) "CØNCENTRATIØN GRADIENT FØUND AFTER XXX TRIES"

   (b) "CP(X) AT PARTICLE SURFACE = .XXXXX ± XX"

   (c) "KC3* (CI3-CPS) = .XXXXX ± XX"

   (d) "HC* (T-TPS) = .XXXXX ± XX"

   Print message (a) indicates the number of iterations that were needed to find a converged value for the concentration gradient.

   Print message (b) gives the converged value for the concentration at the particle surface $(c_p)_s$.

   Print messages (c) and (d) give calculated values where KC3 is the mass transfer coefficient for ammonia, CI3 is the interstitial concentration of ammonia at the catalyst surface, HC is the heat transfer coefficient, T is the interstitial temperature, and TPS is the temperature at the surface of the catalyst.

   Print messages (a), (b), (c), and (d) appear at each axial position in the vapor region.

3. "SATISFACTORY XO FOUND AFTER XXX TRIES, XO = .XXXXX ± XX"

When calculating an ammonia concentration radial profile within a catalyst particle it is necessary to determine the radial depth of penetration of ammonia. The approximate radial position of "zero" concentration is referred to as XO in subroutine SGRAD, and when the iterative procedure employed has successfully determined a value of XO, the above message, with iteration count, is printed.

A sample listing of the output for a typical one-dimensional steady-state data case is shown in Figs. 3a through 3f.

LISTING OF OUTPUT FOR SAMPLE DATA CASE
ONE-DIMENSIONAL STEADY-STATE

```
**SAMPLE DATA CASE (1-DIM SS)**     MIXED BED * G0 = 3.0 * P = 100.

                                       INPUT CONSTANTS
   HF        HL         HV         TF         TVAP       CFL       PRESSURE     KP         F          G0
 .000000   .212628+03 .715478+03 .530000+03 .820000+03 .733200-00 .100000+03 .400000-04 .000000   .300000+01

   R        ALPHA3      CGM        DIF3       DIF4       WM4        WM3        WM2        WM1        ZEND
 .107300+02 .214000+11 .330000+05 .170000-03 .950000-04 .320480+02 .170320+02 .280160+02 .201600+01 .250000-00

   AGM        BGM       ALPHA1     ALPHA2      N1         N2         N3        ENMX1      ENMX2      ENMX3      Z0
 .250000+04 .500000+05 .100000+11 .100000+12 .100000+01 .100000+01-.160000+01 .200000+03 .400000+02 .800000+02

 .000000

                                        Z VS A TABLE
                                 .000000    .100000+01 .210000+02 .000000
 .000000    .550000-02 .111000-01 .167000-01 .168000-01 .439000-01 .575000-01 .711000-01 .847000-01 .983000-01
 .111900+00 .125500-00 .139100-00 .152700-00 .166300-00 .179900-00 .193500-00 .207100-00 .220700-00 .234300-00
 .250000-00
 .100000-02 .100000-02 .100000-02 .100000-02 .640000-02 .640000-02 .640000-02 .640000-02 .640000-02 .640000-02
 .640000-02 .640000-02 .640000-02 .640000-02 .640000-02 .640000-02 .640000-02 .640000-02 .640000-02 .640000-02
 .640000-02

                                        Z VS AP TABLE
                                 .000000    .100000+01 .210000+02 .000000
 .000000    .550000-02 .111000-01 .167000-01 .168000-01 .439000-01 .575000-01 .711000-01 .847000-01 .983000-01
 .111900+00 .125500-00 .139100-00 .152700-00 .166300-00 .179900-00 .193500-00 .207100-00 .220700-00 .234300-00
 .250000-00
 .210000+04 .210000+04 .210000+04 .210000+04 .330000+03 .330000+03 .330000+03 .330000+03 .330000+03 .330000+03
 .330000+03 .330000+03 .330000+03 .330000+03 .330000+03 .330000+03 .330000+03 .330000+03 .330000+03 .330000+03
 .330000+03

                                        Z VS DELTA TABLE
                                 .000000    .100000+01 .210000+02 .000000
 .000000    .550000-02 .111000-01 .167000-01 .168000-01 .439000-01 .575000-01 .711000-01 .847000-01 .983000-01
 .111900+00 .125500-00 .139100-00 .152700-00 .166300-00 .179900-00 .193500-00 .207100-00 .220700-00 .234300-00
 .250000-00
 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00
 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00 .340000-00
 .340000-00
```

FIG. 3a

******************************* ENTERING LIQUID REGION *******************************

Z	TEMP	H	DHDZ
.000000	.530000+03	.000000	.377541
.252216-03	.542936+03	.948446+01	.538926+05
.427074-03	.555862+03	.189619+02	.945157+05
.527298-03	.568781+03	.284346+02	.143787+06
.593145-03	.581695+03	.379026+02	.221126+06
.635941-03	.594602+03	.473658+02	.322530+06
.665267-03	.607502+03	.568244+02	.467775+06
.685477-03	.620396+03	.662782+02	.675305+06
.699470-03	.633283+03	.757274+02	.962125+06
.709286-03	.646164+03	.851718+02	.132107+07
.716432-03	.659039+03	.946115+02	.183241+07
.721580-03	.671907+03	.104047+03	.242181+07
.725474-03	.684769+03	.113477+03	.316562+07
.728452-03	.697625+03	.122902+03	.412827+07
.730734-03	.710474+03	.132323+03	.577362+07

G910461-30

FIG. 3c

Z	TEMP	H	DHDZ
.732365-03	.723316+03	.141740+03	.750974+07
Z	TEMP	H	DHDZ
.733618-03	.736154+03	.151152+03	.935122+07
Z	TEMP	H	DHDZ
.734627-03	.748989+03	.160563+03	.117621+08
Z	TEMP	H	DHDZ
.735427-03	.761822+03	.169972+03	.151922+08
Z	TEMP	H	DHDZ
.736046-03	.774653+03	.179380+03	.187659+08
Z	TEMP	H	DHDZ
.736547-03	.787482+03	.188786+03	.225211+08
Z	TEMP	H	DHDZ
.736964-03	.800308+03	.198190+03	.269846+08
Z	TEMP	H	DHDZ
.737313-03	.813133+03	.207593+03	.342904+08
Z	TEMP	H	DHDZ
.737459-03	.820000+03	.212628+03	.383323+08

******************************* ENTERING LIQUID-VAPOR REGION ***

Z	TEMP	H	WFV
.73770-03	.82000+03	.25963+03	.93472-01
.73893-03	.82000+03	.30663+03	.18694-00
.74016-03	.82000+03	.35363+03	.28041-00
.74138-03	.82000+03	.40064+03	.37389-00
.74261-03	.82000+03	.44764+03	.46736-00
.74384-03	.82000+03	.49464+03	.56083-00
.74506-03	.82000+03	.54164+03	.65430-00
.74629-03	.82000+03	.58865+03	.74777-00
.74751-03	.82000+03	.63565+03	.84124-00
.74874-03	.82000+03	.68265+03	.93472-00
.75082-03	.82000+03	.71548+03	.10000+01

G910461-30

*********************************** ENTERING VAPOR REGION ***********************************

Z	TEMP	PRES	H	C1	C2	C3	C4
.75082274-03	.82000000+03	.10000000+03	.71547798+03	.31579918-02	.43886062-01	.53360037-01	.16743158-00

MFRAC1	MFRAC2	MFRAC3	MFRAC4	FRAC3D
.13782692-00	.13782692-00	.27565384-00	.44869231-00	-.00000000

Z	TEMP	PRES	H	C1	C2	C3	C4
.90740574-03	.86645369+03	.99981377+02	.73897909+03	.32506140-02	.43334869-01	.50454650-01	.14735426-00

MFRAC1	MFRAC2	MFRAC3	MFRAC4	FRAC3D
.15041867-00	.14429730-00	.27635187-00	.42893217-00	.21670607-01

Z	TEMP	PRES	H	C1	C2	C3	C4
.10665796-02	.91158767+03	.99960899+02	.76246590+03	.33173817-02	.42790974-01	.48003883-01	.13356108-00

MFRAC1	MFRAC2	MFRAC3	MFRAC4	FRAC3D
.16197901-00	.15034878-00	.27743711-00	.41023511-00	.40233626-01

Z	TEMP	PRES	H	C1	C2	C3	C4
.12278735-02	.95559712+03	.99938571+02	.78594348+03	.33603019-02	.42236826-01	.45931103-01	.12162228+00

MFRAC1	MFRAC2	MFRAC3	MFRAC4	FRAC3D
.17243814-00	.15596628-00	.27898882-00	.39260677-00	.55749761-01

FIG. 3e

Z	TEMP	PRES	H	C1	C2	C3	C4
.17155202-00	.19507243+04	.78863929+02	.14092872+04	.39661221-02	.31522408-01	.96[illegible]9835?-02	.00000000

MFRAC1	MFRAC2	MFRAC3	MFRAC4	FRAC3D
.53774555-00	.30754914-00	.15470531-00	.00000000	.59806513-00

Z	TEMP	PRES	H	C1	C2	C3	C4
.24999999-00	.19053842+04	.71680713+02	.13780029+04	.38096090-02	.29667359-01	.77733879-02	.00000000

MFRAC1	MFRAC2	MFRAC3	MFRAC4	FRAC3D
.55496938-00	.31099391-00	.13403673-00	.00000000	.64541664-00

Z'S FROM VAPOR REGION

.7508227-03	.9074057-03	.1066580-02	.1227874-02	.1392110-02	.1559678-02	.1730142-02	.1905576-02	.2084807-02	.2269192-02
.2459069-02	.2655209-02	.2858234-02	.3068889-02	.3267984-02	.3516443-02	.3755323-02	.4005866-02	.4269497-02	.4547898-02
.4863068-02	.5157416-02	.5493980-02	.5856422-02	.6249363-02	.6678468-02	.7151910-02	.7680163-02	.8276725-02	.8971330-02
.9737482-02	.1083580-01	.1225605-01	.1465600-01	.1476369-01	.1487130-01	.1497891-01	.1530174-01	.1562457-01	.1659306-01
.1756156-01	.2046704-01	.2337252-01	.3208896-01	.4080540-01	.6695473-01	.9310405-01	.1127160+00	.1323280-00	.1519400-00
.1715520-00	.1911640-00	.2107760-00	.2303800-00	.2500000-00					

STEADY STATE VALUES FOR MBAR AND G AT END OF BED
MBAR = .12115+02 G = .30000+01

***** OPERATIONS COMPLETE *****

FIG. 3f

Common Operational Problems

Many different data cases have been run with the one-dimensional steady-state computer program. During these runs, most of the problems which have developed have been eliminated through program modification. However, two problems which may still occur are noted below, together with appropriate techniques for solving them.

1. "UNABLE TØ FIND SUITABLE XO AFTER FØUR TRIES ØF 25 ITERATIØNS EACH ... PRØGRAM STØP FØLLØWS"

   If a satisfactory value for XO cannot be found after four attempts, this message is printed and program execution is terminated. An appropriate solution to this problem would be to try different values for f_i |Eq. (I-11) in discussion of SGRAD, Appendix I|. These values could be greater than 0.95. To make this change, subroutine SGRAD would have to be recompiled using the new values of f_i.

2. "THERE IS A PUDDLE ØF CØLD HYDRAZINE AT THE LIQUID-VAPØR/VAPØR INTERFACE --- TRY USING A LARGER VALUE FØR GO"

   When using a buried injector scheme it is possible to "flood" the region surrounding the injector tip with cold, liquid hydrazine. A sudden drop in axial temperatures at the liquid-vapor/vapor interface indicates that this has occurred, and in such cases the above message in printed and no further calculations are made. An appropriate solution to this problem would be to try a larger input value for GO and rerun the program with the revised input.

Two-Dimensional Steady-State Model

Input Description

The following is a description of the necessary input for the two-dimensional steady-state computer program. The input format is given in Table II. The coding of the sample data case for this program is shown in Figs. 4a and 4b, and a listing of the input data punch cards corresponding to this sample data case is shown in Figs. 5a and 5b. The statement numbers in the text below refer to the card numbers (first column) of Table II. For each run there will be only one card number one. Cards two through twenty-one should be included for each data case to be run.

1. The first card contains the number NCASE. This number indicates the number of data cases with each run. $1 \leq$ NCASE ≤ 999.

2. The second card is the title card used for individual data case identification. The title may be any alpha numeric information desired.

3. The third card contains the indicators NRINGS and NØFZ. NRINGS indicates the number of evenly spaced radial stations at which calculations are to be made where radial station number one is that one nearest the center of the reactor and radial station number (NRINGS) is that station nearest the reactor wall. For typical runs, NRINGS = 10 was found adequate to insure good results. Increasing this number would allow more detailed radial analysis, but it would also increase computer run time. NØFZ is the number of axial stations (Z's) to be used in the three tables input on cards 10 through 21.

4. Cards four contain the values of F(I), (the rates of feed of hydrazine from buried injectors (Ref. 1) into the system in lb/ft^3-sec). One value of F for each radial station (total number of radial stations = NRINGS) should be input. Ten numbers are allowed to a card. For the suggested NRINGS of 10, there would be one card with ten values of F.

5. Cards five contain the values of GO(I), (the inlet mass flow rates in lb/ft^2-sec) for each radial station. Ten numbers are allowed to a card. For the suggested NRINGS of 10. there would be one card with ten values of GO. All values of GO must be greater than zero.

6. Cards six contain the values of ZO(I), (the axial distance to the end of a buried injector in ft) for each radial station. Ten numbers are allowed to a card. For the suggested NRINGS of 10, there would be one card with ten values of ZO.

7. The seventh card contains the eight constants ALPHA3, HF, R, MN2H4, MNH3, MN2, MH2, and ALPHA1.

ALPHA3 is the preexponential factor in the rate equation for the thermal decomposition of hydrazine. It equals $2.14 \times 10^{10} sec^{-1}$.

HF is the enthalpy of liquid hydrazine entering the bed in deg R.

R is the gas constant. It equals 10.73 $(psia\text{-}ft^3)/(lb\text{-}mole\text{-}deg\ R)$.

MN2H4 is the molecular weight of hydrazine. It equals 32.048 lb/lb mole.

MNH3 is the molecular weight of ammonia. It equals 17.032 lb/lb mole.

MN2 is the molecular weight of nitrogen. It equals 28.016 lb/lb mole.

MH2 is the molecular weight of hydrogen. It equals 2.016 lb/lb mole.

ALPHA1 is the preexponential factor in the rate equation for the catalytic decomposition of hydrazine. For the Shell 405 catalyst it equals $10^{10} sec^{-1}$.

8. The eighth card contains the eight constants ALPHA2, AGM, BGM, KP, TF, CF, NMAX1, and NMAX2.

ALPHA2 is the preexponential factor in the rate equation for the catalytic decomposition of ammonia. For the Shell 405 catalyst it equals $10^{11} sec^{-1}$.

AGM is the activation energy for the catalytic decomposition of hydrazine, divided by the gas constant. For the Shell 405 catalyst it equals 2,500 deg R.

BGM is the activation energy for the catalytic decomposition of ammonia, divided by the gas constant. For the Shell 405 catalyst it equals 50,000 deg R.

KP is the effective thermal conductivity of the porous catalyst particle. For the Shell 405 catalyst it equals 0.4×10^{-4} Btu/ft-sec-deg R.

TF is the temperature of liquid hydrazine entering the bed in deg R.

CF is the specific heat of liquid hydrazine. It equals 0.7332 Btu/lb-deg R.

NMAX1 is the constant used to determine the size of axial station increments in the liquid region. It equals 200. Increasing this number would result in a decrease in size of axial station increments (and an increase in computer run time).

NMAX2 is the constant used to determine the size of axial station increments in the liquid-vapor region. It equals 40. Increasing this number would result in a decrease in size of axial station increments (and an increase in computer run time).

9. The ninth card contains the inlet value of P and five constants ZEND, DON2H4, DONH3, CGM, and RADIUS.

P is the inlet chamber pressure in psia.

ZEND is the catalyst bed length in feet.

DON2H4 is the diffusion coefficient of hydrazine in the gas phase at STP. It equals $0.95 \times 10^{-4} ft^2/sec$.

DONH3 is the diffusion coefficient of ammonia in the gas phase at STP. It equals $0.17 \times 10^{-3} ft^2/sec$.

CGM is the activation energy for the thermal decomposition of hydrazine, divided by the gas constant. It equals 33,000 deg R.

RADIUS is the radius of the catalyst bed in feet.

10. Cards ten through thirteen contain AVSZ(I), the bivariate interpolation table used to obtain the catalyst particle radius, A(z,r)*. These A values are obtained from subroutine UNBAR, an interpolation routine developed at the United Aircraft Research Laboratories, as functions of axial distance, Z, and radial distance, RAD. For this table there should be a total of (NØFZ) Z's, (NRINGS) RAD's and (NØFZ x NRINGS) A's. The table is set up as follows:

*This variable is not subscripted in the program. This notation is used to show that the variable is a function of both axial distance and radial distance and to clarify the way the table is set up.

CARD NO.

10 This card contains the four table descriptors used by UNBAR. The first descriptor signifies the table number. For this program it equals 0.0. The second descriptor signifies the location in the array at which the table starts; the tables in this program are read in such that this number equals 1.0. The third descriptor for a bivariate table such as this one is the number of elements in the first set of independent variables in the table (in this case, the number of Z's). This number equals NØFZ. The fourth descriptor is the number of elements in the second set of independent variables in the table (in this case, the number of RAD's). This number equals NRINGS.

11 These cards contain the monatonically increasing Z values. Enough cards should be used to contain NØFZ values of Z at the rate of ten per card. For example, if NØFZ = 12, 12 values of Z should be input using 2 cards with ten values on the first card and the 2 remaining values on the second card.

12 These cards contain the monatonically increasing RAD's. Enough cards should be used to contain NRINGS values of RAD at the rate of ten per card.

13 These cards contain the values for A(z, r). The A values are input at each Z value for all RAD's (i.e., (NRINGS) values of A for each Z) at the rate of ten per card.

Example 1: if NØFZ = 10 and NRINGS = 5, the first card would contain five A values corresponding to the five RAD's on card 12 for Z(1); the second card would contain the five A values corresponding to the five RAD's for Z(2); ... etc. ...; the 10th card would contain the five A values corresponding to the five RAD's for Z(10).

Example 2: if NØFZ = 10 and NRINGS = 12, the first card would contain 10 A values corresponding to the first ten RAD's (on card 12a) for Z(1); the second card would contain the two remaining A's corresponding to the last two RAD's (on card 12b) for Z(1); the third card would contain the 10 A's corresponding to the first ten RAD's for Z(2); the fourth card would contain the 2 remaining A's for Z(2); ... etc. ...; the 19th card would contain the ten A's corresponding to the first ten RAD's at Z(10); the 20th card would contain the two A's corresponding to the last two RAD's at Z(10).

11. Cards 14 through 17 contain APVSZ(I), the bivariate interpolation table used to obtain the catalyst particle surface area, AP(z,r)*. These AP values are obtained from UNBAR as functions of axial distance, Z, and radial distance, RAD, as in the AVSZ table discussed above. For this table there should be a total of (NØFZ) Z's, (NRINGS) RAD's, and (NØFZ x NRINGS) AP's. The table is set up as follows:

CARD NO.

14 This card is exactly the same as card 10.

15 These cards are exactly the same as cards 11.

16 These cards are exactly the same as cards 12.

17 These cards contain the values for AP(z,r). These values are input at each Z value for all RAD's at the rate of ten values per card. (See examples in the discussion of the AVSZ table as the table setup is the same.)

12. Cards 18 through 21 contain DELVSZ(I), the bivariate interpolation table used to obtain the interparticle void fraction, DELTA (z,r)*. These DELTA values are obtained from UNBAR as functions of axial distance, Z, and radial distance, RAD, as in the AVSZ table discussed above. For this table there should be a total of (NØFZ) Z's, (NRINGS) RAD's, and (NØFZ x NRINGS) DELTA's. The table is set up as follows:

CARD NO.

18 This card is exactly the same as card 10.

19 These cards are exactly the same as cards 11.

20 These cards are exactly the same as cards 12.

21 These cards contain the values for DELTA (z,r). These values are input at each Z value for all RAD's at the rate of ten values per card. (See examples in the discussion of the AVSZ table as the table setup is the same).

NOTE: The values for the orders of the decomposition reactions (called EN1, EN2, and EN3 in the one-dimensional model) are included in the equations in the two-dimensional model and therefore are not input.

*This variable is not subscripted in the program. This notation is used to show that the variable is a function of both axial distance and radial distance and to clarify the way the table is set up.

TABLE II

Two-Dimensional Computer Program: Input Format

CARD NUMBER	NUMBER OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
1	1	I3*	1-3	NCASE		Number of data cases
2	1	14A6	1-80	Title	-	-
3	1	2I3*	1-3 4-6	NRINGS NØFZ	-	Number of radial stations Number of z's in input tables
4	**	10E8.4	1-8 9-16 ↓ 73-80	F(I)	F	Distributed Feed Rate
5	**	10E8.4	1-8 9-16 ↓ 73-80	GO(I)	G_o	Inlet mass flow rate
6	**	10E8.4	1-8 9-16 ↓ 73-80	ZO(I)	Z_o	Axial distance to injector end

*All I format numbers should be right adjusted.

**Enough cards should be used to contain (NRINGS) values of F(I), GO(I) or ZO(I) at the rate of ten per card.

CARD NUMBER	NUMBER OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
7	1	8E10.5	1-10	ALPHA3	α_{hom}	Constant in rate equation
			11-20	HF	h_F	Enthalpy of feed
			21-30	R	R	Gas constant
			31-40	MN2H4	$M^{N_2H_4}$	Molecular weight of N_2H_4
			41-50	MNH3	M^{NH_3}	Molecular weight of NH_3
			51-60	MN2	M^{N_2}	Molecular weight of N_2
			61-70	MH2	M^{H_2}	Molecular weight of H_2
			71-80	ALFHA1	$\alpha^{N_2H_4}$	Preexponential factor
8	1	8E10.5	1-10	ALPHA2	α^{NH_3}	Preexponential factor
			11-20	AGM	$Q_{het}^{N_2H_4}$ IR	Activation energy, deg R
			21-30	BGM	$Q_{het}^{NH_3}$ IR	Activation energy, deg R
			31-40	KP	K_p	Thermal conductivity
			41-50	TF	T_F	Feed temperature
			51-60	CF	C_F	Specific heat of liquid N_2H_4
			61-70	NMAX1	-	Determ. axial step size (liq. reg.)
			71-80	NMAX2	-	Determ. axial step size(liq.vap.reg.)
9	1	8E10.5	1-10	P	P	Inlet chamber pressure
			11-20	ZEND	-	Bed length
			21-30	DON2H4	$D_o^{N_2H_4}$	Diffusion coefficient of N_2H_4
			31-40	DONH3	$D_o^{NH_3}$	Diffusion coefficient of NH_3
			41-50	CGM	$Q_{hom}^{N_2H_4}/R$	Activation energy, deg R
			51-60	RADIUS	-	Bed radius
10	1	4E8.4	1-8	0.		Table descriptor
			9-16	1.		Table descriptor
			17-24	NØFZ.		Table descriptor
			25-32	NRINGS.		Table descriptor
11		10E8.4	1-8	Z(I)	z	Axial station
			9-16			
			↓			
			73-80			

*Enough cards should be used to contain (NØFZ) values of z at the rate of ten per card.

TABLE II (Cont.)

CARD NUMBER	NUMBER OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
12	**	10E8.4	1-8 9-16 ↓ 73-80	RAD(I)	r	Radial station
13	***	10E8.4	1-8 9-16 ↓ 73-80	A(z,r)	a	Catalyst particle radius
14	1	4E8.4	1-8 9-16 17-24 25-32	0. 1. NØFZ. NRINGS.		Table descriptor Table descriptor Table descriptor Table descriptor
15	*	10E8.4	1-8 9-16 ↓ 73-80	Z(I)	z	Axial station
16	**	10E8.4	1-8 9-16 ↓ 73-80	RAD(I)	r	Radial station
17	***	10E8.4	1-8 9-16 ↓ 73-80	AP(z,r)	Ap	Total external catalyst partial surface area per unit volume of bed

*Enough cards should be used to contain (NØFZ) values of z at the rate of ten per card.

**Enough cards should be used to contain (NRINGS) values of RAD at the rate of ten per card.

***Enough cards should be used to contain (NRINGS) values of A and AP for each z at the rate of ten per card (see detailed example in text).

CARD NUMBER	NUMBER OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
18	1	4E8.4	1-8 9-16 17-24 25-32	0. 1. NØFZ. NRINGS.		Table descriptor Table descriptor Table descriptor Table descriptor
19	*	10E8.4	1-8 9-16 ↓ 73-80	Z(I)	z	Axial station
20	**	10E8.4	1-8 9-16 ↓ 73-80	RAD(I)	r	Radial station
21	***	10E8.4	1-8 9-16 ↓ 73-80	DELTA(z,r)	δ	Interparticle void fraction

*Enough cards should be used to contain (NØFZ) values of z at the rate of ten per card.
**Enough cards should be used to contain (NRINGS) values of RAD at the rate of ten per card.
***Enough cards should be used to contain (NRINGS) values of DELTA for each z at the rate of ten per card.

CODING OF A SAMPLE DATA CASE

TWO - DIMENSIONAL STEADY - STATE MODEL

										Card No.
1										1
SAMPLE DATA CASE (2-DIM SS)**					ALL WIRE, NI-S[illegible]		(AV. C3=3.)NP=10[illegible]			2
10 30										3
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	4
5.	5.	5.	5.	5.	5.	5.	1.	1.	1.	5
0.	0.	0.	0.	0.	0.	0.	0.1	[illegible]	0.	6
2.14 E+10	0.		12.7	[illegible]	17.0[illegible]	[illegible]	[illegible]	10.	E+1[illegible]	7
1. E+11	8500.		6000.	[illegible]	450.	.75[illegible]	[illegible]	[illegible]		8
100.	.35		[illegible]-4	.111 E-5	15000.	.75[illegible]				9
.0	1.		10.							10
.0	.0055	.0111	.0167	.0222	.0559	.0575	.0722	[illegible]	.09[illegible]	11a
.1119	.1355	.1[illegible]	.1587	.1[illegible]	.1[illegible]	.1[illegible]	[illegible]	[illegible]	.25[illegible]	11b
.00625	.01875	.03125	.04375	.05625	.06875	.08125	.09375	.10625	.11875	12
.001	.001	.001	.001	.001	.001	.001	.001	.001	.001	13a
.001	.001	.001	.001	.001	.001	.001	.001	.001	.001	13b
.001	.001	.001	.001	.001	.001	.001	.001	.001	.001	13c
.001	.001	.001	.001	.001	.001	.001	.001	.001	.001	13d
.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	13e
.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	13f
↓	↓	↓							↓	↓
.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	.0064	13t
.0	1.	30.	10.							14
.0	.0055	.0111	.0167	.0[illegible]	.0559	.0575	.0711	.0067	[illegible]	15a
.1119	.1355	.1381	.1537	.1[illegible]	.1779	.1935	.2007	[illegible]	[illegible]	15b
.00625	.01875	.03125	.04375	.05625	.06875	.08125	.09375	.10625	.11875	
2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	17a
2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	17b
2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	17c
2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	2100.	17d
330.	330.	330.	330.	330.	330.	330.	330.	330.	330.	17e
330.	330.	330.	330.	330.	330.	330.	330.	330.	330.	17f
↓	↓	↓		↓					↓	↓
330.	330.	330.	330.	330.	330.	330.	330.	330.	330.	17t
.0	1.	30.	1[illegible].							18

FIG. 4a

(CONT.)

CODING OF A SAMPLE DATA CASE (CONTINUED)
TWO - DIMENSIONAL STEADY - STATE MODEL

1–8	9–16	17–24	25–32	33–40	41–48	49–56	57–64	65–72	73–80	Card No.
.0	.0055	.0111	.[illegible]167	.0166	.[illegible]49	.0575	.0711	.0847	.0983	[illegible]a
.1119	.1255	.1391	.1527	.1663	.1799	.1935	.2207	.2343	.2579	[illegible]b
.00625	.01875	.03125	.0[illegible]75	.05625	.06[illegible]75	.08125	.09375	.10625	.11[illegible]	[illegible]
.34	.34	.34	.[illegible]4	.34	.[illegible]	.34	.34	.34	.[illegible]	[illegible]a
.34	.34	.34	.[illegible]4	.34	.[illegible]	.34	.34	.34	.[illegible]	21b
↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓
.34	.34	.34	.[illegible]4	.34	.[illegible]4	.34	.34	.34	.[illegible]	21t

FIG. 4b

LISTING OF INPUT DATA PUNCH CARDS: SAMPLE CASE

TWO - DIMENSIONAL STEADY - STATE MODEL

```
                                                                                  Card No.
 1                                                                                 1
**SAMPLE DATA CASE (2-DIM SS)**    ALL MIXED*1-STEP GO (AV. C0=3.)*P=100           2
 10 20                                                                             3
  0.      0.      0.      0.      0.      0.      0.      0.      0.      0.       4
  5.      5.      5.      5.      5.      5.      5.      1.      1.      1.       5
  0.      0.      0.      0.      0.      0.      0.      0.      0.      0.       6
 2.14 E+10  0.       10.73   32.048  17.032   28.016   2.016   1.   E+10           7
 1.   E+11  2500.    50000.  .4  E-4 530.     .7332    200.    40.                 8
  100.      .25      .95 E-4 .17 E-3 33000.   .125                                 9
  .0      1.      20.     10.                                                      10
  .0     .0055   .0111   .0167   .0168   .0439   .0575   .0711   .0847   .0983     11a
  .1119  .1255   .1391   .1527   .1663   .1799   .1935   .2207   .2343   .2500     11b
.00625  .01875  .03125  .04375  .05625  .06875  .08125  .09375  .10625  .11875     12
 .001    .001    .001    .001    .001    .001    .001    .001    .001    .001      13a
 .001    .001    .001    .001    .001    .001    .001    .001    .001    .001      13b
 .001    .001    .001    .001    .001    .001    .001    .001    .001    .001      13c
 .001    .001    .001    .001    .001    .001    .001    .001    .001    .001      13d
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13e
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13f
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13g
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13h
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13i
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13j
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13k
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13l
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13m
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13n
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13o
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13p
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13q
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13r
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13s
 .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064   .0064     13t
  .0      1.      20.     10.                                                      14
  .0     .0055   .0111   .0167   .0168   .0439   .0575   .0711   .0847   .0983     15a
  .1119  .1255   .1391   .1527   .1663   .1799   .1935   .2207   .2343   .2500     15b
.00625  .01875  .03125  .04375  .05625  .06875  .08125  .09375  .10625  .11875     16
 2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.     17a
 2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.     17b
 2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.     17c
 2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.   2100.     17d
```

FIG. 5a

LISTING OF INPUT DATA PUNCH CARDS : SAMPLE CASE (CONTINUED)
TWO - DIMENSIONAL STEADY - STATE MODEL

										Card No.
330.	330.	330.	330.	330.	330.	330.	330.	330.	330.	17e
330.	330.	330.	330.	330.	330.	330.	330.	330.	330.	17f
330.	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17g
[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17h
[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17i
[illegible]	[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	17j
[illegible]	[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	17k
[illegible]	[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	17l
[illegible]	[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	17m
[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17n
[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17o
330.	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17p
[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17q
[illegible]	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17r
330.	[illegible]	330.	330.	330.	330.	330.	330.	330.	330.	17s
330.	330.	330.	330.	330.	330.	330.	330.	330.	330.	17t
.0	1.	20.	10.							18
.0	.0055	.0111	[illegible]	.0168	.0439	.0575	.0711	.0847	.0983	19a
.1119	.1255	.1391	.1527	.1663	.1799	.1935	.2207	.2343	.2500	19b
.00625	.01875	.03125	.04375	.05625	.06875	.08125	.09375	.10625	.11875	20
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21a
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21b
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21c
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21d
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21e
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21f
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21g
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21h
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21i
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21j
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21k
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21l
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21m
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21n
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21o
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21p
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21q
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21r
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21s
.34	.34	.34	.34	.34	.34	.34	.34	.34	.34	21t

FIG. 5b

Output Description

Output from the two-dimensional steady-state program is entirely in print-out form. There is no print option as in the one-dimensional program; therefore, all printing described below is "standard" and could possibly occur with each data case run. The print statements generated from each routine are described below; they include all printing normally done during execution of any representative data case, error messages, and certain comments pertaining to calculations which do not follow the normal pattern in a typical run.

Standard Output

MAIN Program

1. A complete listing of the punch card input with appropriate headings and FØRTRAN variable titles for all input variables.

2. Axial positions, (Z), and temperatures, (T), in each annular region for both liquid and liquid-vapor regions.

3. Axial position, radial position and temperature at the liquid/liquid-vapor interface for each annular region.

4. Axial position, radial position and temperature at the liquid-vapor/vapor interface for each annular region.

Subroutine VAPØR

1. Concentrations of hydrazine, (C4), ammonia, (C3), nitrogen, (C2), and hydrogen, (C1), and mole fractions of hydrazine, (MFRAC4), ammonia, (MFRAC3), nitrogen, (MFRAC2), and hydrogen, (MFRAC1), at the liquid-vapor/vapor interfaces (these values will be indentical for each ring).

2. Axial position, (Z), temperature, (TEMP), and concentrations of hydrazine, (N2H4), ammonia, (NH3), nitrogen, (N2), and hydrogen, (H2), for each annular region at every axial increment along the reactor.

3. Assumed uniform pressure (calculated by averaging the pressure drop calculated for each ring over the reactor cross-section) in the reactor at each axial increment.

4. Mole fractions of hydrazine, (MFRAC4), ammonia, (MFRAC3), nitrogen, (MFRAC2), and hydrogen, (MFRAC1), and the equivalent fractional ammonia dissociation, (EQUIVALENT FRAC3D), for each annular ring at every axial increment.

5. "THERE IS A PUDDLE ØF CØLD HYDRAZINE AT THE LIQUID-VAPØR/VAPØR INTERFACE --- TRY USING A LARGER VALUE FØR GO"
   When using a buried injector scheme it is possible to "flood" the region surrounding the injector tip with cold, liquid hydrazine. A sudden drop in axial temperatures at the liquid-vapor/vapor interface in any annular ring indicates that this has occurred, and in such cases the above message is printed and no further calculations are made.

6. "THE PRØGRAM HAS CALCUALTED A NEGATIVE PRESSURE --- RETURN AND TERMINATE"

   If a negative pressure is calculated at some axial station, further calculations for the current data case are stopped and this message is printed out.

7. "THE PRØGRAM HAS CALCULATED A NEGATIVE TEMPERATURE IN RING XX --- RETURN AND TERMINATE"

   If a negative temperature is calculated in any annular region at any axial station, further calculations are stopped and this message, including the current annular ring, is printed.

Subroutine SGRAD

1. "WE HAVE CALCULATED A NEGATIVE XO DURING ITERATIØN NØ. XX. SET XO = 0, CALCULATE TPS = .XXXXXX ± XX, AND CØNTINUE"

   XO represents an approximation of the radial distance to which hydrazine penetrates the catalyst particle before being dissipated. It is determined through an iterative procedure, and in some instances initial guesses do not yield satisfactory results. In this case, corrective measures to yield a better approximation to XO are instituted and the procedure repeated. This message indicates only that corrective calculations to improve on the accuracy of XO are being initiated.

2. "UNABLE TØ FIND SUITABLE XO AFTER FØUR TRIES OF 25 ITERATIONS EACH --- PRØGRAM STØP FØLLØWS"

   If after four corrective attempts to approximate XO the procedure still does not yield satisfactory results, this message along with all unacceptable values for XO is printed and further calculations are stopped. An octal dump of core accompanies the program stop.

3. "UNABLE TØ CØNVERGE ØN CPS IN 50 TRIES --- CP(X/A) = .XXXXX ± XX"

   If subroutine SGRAD cannot calculate a "converged" value for CPS after 50 iterations, the final value for CP at the particle surface is used to approximate CPS. This is a good approximation to CPS, however, and program calculations continue with the above message being printed.

A listing of typical output for the two-dimensional sample data case is shown in Figs. 6a through 6i.

LISTING OF OUTPUT FOR SAMPLE DATA CASE

TWO-DIMENSIONAL STEADY-STATE

SAMPLE DATA CASE (2-DIM SS)   ALL MIXED*1-STEP GO (AV. [illegible])*P=[illegible]

PROGRAM INPUT

RING	F	GO	ZO
1	.00000	.50000+01	.00000
2	.00000	.50000+01	.00000
3	.00000	.50000+01	.00000
4	.00000	.50000+01	.00000
5	.00000	.50000+01	.00000
6	.00000	.50000+01	.00000
7	.00000	.50000+01	.00000
8	.00000	.10000+01	.00000
9	.00000	.10000+01	.00000
10	.00000	.10000+01	.00000

ALPHA3 = .2140+11   HF = .0000   R = .1073+02   MN2H4 = .3205+02   MNH3 = .1703+02   MN2 = .2802+02   MH2 = .2016+01

ALPHA1 = .1000+11   ALPHA2 = .1000+12   AGM = .2500+04   BGM = .5000+05   KP = .4000-04   YF = .5300+03   CF = .7332-00

AMAX1 = .2000+03   AMAX2 = .4000+02   P = .1000+03   ZEND = .2500-00   D04 = .9500-04   D03 = .1700-03   CGM = .3300+05

RADIUS = .1250+06

A VS Z TABLE

			.00000	.10000+01	.20000+02	.10000+02			
.00000	.55000-02	.11100-01	.16700-01	.16800-01	.43900-01	.57500-01	.71100-01	.84700-01	.98300-01
.11190+00	.12550+00	.13910-00	.15270-00	.16630-00	.17990-00	.19350-00	.22070-00	.23430-00	.25900-00
.62500-02	.18750-01	.31250-01	.43750-01	.56250-01	.68750-01	.81250-01	.93750-01	.10625+00	.11875+00
.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02
.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02
.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02
.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02	.10000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02
.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02	.64000-02

FIG. 6a

AP VS Z TABLE

			.00000	.10000+01	.20000+02	.10000+02			
.00000	.55000-02	.11100-01	.16700-01	.16800-01	.43900-01	.57500-01	.71100-01	.84700-01	.98300-01
.11190+00	.12550-00	.13910-00	.15270-00	.16630-00	.17990-00	.19350-00	.22070-00	.23430-00	.25000-00
.62500-02	.18750-01	.31250-01	.43750-01	.56250-01	.68750-01	.31250-01	.93750-01	.19625+00	.11875+00
.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04
.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04
.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04
.21000+04	.21000+04	.21000+04	.2[illegible]+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04
.33000+03	.33000+03	.33000+03	.3[illegible]+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+05	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03
.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03	.33000+03

DELTA VS Z TABLE

			.00000	.10000+01	.20000+02	.10000+02			
.00000	.55000-02	.11100-01	.16700-01	.16800-01	.43900-01	.57500-01	.71100-01	.84700-01	.98700-01
.11190+00	.12550-00	.13910-00	.15270-00	.16630-00	.17990-00	.19350-00	.22070-00	.23430-00	.25000-00
.62500-02	.18750-01	.31250-01	.43750-01	.56250-01	.68750-01	.81250-01	.93750-01	.10625+00	.11875+00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00
.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00	.34000-00

FIG. 6b

RING 1

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.41918-03	.54294+03	.66785-03	.55586+03	.78786-03	.56878+03	.87086-03	.58169+03
.91775-03	.59460+03	.95120-03	.60750+03	.98024-03	.62040+03	.99989-03	.63328+03	.10119-02	.64616+03
.10222-02	.65904+03	.10290-02	.67191+03	.10343-02	.68477+03	.10388-02	.69762+03	.10426-02	.71047+03
.10453-02	.72332+03	.10474-02	.73615+03	.10491-02	.74899+03	.10505-02	.76182+03	.10515-02	.77465+03
.10523-02	.78746+03	.10530-02	.80031+03	.10536-02	.81313+03	.10534-02	.82000+03	.10557-02	.82000+03
.10579-02	.82000+03	.10602-02	.82000+03	.10625-02	.82000+03	.10647-02	.82000+03	.10670-02	.82000+03
.10693-02	.82000+03	.10716-02	.82000+03	.10738-02	.82000+03	.10761-02	.82000+03	.10777-02	.82000+03

RING 2

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.41918-03	.54294+03	.66785-03	.55586+03	.78786-03	.56878+03	.87086-03	.58169+03
.91775-03	.59460+03	.95120-03	.60750+03	.98024-03	.62040+03	.99989-03	.63328+03	.10119-02	.64616+03
.10222-02	.65904+03	.10290-02	.67191+03	.10343-02	.68477+03	.10388-02	.69762+03	.10426-02	.71047+03
.10453-02	.72332+03	.10474-02	.73615+03	.10491-02	.74899+03	.10505-02	.76182+03	.10515-02	.77465+03
.10523-02	.78746+03	.10530-02	.80031+03	.10536-02	.81313+03	.10534-02	.82000+03	.10557-02	.82000+03
.10579-02	.82000+03	.10602-02	.82000+03	.10625-02	.82000+03	.10647-02	.82000+03	.10670-02	.82000+03
.10693-02	.82000+03	.10716-02	.82000+03	.10738-02	.82000+03	.10761-02	.82000+03	.10777-02	.82000+03

RING 3

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.41915-03	.54294+03	.66786-03	.55586+03	.78787-03	.56878+03	.87087-03	.58169+03
.91777-03	.59460+03	.95121-03	.60750+03	.98026-03	.62040+03	.99991-03	.63328+03	.10119-02	.64616+03
.10222-02	.65904+03	.10289-02	.67191+03	.10343-02	.68477+03	.10388-02	.69762+03	.10426-02	.71047+03
.10453-02	.72332+03	.10474-02	.73615+03	.10491-02	.74899+03	.10504-02	.76182+03	.10515-02	.77465+03
.10523-02	.78746+03	.10533-02	.80031+03	.10536-02	.81313+03	.10533-02	.82000+03	.10556-02	.82000+03
.10579-02	.82000+03	.10602-02	.82000+03	.10624-02	.82000+03	.10647-02	.82000+03	.10670-02	.82000+03
.10693-02	.82000+03	.10715-02	.82000+03	.10738-02	.82000+03	.10761-02	.82000+03	.10777-02	.82000+03

RING 4

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.41918-03	.54294+03	.66785-03	.55586+03	.78786-03	.56878+03	.87056-03	.58169+03
.91775-03	.59460+03	.95120-03	.60750+03	.98024-03	.62040+03	.99989-03	.63328+03	.10119-02	.64616+03
.10222-02	.65904+03	.10290-02	.67191+03	.10343-02	.68477+03	.10388-02	.69762+03	.10426-02	.71047+03
.10453-02	.72332+03	.10474-02	.73615+03	.10491-02	.74899+03	.10505-02	.76182+03	.10515-02	.77465+03
.10523-02	.78746+03	.10530-02	.80031+03	.10536-02	.81313+03	.10534-02	.82000+03	.10557-02	.82000+03
.10579-02	.82000+03	.10602-02	.82000+03	.10625-02	.82000+03	.10647-02	.82000+03	.10670-02	.82000+03
.10693-02	.82000+03	.10716-02	.82000+03	.10738-02	.82000+03	.10761-02	.82000+03	.10777-02	.82000+03

RING 5

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.41918-03	.54294+03	.66785-03	.55586+03	.78786-03	.56878+03	.87086-03	.58169+03
.91775-03	.59460+03	.95120-03	.60750+03	.98024-03	.62040+03	.99989-03	.63328+03	.10119-02	.64616+03
.10222-02	.65904+03	.10290-02	.67191+03	.10343-02	.68477+03	.10388-02	.69762+03	.10426-02	.71047+03
.10453-02	.72332+03	.10474-02	.73615+03	.10491-02	.74899+03	.10505-02	.76182+03	.10515-02	.77465+03
.10523-02	.78746+03	.10530-02	.80031+03	.10536-02	.81313+03	.10534-02	.82000+03	.10557-02	.82000+03
.10579-02	.82000+03	.10602-02	.82000+03	.10625-02	.82000+03	.10647-02	.82000+03	.10670-02	.82000+03
.10693-02	.82000+03	.10716-02	.82000+03	.10738-02	.82000+03	.10761-02	.82000+03	.10777-02	.82000+03

RING 6

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.41918-03	.54294+03	.66785-03	.55586+03	.78786-03	.56878+03	.87086-03	.58169+03
.91775-03	.59460+03	.95120-03	.60750+03	.98024-03	.62040+03	.99989-03	.63328+03	.10119-02	.64616+03

FIG. 6c

.10222-02	.65904+03	.10290-02	.67191+03	.10343-02	.68477+03	.10388-02	.69762+03	.10426-02	.71047+03
.10453-02	.72332+03	.10474-02	.73615+03	.10491-02	.74899+03	.10505-02	.76182+03	.10515-02	.77465+03
.10523-02	.78748+03	.10530-02	.80031+03	.10536-02	.81313+03	.10534-02	.82000+03	.10557-02	.82000+03
.10579-02	.82000+03	.10602-02	.82000+03	.10625-02	.82000+03	.10647-02	.82000+03	.10670-02	.82000+03
.10693-02	.82000+03	.10716-02	.82000+03	.10738-02	.82000+03	.10761-02	.82000+03	.10777-02	.82000+03

RING 7

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.41918-03	.54294+03	.66785-03	.55586+03	.78786-03	.56878+03	.87086-03	.58169+03
.91773-03	.59460+03	.95120-03	.60750+03	.98024-03	.62040+03	.99989-03	.63328+03	.10119-02	.64616+03
.10222-02	.65904+03	.10290-02	.67191+03	.10343-02	.68477+03	.10388-02	.69762+03	.10426-02	.71047+03
.10453-02	.72332+03	.10474-02	.73615+03	.10491-02	.74899+03	.10505-02	.76182+03	.10515-02	.77465+03
.10523-02	.78748+03	.10530-02	.80031+03	.10536-02	.81313+03	.10534-02	.82000+03	.10557-02	.82000+03
.10579-02	.82000+03	.10602-02	.82000+03	.10625-02	.82000+03	.10647-02	.82000+03	.10670-02	.82000+03
.10693-02	.82000+03	.10716-02	.82000+03	.10738-02	.82000+03	.10761-02	.82000+03	.10777-02	.82000+03

RING 8

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.83836-04	.54294+03	.13358-03	.55586+03	.15758-03	.56878+03	.17418-03	.58169+03
.18356-03	.59460+03	.19025-03	.60750+03	.19606-03	.62040+03	.19999-03	.63328+03	.20239-03	.64616+03
.20445-03	.65904+03	.20582-03	.67191+03	.20688-03	.68477+03	.20778-03	.69762+03	.20854-03	.71047+03
.20909-03	.72332+03	.20951-03	.73615+03	.20984-03	.74899+03	.21011-03	.76182+03	.21032-03	.77465+03
.21048-03	.78748+03	.21062-03	.80031+03	.21074-03	.81313+03	.21070-03	.82000+03	.21115-03	.82000+03
.21161-03	.82000+03	.21206-03	.82000+03	.21251-03	.82000+03	.21297-03	.82000+03	.21342-03	.82000+03
.21388-03	.82000+03	.21433-03	.82000+03	.21479-03	.82000+03	.21524-03	.82000+03	.21556-03	.82000+03

RING 9

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.83836-04	.54294+03	.13358-03	.55586+03	.15758-03	.56878+03	.17418-03	.58169+03
.18356-03	.59460+03	.19025-03	.60750+03	.19606-03	.62040+03	.19999-03	.63328+03	.20239-03	.64616+03
.20445-03	.65904+03	.20582-03	.67191+03	.20688-03	.68477+03	.20778-03	.69762+03	.20854-03	.71047+03
.20909-03	.72332+03	.20951-03	.73615+03	.20984-03	.74899+03	.21011-03	.76182+03	.21032-03	.77465+03
.21048-03	.78748+03	.21062-03	.80031+03	.21074-03	.81313+03	.21070-03	.82000+03	.21115-03	.82000+03
.21161-03	.82000+03	.21206-03	.82000+03	.21251-03	.82000+03	.21297-03	.82000+03	.21342-03	.82000+03
.21388-03	.82000+03	.21433-03	.82000+03	.21479-03	.82000+03	.21524-03	.82000+03	.21556-03	.82000+03

RING 10

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.83836-04	.54294+03	.13358-03	.55586+03	.15758-03	.56878+03	.17418-03	.58169+03
.18356-03	.59460+03	.19025-03	.60750+03	.19606-03	.62040+03	.19999-03	.63328+03	.20239-03	.64616+03
.20445-03	.65904+03	.20582-03	.67191+03	.20688-03	.68477+03	.20778-03	.69762+03	.20854-03	.71047+03
.20909-03	.72332+03	.20951-03	.73615+03	.20984-03	.74899+03	.21011-03	.76182+03	.21032-03	.77465+03
.21048-03	.78748+03	.21062-03	.80031+03	.21074-03	.81313+03	.21070-03	.82000+03	.21115-03	.82000+03
.21161-03	.82000+03	.21206-03	.82000+03	.21251-03	.82000+03	.21297-03	.82000+03	.21342-03	.82000+03
.21388-03	.82000+03	.21433-03	.82000+03	.21479-03	.82000+03	.21524-03	.82000+03	.21556-03	.82000+03

FIG. 6d

POSITION AND TEMPERATURE AT LIQUID - LIQUID VAPOR INTERFACE FOR EACH ANNULAR REGION

RING	AXIAL POSITION	RADIAL POSITION	TEMPERATURE
1	.10534-02	.62500-02	.82000+03
2	.10534-02	.18750-01	.82000+03
3	.10534-02	.31250-01	.82000+03
4	.10534-02	.43750-01	.82000+03
5	.10534-02	.56250-01	.82000+03
6	.10534-02	.68750-01	.82000+03
7	.10534-02	.81250-01	.82000+03
8	.21070-03	.93750-01	.82000+03
9	.21070-03	.10625+00	.82000+03
10	.21070-03	.11875+00	.82000+03

********************** LIQUID-VAPOR REGION **********************

POSITION AND TEMPERATURE AT LIQUID VAPOR - VAPOR INTERFACE FOR EACH ANNULAR REGION

RING	AXIAL POSITION	RADIAL POSITION	TEMPERATURE
1	.10777-02	.62500-02	.82000+03
2	.10777-02	.18750-01	.82000+03
3	.10777-02	.31250-01	.82000+03
4	.10777-02	.43750-01	.82000+03
5	.10777-02	.56250-01	.82000+03
6	.10777-02	.68750-01	.82000+03
7	.10777-02	.81250-01	.82000+03
8	.21556-03	.93750-01	.82000+03
9	.21556-03	.10625+00	.82000+03
10	.21556-03	.11875+00	.82000+03

FIG. 6e

G910461-30

************************* VAPOR REGION *************************

CONCENTRATIONS AT LIQUID VAPOR – VAPOR INTERFACE

N2H4	NH3	N2	H2
.16343-00	.53360-01	.43886-01	.31580-02

MFRAC1	MFRAC2	MFRAC3	MFRAC4	FRAC3D
.13783-00	.13783-00	.27565-00	.44869-00	-.00000

RING	Z	TEMP	N2H4	NH3	N2	H2
1	.00000	.00000	.00000	.00000	.00000	.00000
2	.00000	.00000	.00000	.00000	.00000	.00000
3	.00000	.00000	.00000	.00000	.00000	.00000
4	.00000	.00000	.00000	.00000	.00000	.00000
5	.00000	.00000	.00000	.00000	.00000	.00000
6	.00000	.00000	.00000	.00000	.00000	.00000
7	.00000	.00000	.00000	.00000	.00000	.00000
8	.25004-03	.83487+03	.15807-00	.52357-01	.43798-01	.32047-02
9	.25004-03	.83487+03	.15807-00	.52357-01	.43798-01	.32047-02
10	.25004-03	.83487+03	.15807-00	.52357-01	.43798-01	.32047-02

PRESSURE = .10000+03

MFRAC1	MFRAC2	MFRAC3	MFRAC4	EQUIVALENT FRAC3D
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.14245-00	.14009-00	.27547-00	.44199-00	.84848-02
.14245-00	.14009-00	.27547-00	.44199-00	.84848-02
.14245-00	.14009-00	.27547-00	.44199-00	.84848-02

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RING	Z	TEMP	N2H4	NH3	N2	H2
1	.00000	.00000	.00000	.00000	.00000	.00000
2	.00000	.00000	.00000	.00000	.00000	.00000
3	.00000	.00000	.00000	.00000	.00000	.00000
4	.00000	.00000	.00000	.00000	.00000	.00000
5	.00000	.00000	.00000	.00000	.00000	.00000
6	.00000	.00000	.00000	.00000	.00000	.00000
7	.00000	.00000	.00000	.00000	.00000	.00000
8	.28453-03	.84959+03	.15297-00	.51410-01	.43699-01	.32466-02
9	.28453-03	.84959+03	.15297-00	.51410-01	.43699-01	.32466-02
10	.28453-03	.84959+03	.15297-00	.51410-01	.43699-01	.32466-02

PRESSURE = [illegible]

FIG. 6f

MFRAC1	MFRAC2	MFRAC3	MFRAC4	EQUIVALENT FRAC3D
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.14691-00	.14229-00	.27535-00	.43544-00	.16485-01
.14691-00	.14229-00	.27535-00	.43544-00	.16485-01
.14691-00	.14229-00	.27535-00	.43544-00	.16485-01

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RING	Z	TEMP	N2H4	NH3	N2	H2
1	.00000	.00000	.00000	.00000	.00000	.00000
2	.00000	.00000	.00000	.00000	.00000	.00000
3	.00000	.00000	.00000	.00000	.00000	.00000
4	.00000	.00000	.00000	.00000	.00000	.00000
5	.00000	.00000	.00000	.00000	.00000	.00000
6	.00000	.00000	.00000	.00000	.00000	.00000
7	.00000	.00000	.00000	.00000	.00000	.00000
8	.31901-03	.86423+03	.14813-00	.50520-01	.43585-01	.32828-02
9	.31901-03	.86423+03	.14813-00	.50520-01	.43585-01	.32828-02
10	.31901-03	.86423+03	.14813-00	.50520-01	.43585-01	.32828-02

PRESSURE = .99989+02

MFRAC1	MFRAC2	MFRAC3	MFRAC4	EQUIVALENT FRAC3D
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.00000	.00000	.00000	.00000	.00000
.15116-00	.14442-00	.27535-00	.42907-00	.23903-01
.15116-00	.14442-00	.27535-00	.42907-00	.23903-01
.15116-00	.14442-00	.27535-00	.42907-00	.23903-01

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. . .

FIG. 6g

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RING	Z	TEMP	N2H4	NH3	N2	H2
1	.24607-00	.19963+04	.33006-05	.70498-02	.21648-01	.26983-02
2	.24607-00	.19959+04	.22659-05	.70381-02	.21658-01	.27004-02
3	.24607-00	.19939+04	.31883-05	.69988-02	.21694-01	.27079-02
4	.24607-00	.19888+04	.24045-05	.69042-02	.21784-01	.27265-02
5	.24607-00	.19770+04	.31228-05	.67054-02	.21985-01	.27671-02
6	.24607-00	.19536+04	.18765-05	.63345-02	.22378-01	.28457-02
7	.24607-00	.19127+04	.25429-05	.57225-02	.23071-01	.29817-02
8	.24607-00	.18513+04	.00000	.48489-02	.24240-01	.32016-02
9	.24607-00	.18224+04	.14423-05	.44166-02	.24762-01	.33023-02
10	.24607-00	.18108+04	.00000	.42343-02	.24980-01	.334 -02

PRESSURE = .55026+02

MERAC1	MERAC2	MERAC3	MERAC4	EQUIVALENT FRAC3D
.53004-00	.30600-00	.16392-00	.40785-04	.57749-00
.53031-00	.30606-00	.16360-00	.27992-04	.57819-00
.53121-00	.30623-00	.16251-00	.39345-04	.58061-00
.53341-00	.30668-00	.15988-00	.29592-04	.58646-00
.53804-00	.30760-00	.15432-00	.38196-04	.59891-00
.54663-00	.30932-00	.14403-00	.22675-04	.62231-00
.56053-00	.31210-00	.12734-00	.30072-04	.66113-00
.58002-00	.31600-00	.10398+00	.00000	.71744-00
.58896-00	.31779-00	.93237-01	.16181-04	.74414-00
.59266-00	.31853-00	.88814-01	.00000	.75529-00

FIG. 6h

****

RING	Z	TEMP	N2H4	NH3	N2	H2
1	.25000-00	.19944+04	.30099-05	.69183-02	.21362-01	.20649-02
2	.25000-00	.19939+04	.22178-05	.69062-02	.21372-01	.20671-02
3	.25000-00	.19919+04	.29393-05	.68667-02	.21408-01	.25746-02
4	.25000-00	.19867+04	.23224-05	.67723-02	.21498-01	.26932-02
5	.25000-00	.19748+04	.28764-05	.65756-02	.21698-01	.27335-02
6	.25000-00	.19515+04	.18411-05	.62114-02	.22085-01	.28108-02
7	.25000-00	.19108+04	.22974-05	.56117-02	.22765-01	.29442-02
8	.25000-00	.18501+04	.13439-06	.47590-02	.23908-01	.31592-02
9	.25000-00	.18213+04	.12229-05	.43353-02	.24420-01	.32579-02
10	.25000-00	.18097+04	.46398-07	.41570-02	.24634-01	.32992-02

PRESSURE = .54222+02

MFRAC1	MFRAC2	MFRAC3	MFRAC4	EQUIVALENT FRAC3D
.53073-00	.30614-00	.16309-00	.37709-04	.57933-00
.53102-00	.30620-00	.16276-00	.27777-04	.58006-00
.53194-00	.30638-00	.16165-00	.36780-04	.58252-00
.53416-00	.30683-00	.15899-00	.28975-04	.58846-00
.53880-00	.30775-00	.15342-00	.35665-04	.60096-00
.54734-00	.30946-00	.14317-00	.22552-04	.62427-00
.56115-00	.31222-00	.12660-00	.27545-04	.66287-00
.58042-00	.31608-00	.10349+00	.15532-05	.71864-00
.58931-00	.31786-00	.92822-01	.13915-04	.74518-00
.59297-00	.31859-00	.88434-01	.52458-06	.75625-00

****

****** OPERATIONS COMPLETE ******

FIG. 6i

Common Operational Problems

The two-dimensional steady-state computer program has been run with a large variety of data cases. During these runs, most of the problems which developed were eliminated by modifying the program. However, a few problems may still remain; these problems are outlined below together with appropriate techniques for solving them.

1. "THE PRØGRAM HAS CALCULATED A NEGATIVE PRESSURE---RETURN AND TERMINATE"

   If a negative pressure is calculated at some axial station in the vapor region, further calculations for the current data case are stopped and this message is printed out. This diagnostic statement indicates that a physical limitation of the reactor system has been exceeded. Therefore, this particular case cannot be run. A lower mass flow rate or a higher feed pressure should work.

2. "THE PRØGRAM HAS CALCULATED A NEGATIVE TEMPERATURE IN RING XX---RETURN AND TERMINATE"

   If a negative temperature is calcualted in any annular region at any axial station in the vapor region, further calculations are stopped and this message, including the current annular ring, is printed. An appropriate solution to this problem would be to increase the number of radial regions into which the reactor is divided.

3. "UNABLE TØ FIND SUITABLE XO AFTER FØUR TRIES ØF 25 ITERATIØNS EACH ---PRØGRAM STØP FØLLØWS"

   If a satisfactory value for XO cannot be found after four attempts, this message is printed and program execution is terminated. An appropriate solution to this problem would be to try different values for f_i [Eq. (I-11) in discussion of SGRAD, Appendix I]. These values could be greater than 0.95. To make this change, subroutine SGRAD would have to be recompiled using the new values of f_i.

4. "THERE IS A PUDDLE ØF CØLD HYDRAZINE AT THE LIQUID-VAPØR/VAPØR INTERFACE --- TRY USING A LARGER VALUE FØR GO"

   When using a buried injector scheme it is possible to "flood" the region surrounding the injector tip with cold, liquid hydrazine. A sudden drop in axial temperatures at the liquid-vapor/vapor interface in any annular ring indicates that this has occurred, and in such cases the above message is printed and no further calculations are made. An appropriate solution to this problem would be to try a larger input value for GO, and rerun the program with the revised input.

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LIST OF SYMBOLS

a Radius of spherical particle, ft

A_p Total external surface of catalyst particle per unit volume of bed, ft^{-1}

c_i Reactant concentration in interstitial fluid, lb/ft^3

c_p Reactant concentration in gas phase within the porous particle, lb/ft^3

C_F Specific heat of fluid in the interstitial phase, Btu/lb - deg R

$\overline{C_F}$ Average specific heat of fluid in the interstitial phase, Btu/lb - deg R

D_i Diffusion coefficient of reactant gas in the interstitial fluid, ft^2/sec

D_o Diffusion coefficient of reactant gas in the interstitial fluid at STP, ft^2/sec

D_p Diffusion coefficient of reactant gas in the porous particle, ft^2/sec

f_i Weighting factor in Eq. (I-11)

F Rate of feed of hydrazine from buried injectors into the system (Ref. 1), lb/ft^3-sec

g_C Conversion factor, (lb_m/lb_f) ft/sec^2

G Mass flow rate, lb/ft^2-sec

h Enthalpy, Btu/lb

h_c Heat transfer coefficient, Btu/ft^2-sec-deg R

H Heat of reaction (negative for exothermic reaction), Btu/lb

k_c Mass transfer coefficient, ft/sec

k_o Reaction rate constant, equals $\alpha e^{-\gamma}$

K_p Thermal conductivity of the porous catalyst particle, Btu/ft-sec-deg R

M	Molecular weight, lb/lb mole
$\bar{M}$	Average molecular weight, lb/lb mole
n	Order of decomposition reaction
N_r	Radial mass flux, lb/ft^2-sec
P	Chamber pressure, psia
q_r	Radial heat flux, Btu/ft^2-sec
Q_{het}	Activation energy for (heterogeneous) chemical reaction on the catalyst surfaces, Btu/lb mole
Q_{hom}	Activation energy for (homogeneous) chemical reaction in the interstitial phase, Btu/lb mole
r	Radial distance from the center of the cylindrical reaction chamber, ft
r_{het}	Rate of (heterogeneous) chemical reaction on the catalyst surfaces, lb/ft^3-sec
r_{hom}	Rate of (homogeneous) chemical reaction in the interstitial phase, lb/ft^3-sec
R	Gas constant, equals 10.73 psia - ft^3/lb mole - deg R, or, Radius of reactor
T	Temperature, deg R
T_{vap}	Vaporization temperature, deg R
w_i	Weight fraction of reactant in interstitial phase
x	Radial distance from the center of the spherical catalyst particle, ft
X_o	Defined in Appendix I (Discussion of Subroutine SGRAD)
z	Axial distance, ft
z_o	Axial distance to the end of buried injectors, ft
α	Preexponential factor in rate equation

β Equals $\left[-(C_p)_s \; HD_p\right] / \left[K_p \; (T_p)_s\right]$

γ Equals $Q_{net}/R \; (T_p)_s$

δ Interparticle void fraction

ϵ Eddy diffusivity, ft^2/sec

λ Eddy conductivity, Btu/ft-sec-deg R

μ Viscosity of interstitial fluid, lb/ft - sec

ρ_i Density of interstitial fluid, lb/ft^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

J Refers to chemical species

L Refers to liquid at vaporization temperature

V Refers to vapor at vaporization temperature

APPENDIX I

Description of Subroutines

The following is a list and brief description of the subroutines which comprise the UNIVAC 1108 computer programs describing the one- and two-dimensional steady-state models of a hydrazine catalytic reactor. Subroutine SGRAD, since it is the key subroutine in each program is described in detail. The flow charts for the main programs and major subroutines are included immediately after this list in Figs. I-1 through I-8. The number outside of and next to any block on the flow charts indicates the approximate statement number in that routine at which that particular operation occurs.

<u>One-Dimensional Model</u>

MAIN (Fig. I-1)	Controls input and calculates concentrations and temperatures in the liquid region of the reactor.
SLØPE (Fig. I-1)	Calculates concentration and temperature profiles within the catalyst particles for the liquid and liquid vapor regions of the reactor. This subroutine is similar to SGRAD which is described in detail later in this section.
LQVP (Fig. I-2)	Calculates enthalpy during the liquid vapor region of the reactor (concentration of N_2H_4 and temperature remain constant).
LQV2 (Fig. I-2)	Calculates hydrazine concentration, enthalpy and temperatures during the liquid-liquid vapor region of the reactor (concentration of hydrazine varies).
VAPØR (Figs. I-3 & I-4)	Calculates concentrations, temperatures and pressures in the vapor region of the reactor.
PARAM (Fig. I-5)	Calculates parameters needed for calculations done in subroutine SLØPE.
CØNC (Fig. I-5)	Calculates reactant concentrations at the liquid vapor-vapor interface of the reactor.
UNBAR	Interpolation routine used to obtain values from a table.
BLØCK DATA TABLES	Tables of: (1) temperature vs. viscosity (2) temperature vs. vapor pressure

(3) temperature vs. heats of reaction
(4) temperature vs. specific heat
(5) vapor pressure vs. temperature
(6) enthalpy vs. temperature

SGRAD (Fig. I-5) — This routine is the same as it is in the two-dimensional model. For a detailed description, see the section describing two-dimensional subroutines.

Two-Dimensional Model

MAIN (Fig. I-6) — Controls input and calculates concentrations and temperatures in the liquid region of the reactor for all annular regions.

SLØPE (Fig. I-6) — Calculates concentration and temperature profiles within the catalyst particles for the liquid and liquid vapor regions of the reactor for all annular regions. This subroutine is similar to SGRAD which is described in detail later in this section.

LQVP (Fig. I-6) — Calculates enthalpy during the liquid vapor region of the reactor for all annular regions (concentration of N_2H_4 and temperature remain constant).

VAPØR (Fig. I-7) — Calculates concentrations, temperatures and pressures in the vapor region of the reactor for all annualr regions.

DELTAZ (Fig. I-8) — Calculates axial increments for the vapor region.

ØRDER (Fig. I-8) — Arranges an array of numbers in ascending order

UNBAR — Interpolation routine used to obtain values from a table.

BLØCK DATA TABLES — Tables of:

(1) temperature vs. viscosity
(2) temperature vs. vapor pressure
(3) temperature vs. heats of reaction
(4) temperature vs. specific heat
(5) vapor pressure vs. temperature
(6) enthalpy vs. temperature

SGRAD (Fig. I-8) — Detailed description follows:

SGRAD (Fig. I-8)

The purpose of subroutine SGRAD is to solve the implicit integral equations describing reactant concentration and temperature profiles in the porous catalyst particles and to calculate the slope of the reactant concentration gradient at the surface of the catalyst particles. This routine is used for calculations in the vapor region of the reactor only. In the hydrazine catalytic reactor system, ammonia concentration profiles are calculated but the subroutine is very general and can be used for many other reactants. The key equation to be solved is an implicit integral equation of the form (Refs. 2 and 9):

$$c_p^{NH_3}(x/a) = c_i^{NH_3} - a^2\left[\frac{1}{x/a} - \frac{a k_c^{NH_3}\ D_p^{NH_3}}{a k_c^{NH_3}}\right]\int_{x_0/a}^{x/a} \xi^2\, \frac{r_{het}^{NH_3}\left[c_p^{NH_3}(x/a)\right]}{D_p^{NH_3}}\, d\xi - a^2\int_{x/a}^{1}\left[\frac{1}{\xi} - \frac{a k_c^{NH_3} - D_p^{NH_3}}{a k_c^{NH_3}}\right]\xi^2\, \frac{r_{het}^{NH_3}\left[c_p^{NH_3}(x/a)\right]}{D_p^{NH_3}}\, d\xi \qquad \text{(I-1)}$$

where $c_p^{NH_3}(x)$ is the reactant (ammonia) concentration as a function of x (the radial position within the catalyst particle), $c_i^{NH_3}$ is the interstitial reactant concentration and a is the radius of the spherical catalyst particle. To solve this equation, a two-phase iterative scheme is used. First, an initial estimate for $c_p^{NH_3}(x)$ is found through an iterative method of calculating successively better approximations. Second, using the good initial estimate found in the first phase, a similar iterative method is used to arrive at converged values of the actual $c_p^{NH_3}(x)$ distribution.

Phase I

It was found through hand calculation that solutions of Eq. (I-1) were very likely to diverge if the initial estimate was not a very good estimate. Therefore, in the first phase of this subroutine the iterative scheme is used to find this good first estimate. A linear function of the type shown in Fig. I-9 was found to be a fairly close approximation to the actual concentration distribution. The point at which the reactant concentration profile changes slope is referred to as X_0.

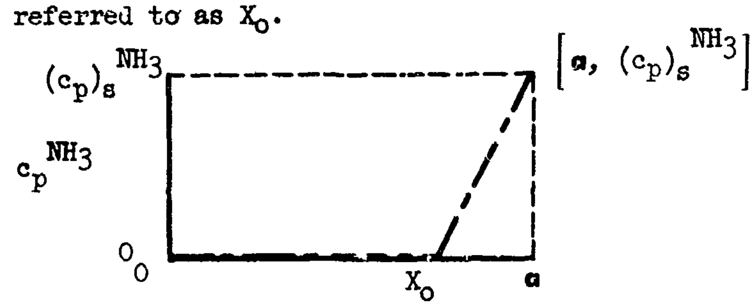


Fig. (I-9)

The final solution to Phase I is a distribution of this type.

Iterative Procedure: Phase I

1. First a guess is made at a value for the reactant concentration at the surface of the catalyst particle: $(c_p)_s^{NH_3} = c_i^{NH_3}/2$.

2. Using this value, a value is found for the slope of the concentration profile at the surface, $\left[dc_p^{NH_3}/dx\right]_{x=a}$.

$$\left[dc_p^{NH_3}/dx\right]_{x=a} = \frac{k_c^{NH_3}}{D_p^{NH_3}}\left[c_i - (c_p)_s\right]^{NH_3} \qquad \text{(I-2)}$$

where $k_c^{NH_3}$ is calculated from an equation given in Ref. 1 and $D_p^{NH_3}$ is calculated from Eq. (I-3).

$$D_p^{NH_3} = D_0^{NH_3}\left\{\left(\frac{(T_p)_s}{492}\right)^{1.823} \cdot \left(\frac{14.7}{P}\right) \cdot \left[1 - e^{-0.0672\,(P/14.7)(492/(T_p)_s)}\right]\right\} \qquad \text{(I-3)}$$

3. The temperature at the particle surface, $(T_p)_s$, is calculated from

$$(T_p)_s = T_i - \frac{1}{h_c}\left[(H\cdot k_c\cdot c_i)^{N_2H_4} + \left(H\cdot D_p\cdot\left[dc_p/dx\right]_{x=a}\right)^{NH_3}\right] \qquad \text{(I-4)}$$

where T_i and $c_i^{N_2H_4}$ are input to the subroutine, $H^{N_2H_4}$ and H^{NH_3} are taken from tables in the computer program, and h_c and $k_c^{N_2H_4}$ are calculated according to the equations in Ref. 1.

4. Using the point $\left[a,\ (c_p)_s^{NH_3}\right]$ and the slope $\left[dc_p^{NH_3}/dx\right]_{x=a}$, a line is established and extrapolated to the $c_p^{NH_3} = 0$ axis line, intersecting the axis line at X_0 (as in Fig. I-9).

5. The value for X_0 is calculated from

$$x_0 = a - \left\{(c_p)_s / \left[dc_p/dx\right]_{x=a}\right\}^{NH_3} \qquad \text{(I-5)}$$

Since the region of primary interest is the particle surface, it is at this point that convergence on a value for $c_p^{NH_3}(x)$ is tested. To test for convergence, a new $(c_p)_s^{NH_3}$ is calculated and compared to the previous $(c_p)_s^{NH_3}$. The new value for $(c_p)_s^{NH_3}$ can be calculated from Eq. (I-1) by noting that, at the catalyst particle surface, where $x=a$, the second integral term in Eq. (I-1) drops out leaving

$$(c_p)_s^{NH_3} = c_i^{NH_3} - \left[\frac{1}{x} - \frac{a k_c - D_p^{NH_3}}{a^2 k_c^{NH_3}}\right]\int_0^a \xi^2\,\frac{r_{het}\left[c_p^{NH_3}(x)\right]}{D_p^{NH_3}}\,d\xi \qquad \text{(I-6)}$$

As can be seen in Fig. (I-9) in distributions of this type all values of $c_p^{NH_3}(x)$ between 0 and X_o are zero. Therefore, in evaluating the integrals, all points between 0 and X_o can be ignored. If this is done and if x is normalized by dividing by a, Eq. (I-6) reduces to

$$(c_p)_S^{NH_3} = c_i^{NH_3} - a^2 \left[1 - \frac{a k_c^{NH_3} - D_p^{NH_3}}{a k_c^{NH_3}}\right] \int_{X_o/a}^{1} \xi^2 \, \frac{r_{het}\left[c_p^{NH_3}(x)\right]}{D_p^{NH_3}} \, d\xi \qquad \text{(I-7)}$$

where all terms have been previously determined except r_{het} which is calculated from

$$r_{het}^{NH_3} = k_o \left(c_i^{NH_3}\right)^{1-n} \cdot \left[c_p^{NH_3}(x)\right]^n \exp\left\{\gamma\beta\left(1 - c_p^{NH_3}(x)/c_i^{NH_3}\right) \Big/ \left[1 + \beta\left(1 - c_p^{NH_3}(x)/c_i^{NH_3}\right)\right]\right\} \qquad \text{(I-8)}$$

where n, k_o, γ, and β are defined in the List of Symbols.

6. A new value for $(c_p)_s^{NH_3}$ is calculated using Eq. (I-7) where the integral is evaluated numerically using the trapezoidal method.

7. A new value for $\left[dc_p^{NH_3}/dx\right]_{x=a}$ is calculated from Eq. (I-3) using the newly calculated $(c_p)_s^{NH_3}$.

8. New values are calculated for $(T_p)_s$, $D_p^{NH_3}$, γ, β, k_o.

9. The following convergence tests are made:

$$\left| \frac{\left[T_i - (T_p)_S\right]_{OLD} - \left[T_i - (T_p)_S\right]_{NEW}}{\left[T_i - (T_p)_S\right]_{NEW}} \right| \overset{?}{\leq} 0.05 \qquad \text{(I-9)}$$

and

$$\left| \frac{\left[c_i - (c_p)_S\right]_{OLD}^{NH_3} - \left[c_i - (c_p)_S\right]_{NEW}^{NH_3}}{\left[c_i - (c_p)_S\right]_{NEW}^{NH_3}} \right| \overset{?}{\leq} 0.05 \qquad \text{(I-10)}$$

If these tests are both satisfied, the value of X_o calculated in Eq. (I-5) is saved and the program moves on to Phase II.

If both tests are not satisfied, an averaged value of $(c_p)_s^{NH_3}$ is calculated using as many as three averaging techniques to insure rapid convergence.

Using this new value of $(c_p)_s^{NH_3}$, steps 2 through 9 are repeated up to a maximum of twenty-five times. If no convergence is reached after twenty-five iterations, a "weighted" estimate of X_o is tried:

$$X_o = f_i \cdot (X_o)_{\substack{\text{previously}\\ \text{calculated}}} + (1-f_i) \cdot (X_o)_{\substack{\text{last}\\ \text{calculated}}} \qquad \text{(I-11)}$$

Steps 1 through 9 are repeated up to twenty-five times. Succeeding values f_i = 0.80, 0.85, 0.90, and 0.95 are tried until convergence is reached. If convergence still is not reached and therefore a satisfactory X_o is not found, a program termination with an appropriate error message follows.

Phase II

Using as an initial approximation the straight line determined by the convergent X_o and $\left[dc_p^{NH_3}/dx\right]_{x=a}$ found in Phase I, an iterative scheme similar to that in Phase I is now employed to find convergent values for the entire $c_p^{NH_3}(x)$ distribution within the catalyst particle. It was found through hand calculations that the convergent values of $c_p^{NH_3}(x)$ near the surface were not changed by more than 5 percent when the values of $c_p^{NH_3}(x)$ between 0 and X_o were not considered in the iterative procedure. Therefore, the points in this range are ignored.

Iterative Procedure: Phase II

The values of $c_p^{NH_3}(x)$, $(T_p)_s$, $k_o^{NH_3}$, β^{NH_3}, γ^{NH_3}, etc. found in the last iteration in Phase I are the initial input to the following iteration.

1. A new $c_p^{NH_3}(x)$ profile is calculated from Eq. (I-12).

$$c_p^{NH_3}(x/a) = c_i^{NH_3} - a^2 \left[\frac{1}{x/a} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right] \int_{X_o/a}^{x/a} \xi^2 \, \frac{r_{het}^{NH_3}\left[c_p^{NH_3}(x/a)\right]}{D_p^{NH_3}} \, d\xi$$

$$- \; a^2 \int_{x/a}^{1} \left[\frac{1}{\xi} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right] \xi^2 \, \frac{r_{het}^{NH_3}\left[c_p^{NH_3}(x/a)\right]}{D_p^{NH_3}} \, d\xi \qquad \text{(I-12)}$$

As before, the limits of the integral have been normalized by dividing by a. The integrals are evaluated numerically using the finite sum approximation described below.

To evaluate the integral terms in Eq. (I-12) the following procedure, using a finite sum approximation, is used:

(a) the interval $X_0/a \leq x/a \leq 1$ is divided into 24 equally spaced subdivisions, and an average value for $r_{het}\left[c_p^{NH_3}(x/a)\right]$ is calculated for each of these divisions.

(b) treating $r_{het}\left[c_p^{NH_3}(x/a)\right]$ as constant over each of these subdivisions, Eq. (I-12) can be approximated by

$$c_p^{NH_3}(x/a) = c_i^{NH_3} - \frac{a}{D_p^{NH_3}}\left[\frac{1}{x/a} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right]\left\{r_{het}^{1}\int_{X_0/a}^{X_0/a+\Delta X/a}\xi\, d\xi\right.$$

$$\left. + r_{het}^{2}\int_{X_0/a+\Delta X/a}^{X_0/a+2\Delta X/a}\xi\, d\xi + \cdots + r_{het}^{24}\int_{X_0/a+(k-1)\Delta X/a}^{X_0/a+k\Delta X/a}\xi\, d\xi\right\}$$

$$- \frac{a^2}{D_p^{NH_3}}\left\{r_{het}^{1}\int_{X_0/a+k\Delta X/a}^{X_0/a+(k+1)\Delta X/a}\left[\frac{1}{\xi} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right]\xi^2 d\xi\right.$$

$$\text{(I-13)}$$

$$+ r_{het}^{2}\int_{X_0/a+(k+1)\Delta X/a}^{X_0/a+(k+2)\Delta X/a}\left[\frac{1}{\xi} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right]\xi^2 d\xi + \cdots$$

$$\left. + r_{het}^{24}\int_{X_0/a+23\Delta X/a}^{X_0/a+24\Delta X/a}\left[\frac{1}{\xi} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right]\xi^2 d\xi\right\}$$

where k = 1, 2, . . ., 24

(c) the integrals in Eq. (I-13) can now be evaluated directly

$$\text{viz} \quad \int_a^b \xi\, d\xi = \left.\frac{\xi^2}{2}\right|_a^b = \frac{b^2}{2} - \frac{a^2}{2}$$

$$\int_a^b \text{CONSTANT}\cdot\xi^2 d\xi = \text{CONSTANT}\cdot\left.\frac{\xi^3}{3}\right|_a^b = \text{CONSTANT}\left(\frac{b^3}{3} - \frac{a^3}{3}\right)$$

(d) rearranging and integrating term by term in Eq. (I-13) yields the finite sum approximation for $c_p^{NH_3}(x/a)$ at each subdivision of the interval from X_0/a to 1:

$$c_p^{NH_3}(x/a)_{k+1} = c_i^{NH_3} - \frac{a^2}{D_p^{NH_3}} \left\{ \left(\frac{1}{x_k/a} - \frac{av+1}{av} \right) \cdot \sum_{j=1}^{k} \frac{r_{het}^{j}}{3} \left[\left(\frac{x_j}{a}\right)^3 - \left(\frac{x_{j-1}}{a}\right)^3 \right] + \sum_{j=k}^{24} \frac{r_{het}^{j+1}}{2} \left[\left(\frac{x_{j+1}}{a}\right)^2 - \left(\frac{x_j}{a}\right)^2 \right] - \left(\frac{av+1}{av}\right) \cdot \sum_{j=k}^{24} \frac{r_{het}^{j+1}}{3} \left[\left(\frac{x_{j+1}}{a}\right)^3 - \left(\frac{x_j}{a}\right)^3 \right] \right\} \quad \text{(I-14)}$$

where $v = (ak_c - D_p)^{NH_3} / ak_c^{NH_3}$ and $K = 1, 2, \ldots, 24$.

(e) the values for $c_p^{NH_3}(x/a)\big|_{x=X_0}$ and $c_p^{NH_3}(x/a)\big|_{x=a}$ are special cases where one or the other of the integral terms in Eq. (I-12) vanishes. Evaluation follows from a simple reduction of Eq. (I-14).

2. A new value for $\left[dc_p^{NH_3}/dx\right]_{x=a}$ is calculated from Eq. (I-3) using the newly calculated $(c_p)_s^{NH_3}$.

3. A new value for $(T_p)_s$ is calculated from Eq. (I-4).

4. Convergence tests are made (as they were in Phase I) using Eqs. (I-9) and (I-10).

   (a) If the convergence tests are both satisfied, the quantities GRAD and TGRAD are calculated according to Eqs. (I-15) and (I-16), and the program returns to the point from which the subroutine was called.

$$\text{GRAD} = \left[dc_p^{NH_3}/dx\right]_{x=a} \cdot D_p^{NH_3} \quad \text{(I-15)}$$

$$\text{TGRAD} = k_c \left[T_i - (T_P)_S \right] \qquad \text{(I-16)}$$

(b) If the tests are not both satisfied, a new $c_p^{NH3}(x)$ distribution is calculated using one of various averaging techniques. Corresponding $\left| dc_p^{NH3}/dx \right|_{x=a}$, $(T_p)_s$, k_o, γ, β, etc. are also calculated. Then steps 1 through 4 are repeated up to a maximum of 50 times. If convergence criteria are not met after 50 iterations, approximations to acceptable values of GRAD and TGRAD are made using the results of the Phase I iterative procedure, an appropriate message is printed, and the program returns to the point from which the subroutine was called.

Distributions of the type shown in Fig. (I-10) are typical of those found in this iterative procedure.

(1) converged linear approximation from Phase I

(2) curve calculated from curve (1) using Eq. (I-11) (Phase II, step 1)

(3) averaged curve calculated from curves (1) and (2) (Phase II, step 4b)

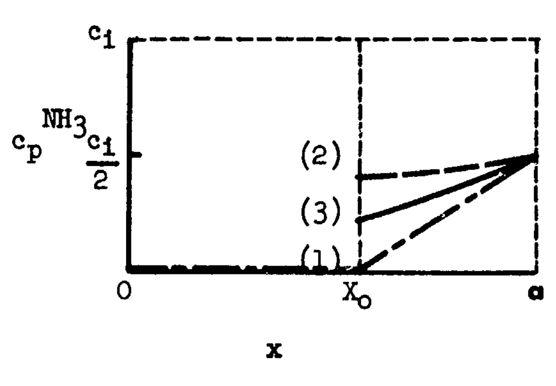


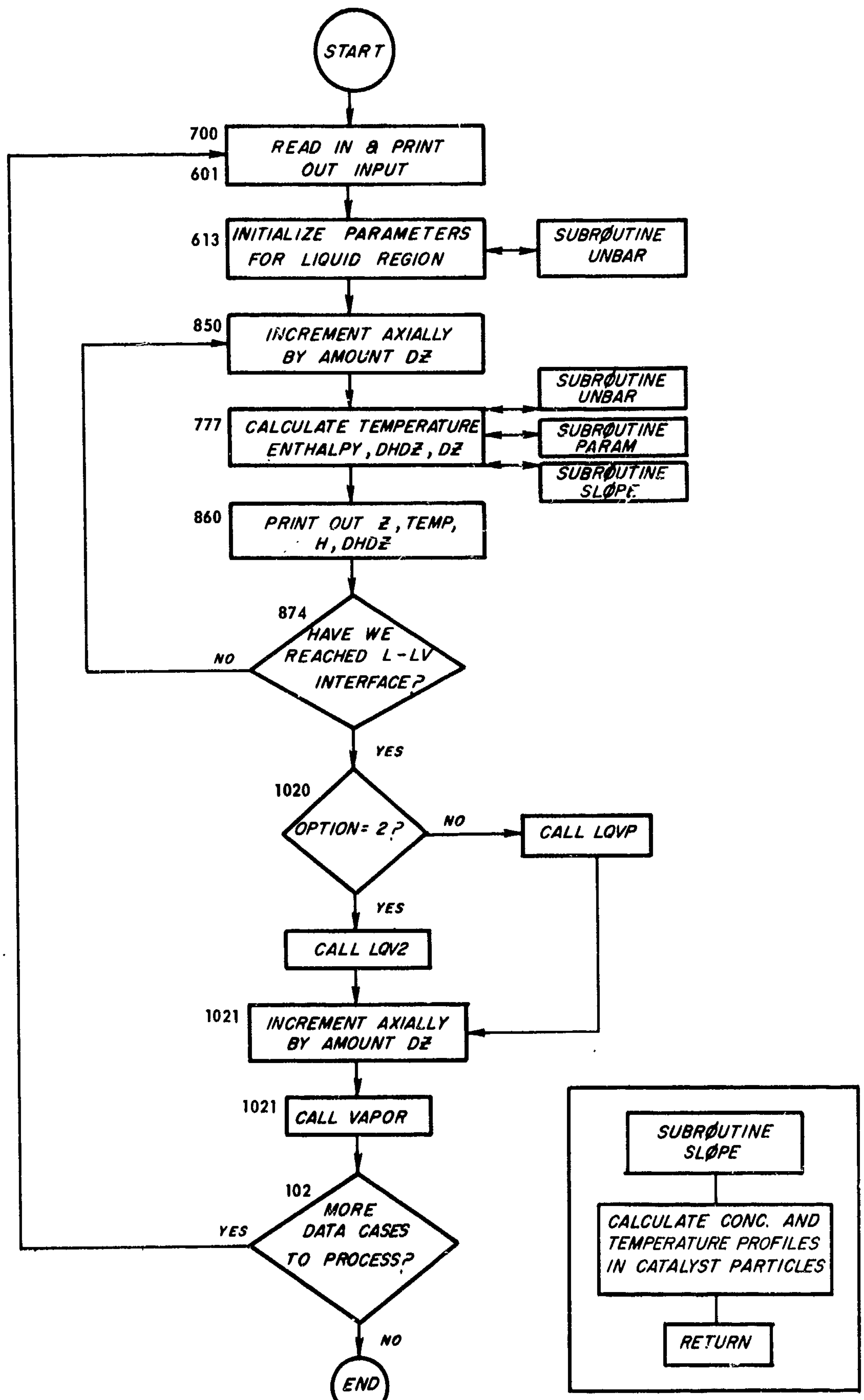
Fig. (I-10)

G910461-30

FIG. I-1

ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

MAIN PROGRAM and SUBRØUTINE SLØPE: Flow Diagrams



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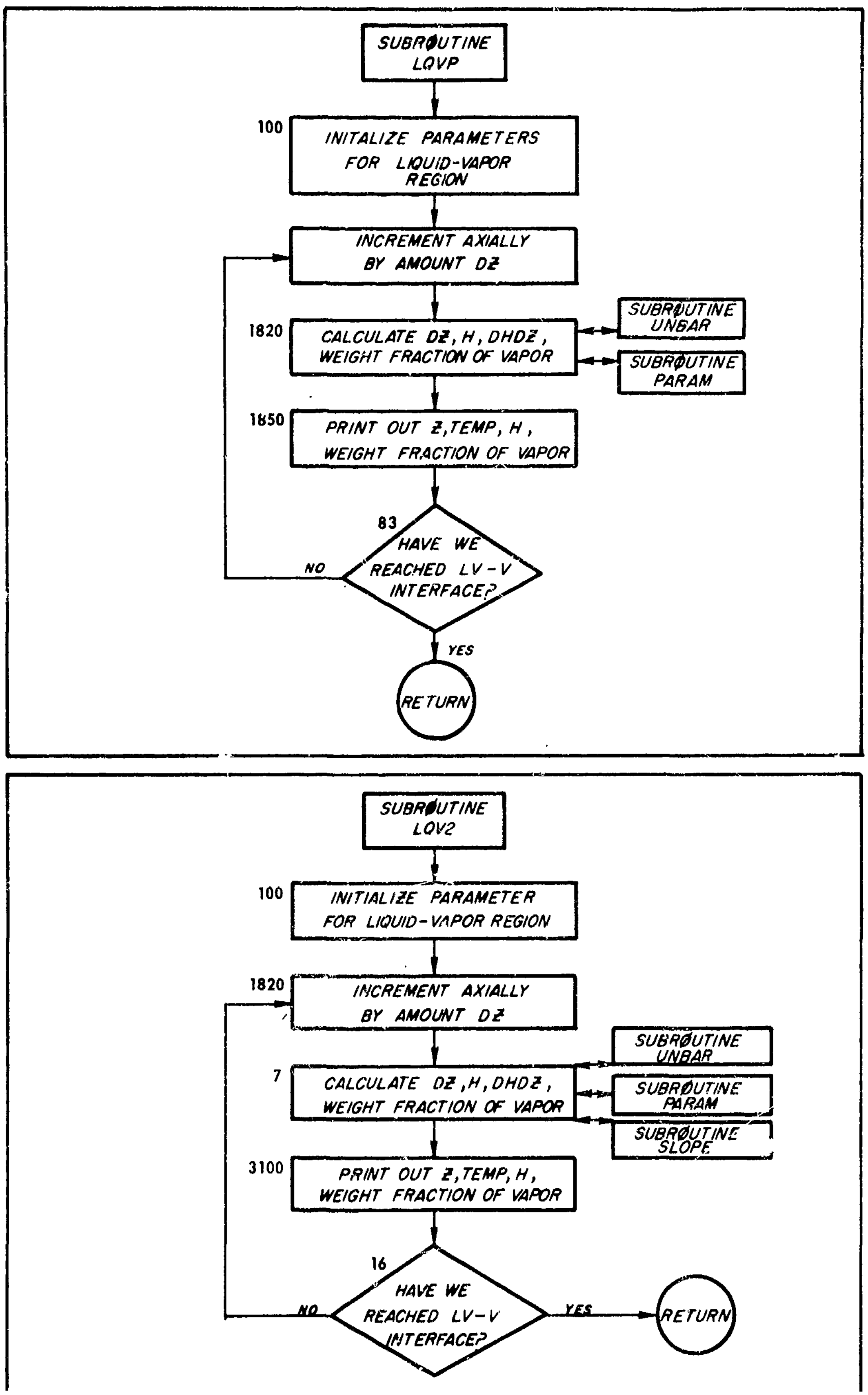
ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

FIG. I-2

SUBRØUTINES LQVP and LQV2 : Flow Diagrams

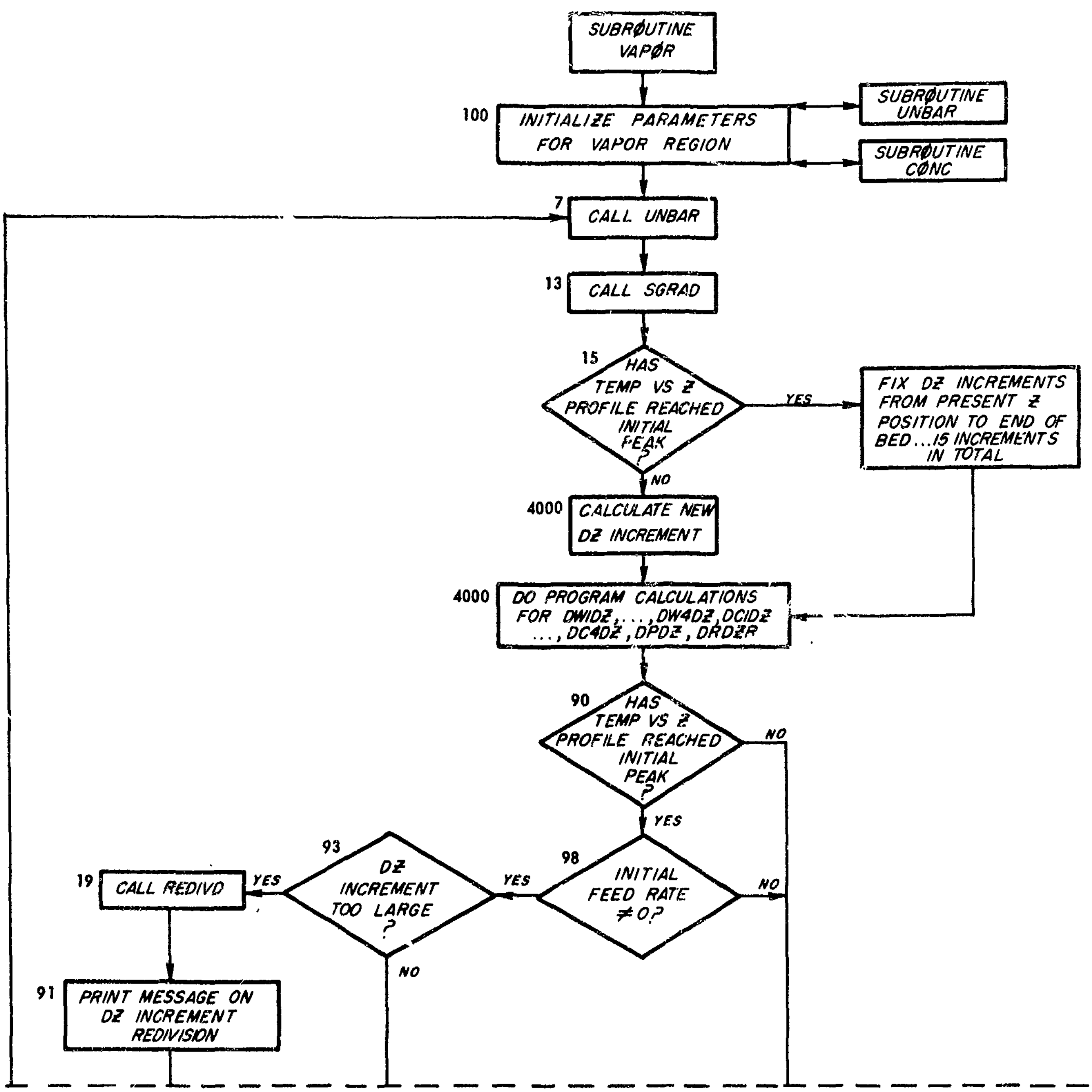


G910461-30

FIG. I-3

ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

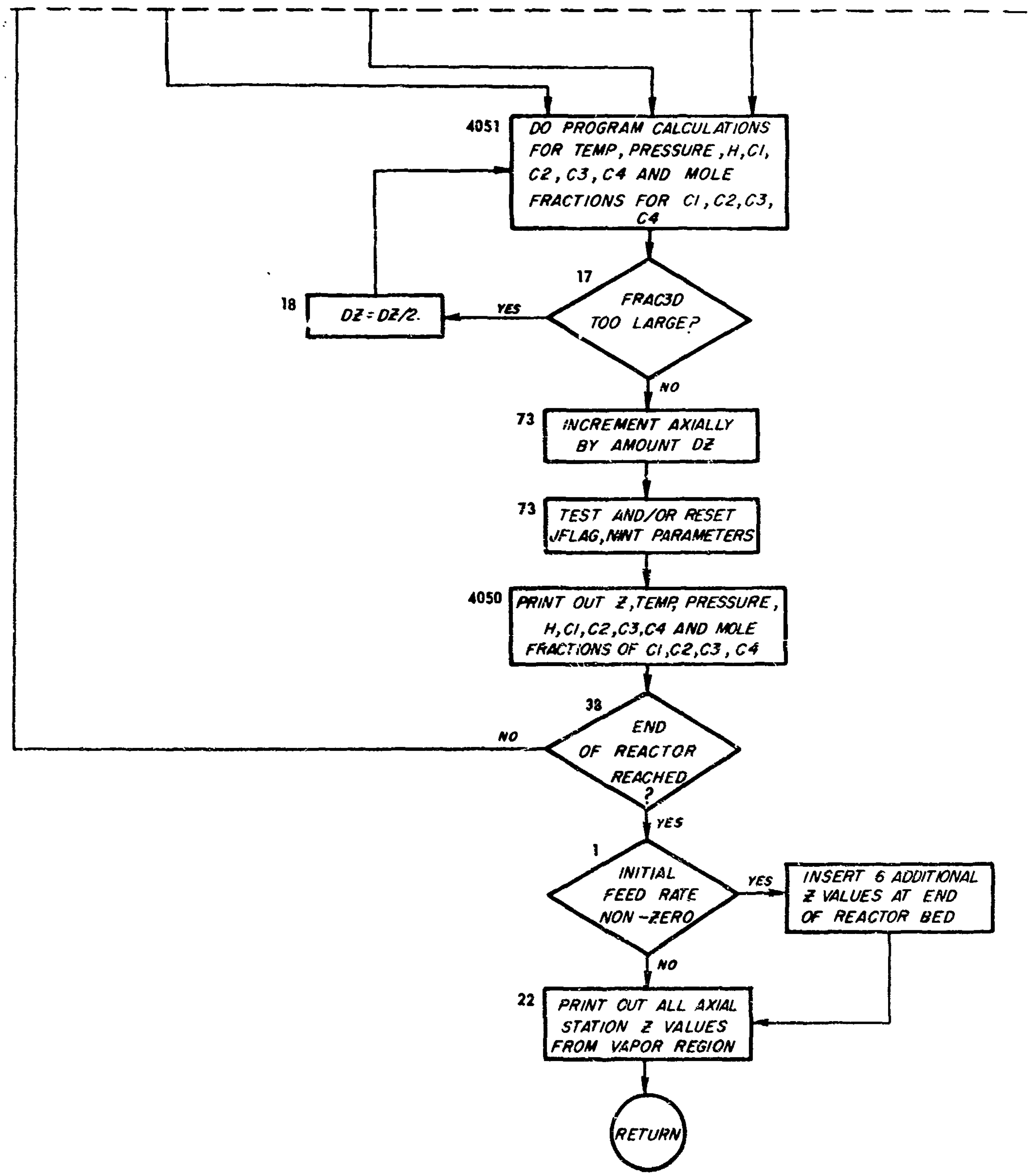
SUBRØUTINE VAPØR : Flow Diagram



(CONTINUED ON PAGE 82)

G910461-30 **ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM** FIG. I-4

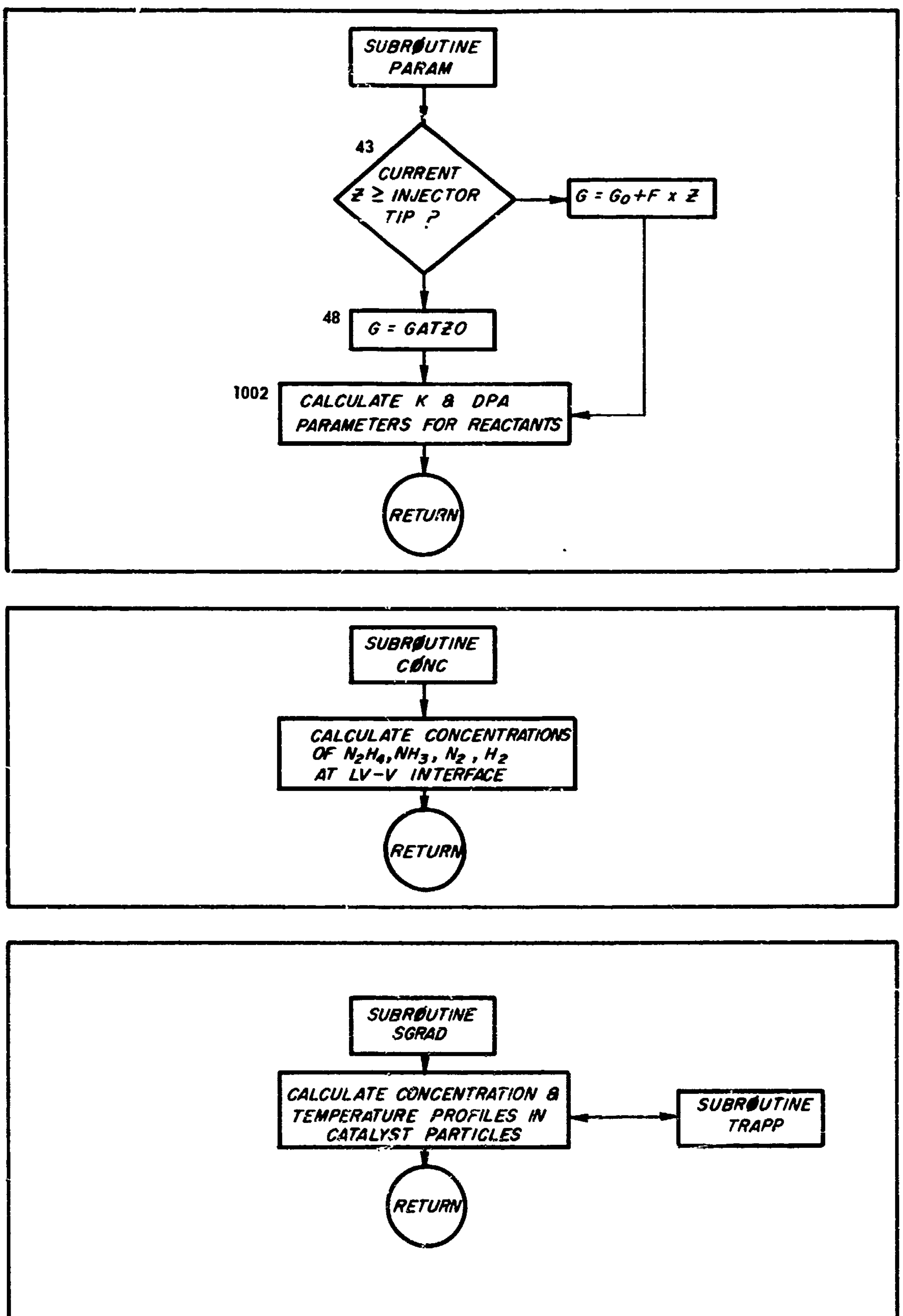
SUBRØUTINE VAPØR (cont.)



G910461-30 FIG. I-5

ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

SUBRØUTINES PARAM, CØNC, and SGRAD: Flow Diagrams



TWO-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

MAIN PROGRAM

FLOW DIAGRAM

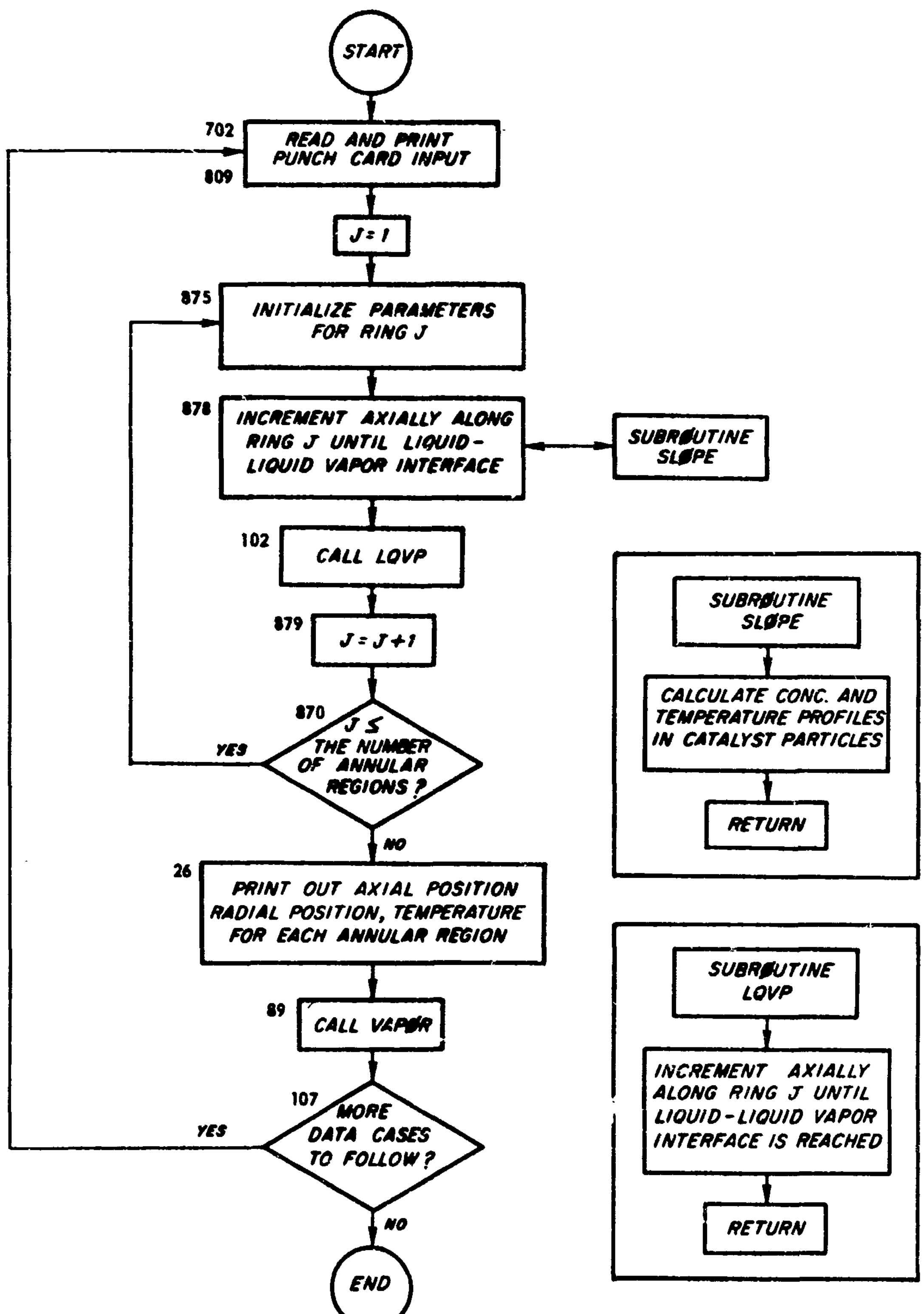


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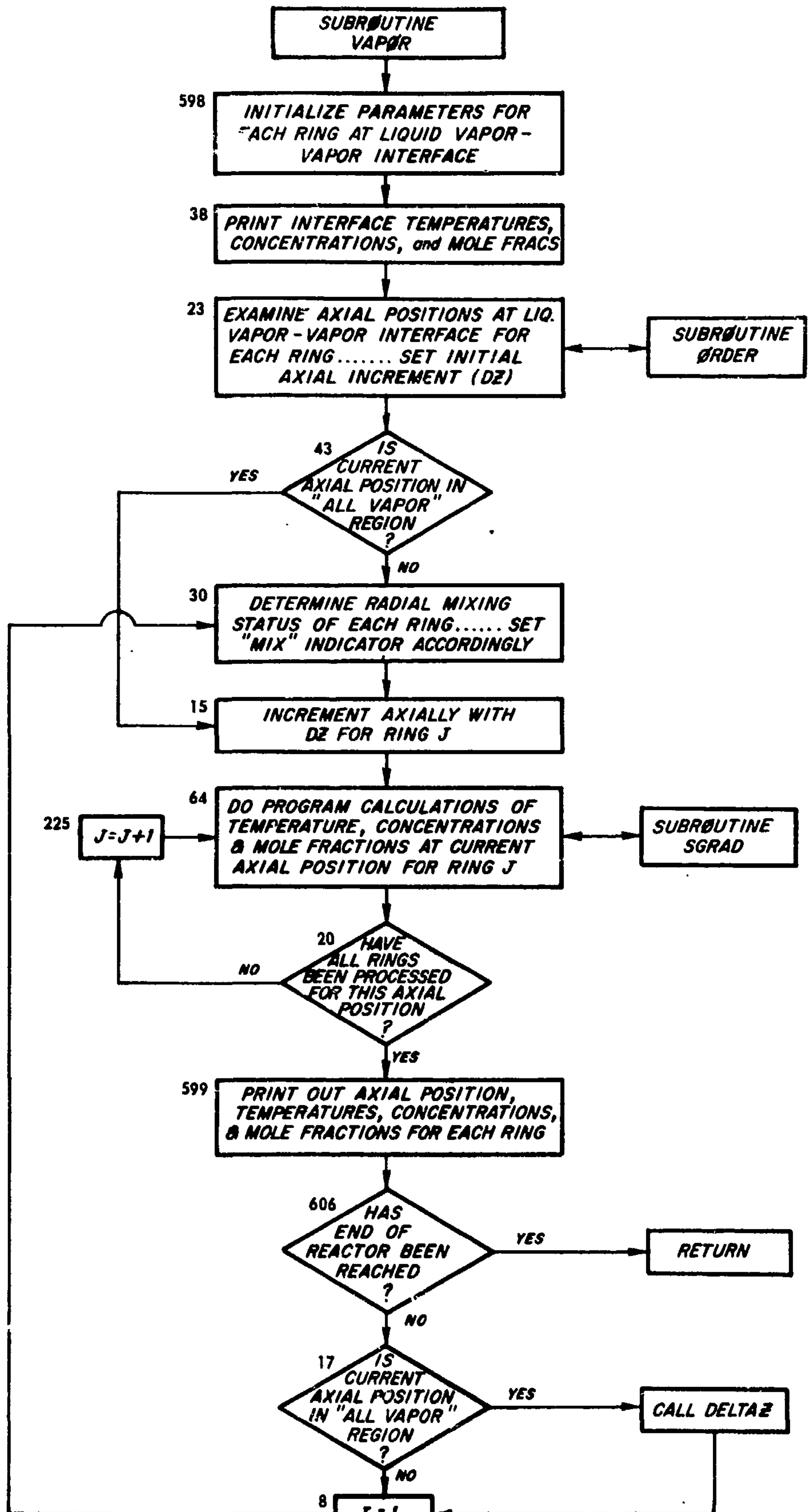
FIG. I-7

TWO-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

SUBRØUTINE VAPØR: Flow Diagram



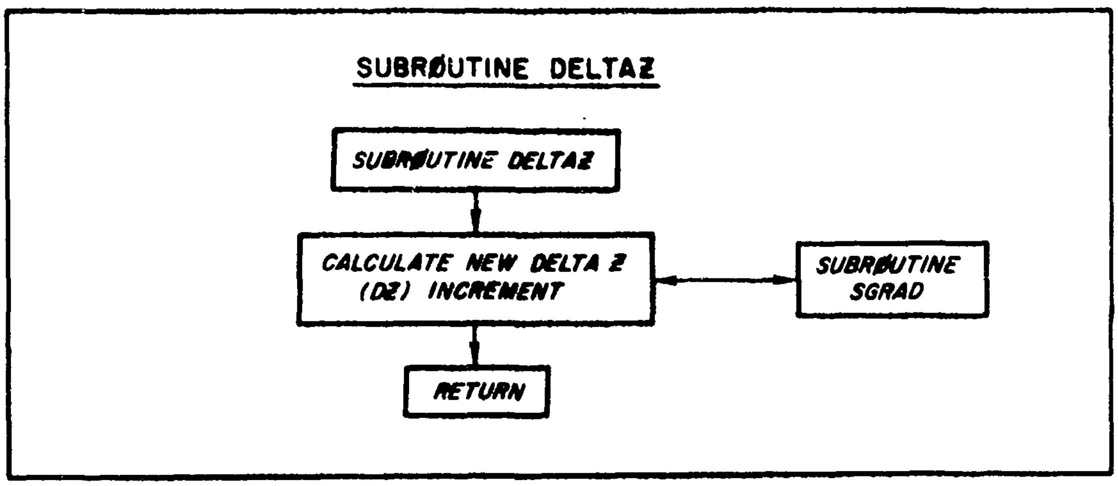
G910461-30

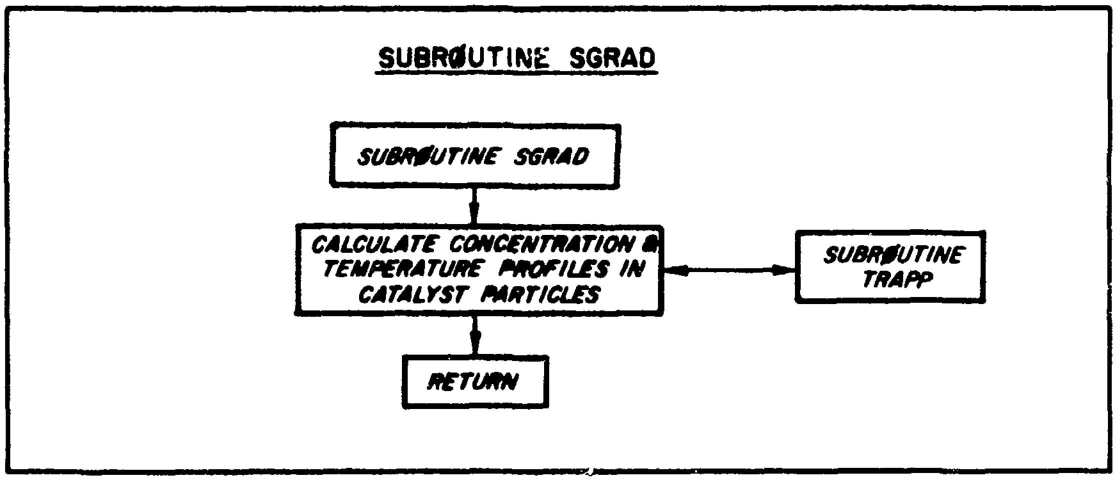
FIG. I-8

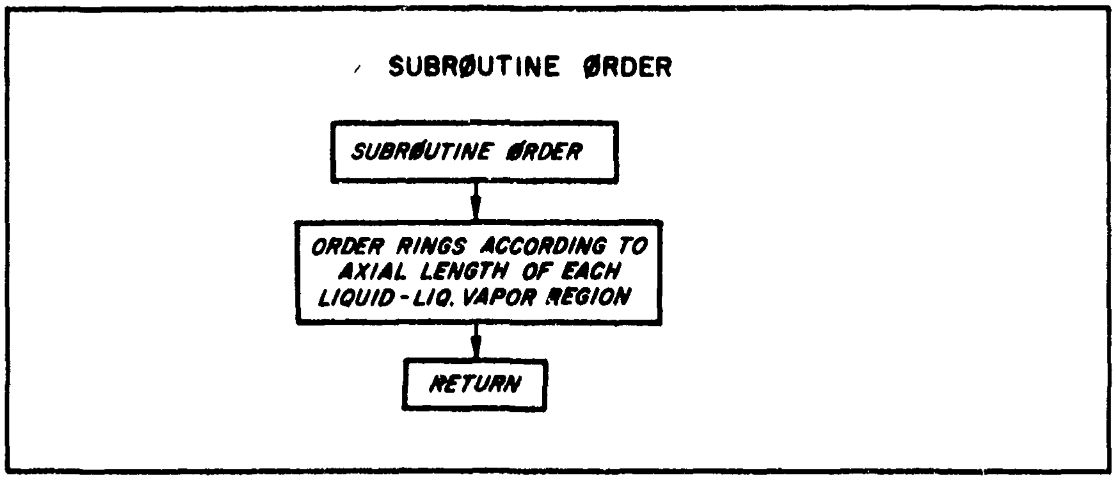
TWO-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

SUBRØUTINES DELTAZ, SGRAD, and ØRDER

Flow Diagrams







G910461-30

APPENDIX II

LISTING OF COMPUTER PROGRAMS

ONE-DIMENSIONAL STEADY-STATE MODEL

```
C ***********************************************************************
C
C DESCRIPTION OF INPUT DATA PUNCH CARDS FOLLOWS ...
C
C                                                                      FORMAT
C  CARD  1       COL'S  1-3    CONTAIN NCASE   (ONLY ONE CARD 1        (I3)
C                                                PER RUN)
C
C                                              (CARDS 2 THRU 16
C                                                SHOULD BE REPEATED
C                                                FOR EACH DATA CASE)
C
C  CARD  2       COL'S  1-80   TITLE CARD ... ANY ALPHANUMERIC         (14A6)
C                                              INFORMATION DESIRED
C
C  CARD  3       COL'S  1-2    CONTAIN OPTION                          (I2)
C                COL'S  3-4    CONTAIN PRINT                           (I2)
C                COL'S  5-7    CONTAIN NOFZ                            (I3)
C
C  CARD  4       COL'S  1-10   CONTAIN Z0 .......................... (E10.5)
C                      11-20   CONTAIN G0 .......................... (E10.5)
C                      21-30   CONTAIN FC .......................... (E10.5)
C                      31-40   CONTAIN ALPHA3 ...................... (E10.5)
C                      41-50   CONTAIN HF .......................... (E10.5)
C                      51-60   CONTAIN R ........................... (E10.5)
C                      61-70   CONTAIN WM4 ......................... (E10.5)
C                      71-80   CONTAIN WM3 ......................... (E10.5)
C  CARD  5       COL'S  1-10   CONTAIN WM2 ......................... (E10.5)
C                      11-20   CONTAIN WM1 ......................... (E10.5)
C                      21-30   CONTAIN ALPHA1 ...................... (E10.5)
C                      31-40   CONTAIN ALPHA2 ...................... (E10.5)
C                      41-50   CONTAIN AGM ......................... (E10.5)
C                      51-60   CONTAIN BGM ......................... (E10.5)
C                      61-70   CONTAIN KP .......................... (E10.5)
C                      71-80   CONTAIN CGM ......................... (E10.5)
C  CARD  6       COL'S  1-10   CONTAIN TF .......................... (E10.5)
C                      11-20   CONTAIN CFL ......................... (E10.5)
C                      21-30   CONTAIN ENMX1 ....................... (E10.5)
C                      31-40   CONTAIN ENMX2 ....................... (E10.5)
C                      41-50   CONTAIN ENMX3 ....................... (E10.5)
C                      51-60   CONTAIN DIF3 ........................ (E10.5)
C                      61-70   CONTAIN DIF4 ........................ (E10.5)
C                      71-80   CONTAIN PRES ........................ (E10.5)
C  CARD  7       COL'S  1-10   CONTAIN ZEND ........................ (E10.5)
C                      11-20   CONTAIN EN1 ......................... (E10.5)
C                      21-30   CONTAIN EN2 ......................... (E10.5)
C                      31-40   CONTAIN EN3 ......................... (E10.5)
C
C
C              (THE TABLE FOR CATALYST PARTICLE RADIUS VS
C               AXIAL DISTANCE ALONG REACTOR BED FOLLOWS)
C
C  CARD  8       COL'S  1- 8   CONTAIN THE NUMBER 0.0                  (E8.4)
C                COL'S  9-16   CONTAIN THE NUMBER 1.0                  (E8.4)
C                COL'S 17-24   CONTAIN NOFZ (FLOATING POINT)           (E8.4)
C                COL'S 25-32   CONTAIN THE NUMBER 0.0                  (E8.4)
C
C  CARDS 9A,9B,...             CONTAIN THE AXIAL STATION Z VALUES
```

```
C                          Z(1),Z(2),...,Z(NOFZ)
C                          10 PER CARD, COL'S 1-80 ........... (10E8.4)
C
C  CARDS 10A,10B,...       CONTAIN THE CATALYST PARTICLE RADII
C                          A(1),A(2),...,A(NOFZ)
C                          10 PER CARD, COL'S 1-80 ........... (10E8.4)
C
C
C            (THE TABLE FOR CATALYST PARTICLE SURFACE AREA
C             VS AXIAL DISTANCE ALONG REACTOR BED FOLLOWS)
C
C  CARD 11              THIS CARD IS IDENTICAL TO CARD 8
C
C  CARDS 12A,12B,...    THESE CARDS (OR SINGLE CARD) ARE IDENTICAL
C                       TO CARDS 9A,9B,...
C
C  CARDS 13A,13B,...    CONTAIN THE CATALYST PARTICLE SURFACE AREAS
C                       AP(1),AP(2),...,AP(NOFZ)
C                       10 PER CARD, COL'S 1-80 .............. (10E8.4)
C
C
C            (THE TABLE FOR INTERPARTICLE VOID FRACTION VS
C             AXIAL DISTANCE ALONG REACTOR BED FOLLOWS)
C
C  CARD 14              THIS CARD IS IDENTICAL TO CARD 8
C
C  CARDS 15A,15B,...    THESE CARDS (OR SINGLE CARD) ARE IDENTICAL
C                       TO CARDS 9A,9B,...
C
C  CARDS 16A,16B,...    CONTAIN THE INTERPARTICLE VOID FRACTIONS
C                       DELA(1),DELA(2),...,DELA(NOFZ)
C                       10 PER CARD, COL'S 1-80 .............. (10E8.4)
C
C
C ***********************************************************************
      REAL KP,K
      INTEGER OPTION,PRINT
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
     1        SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,
     1        WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BOM,HF,DZ,ALPHA1,ALPHA2
     2        ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,
      COMMON /MUVST/VISVST(30)
      COMMON /FLAGS/MFLAG,KFLAG,PRINT
      COMMON /IFCE00/IFC,GATZ0
      COMMON /LIZTBL/DHVST(18),DHLVST(18)
      COMMON /DAVTBL/VPTBL(44)
      DIMENSION  TITLE(14)
      READ (5,700) NCASE
  700 FORMAT (I3)
      KOUNT=1
  705 READ (5,608) TITLE
  608 FORMAT (14A6)
      WRITE (6,609) TITLE
  609 FORMAT (1H1,14A6//)
      IFC=1
      READ (5,809) OPTION,PRINT,NOFZ
  809 FORMAT (2I2,I3)
```

```
      READ (5,800) Z0,G0,FC,ALPHA3,HF,R,WM4,WM3,WM2,WM1,ALPHA1,ALPHA2,
     X        AGM,BGM,KP,CGM,TF,CFL,ENMX1,ENMX2,ENMX3,DIF3,DIF4,PRES,ZEND,
     X        EN1,EN2,EN3,
  800 FORMAT (8E10.5)
      NZTBL = 2*NOFZ+4
      NOFZ4 = NOFZ+4
      NOFZ5 = NOFZ4+1
      CALL UNBAR (VPTBL(1),1,PRES,0.,TVAP,KK)
      CALL UNBAR (DHVST(1),1,TVAP,0.,DELHV,KK)
      CALL UNBAR (DHLVST(1),1,TVAP,0.,DELHL,KK)
      HL=(TVAP-TF)*CFL
      HV=HL+DELHV-DELHL
      GATZ0=G0+FC*Z0
      IF(FC.GT.0.)GO TO 637
      IFC=0
  637 WRITE (6,600)
  600 FORMAT (52X,16H INPUT CONSTANTS/7X,102H HF              HL              HV
     X        TF            TVAP           CFL          PRESSURE         KP             F
     X        G0 )
      WRITE (6,601) HF,HL,HV,TF,TVAP,CFL,PRES,KP,FC,G0
  601 FORMAT (3X,10E11.6//)
      WRITE (6,602)
  602 FORMAT (7X,113H R             ALPHA3          CGM             DIF3            DIF4
     X        WM4            WM3            WM2            WM1            ZEND )
      WRITE (6,601) R,ALPHA3,CGM,DIF3,DIF4,WM4,WM3,WM2,WM1,ZEND
      WRITE (6,603)
  603 FORMAT (6X,113H AGM           BGM            ALPHA1          ALPHA2          N1
     X        N2             N3             ENMX1          ENMX2          ENMX3          )
      WRITE (6,601) AGM,BGM,ALPHA1,ALPHA2,EN1,EN2,EN3,ENMX1,ENMX2,ENMX3
      WRITE (6,617) Z0
  617 FORMAT (// 8X,'Z0' / 3X,E11.6)
      READ (5,20) (ZTBLA(I),I=1,4)
   20 FORMAT (4E8.4)
      READ (5,21) (ZTBLA(I),I=5,NOFZ4)
   21 FORMAT (10E8.4)
      READ (5,21) (ZTBLA(I),I=NOFZ5,NZTBL)
      READ (5,20) (ZTBLAP(I),I=1,4)
      READ (5,21) (ZTBLAP(I),I=5,NOFZ4)
      READ (5,21) (ZTBLAP(I),I=NOFZ5,NZTBL)
      READ (5,20) (ZTBLD(I),I=1,4)
      READ (5,21) (ZTBLD(I),I=5,NOFZ4)
      READ (5,21) (ZTBLD(I),I=NOFZ5,NZTBL)
      WRITE (6,604)
  604 FORMAT (///55X,13H Z VS A TABLE)
      WRITE (6,22) (ZTBLA(I),I=1,4)
   22 FORMAT (40X,4E13.5)
      WRITE (6,23) (ZTBLA(I),I=5,NOFZ4)
   23 FORMAT (1X,10E13.5)
      WRITE (6,25)
   25 FORMAT ( / )
      WRITE (6,23) (ZTBLA(I),I=NOFZ5,NZTBL)
      WRITE (6,24)
   24 FORMAT ( // )
      WRITE (6,606)
  606  FORMAT (54X,14H Z VS AP TABLE )
      WRITE (6,22) (ZTBLAP(I),I=1,4)
      WRITE (6,23) (ZTBLAP(I),I=5,NOFZ4)
      WRITE (6,25)
      WRITE (6,23) (ZTBLAP(I),I=NOFZ5,NZTBL)
      WRITE (6,24)
```

```
      WRITE (6,607)
  607 FORMAT (52X,17H Z VS DELTA TABLE )
      WRITE (6,22) (ZTBLD(I),I=1,4)
      WRITE (6,23) (ZTBLD(I),I=5,NOFZ4)
      WRITE (6,25)
      WRITE (6,23) (ZTBLD(I),I=NOFZ5,NZTBL)
      WRITE (6,613)
  613 FORMAT ('1'18X,'*******************************      ENTERING LIQUID
     A REGION      *******************************' )
      MPLACE=0
      DZ=0.0
      Z(1)=0.0
      H=HF
      II=2
  850 Z(II)=Z(II-1)+DZ
      TEMP=TF+(H-HF)/CFL
      CALL UNBAR (TBLVP(1),1,TEMP,0.,VP,KK)
      CN2H4=(VP+WM4)/(R*TEMP)
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)
      CALL UNBAR (ZTBLAP(1),1,Z(II),0.,AP,KK)
      CALL UNBAR (ZTBLA(1),1,Z(II),0.,A,KK)
      CALL PARAM(TEMP,Z(II),1,CN2H4,H4,0,G,GMMA,K,DPA,BETA)
      CALL SLOPE (CN2H4,GMMA,K,BETA,EN1,DERIV(II),DPA,A,DIF4)
      IF(H-HL)777,776,777
  776 IF(H1.GT.20)DERIV(II)=DERIV(II-1)
  777 DHDZ(II)=-(H4*DPA*AP*DERIV(II)+FC*(H-HF))/G
      DZ=-H4/(EMMX1*DHDZ(II))
      WRITE(6,820)
  820 FORMAT (/39X,4HH Z           TEMP            H               DHDZ )
      WRITE(6,860) Z(II),TEMP,H,DHDZ(II)
  860 FORMAT (/30X,4E15.6)
      IF(H-HL)874,1020,874
  874 H=H+DHDZ(II)*DZ
      IF(H-HL)875,1020,1000
  875 II=II+1
      GO TO 850
C     BACKSTEP TO L-L-V-BOUNDARY
 1000 DZ=(HL-H)/DHDZ(II)+DZ
      H=HL
      II=II+1
      GO TO 850
 1020 IF(OPTION.EQ.2)CALL LQV2(H,Z(II),DERIV(II),II,DHDZ(II),TEMP,CN2H4)
      IF(OPTION.EQ.2)GO TO 1021
      CALL LQVP(H,Z(II),DERIV(II),II,DHDZ(II),TEMP)
C     START VAPOR REGION
 1021 DZ=-H4/(EMMX3*DHDZ(II))
      CALL VAPOR(TEMP,Z(II),II,DHDZ(II),DERIV(II),H)
      KOUNT=KOUNT+1
      IF(KOUNT.LE.NCASE)GO TO 705
      WRITE (6,102)
  102 FORMAT (////41X,36H *****   OPERATIONS COMPLETE    *****  )
      STOP
      END


      SUBROUTINE LQVP (H,ZLV,Q,JJ,Q1,TEMP)
      REAL KP,K
      INTEGER PRINT
```

```
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
     1          SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,
     1          WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2
     2          ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,
      COMMON /MUVST/VISVST(30)
      COMMON /FLAGS/MFLAG,KFLAG,PRINT
      WRITE(6,100)
  100 FORMAT(109H1          ******************************      ENTERING L
     1IQUID-VAPOR REGION        ******************************    //)
      DERIV(JJ)=Q
      DHDZ(JJ)=Q1
      WRITE(6,1750)
 1750 FORMAT(//30X, 3H Z , 11X,5H TEMP 11X, 3H H  12X, 3HWFV)
      Z(JJ)=ZLV
      JJ=JJ+1
 1800 CONTINUE
 1820 DERIV(JJ)=DERIV(JJ-1)
      Z(JJ)=Z(JJ-1)+DZ
      TEMP=TVAP
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)
      CALL UNBAR (ZTBLAP(1),1,Z(JJ),0.,AP,KK)
      CALL PARAM(TEMP,Z(JJ),1,0.0,0.0,0,G,GMMA,K,DPA,BETA)
      DHDZ(JJ)=-(H4*DPA*AP*DERIV(JJ)+FC*(H-HF))/G
      DZ=-H4/(ENMX2*DHDZ(JJ))
      IF(H-HV)82,1850,82
   82 H=H+DHDZ(JJ)*DZ
      IF(H-HV) 1850,1850,2000
 1850 WFV=(H-HL)/(HV-HL)
      WRITE (6,1900) Z(JJ),TEMP,H,WFV
 1900 FORMAT(22X,E14.5,1X,E14.5,1X,E14.5,1X,E14.5)
      IF(H-HV)83,1950,83
   83 JJ=JJ+1
      GO TO 1800
 2000 DZ=(HV-H)/DHDZ(JJ)+DZ
      H=HV
      JJ=JJ+1
      GO TO 1820
 1950 RETURN
      END
```

```
      SUBROUTINE LGV2 (H,ZLV,Q,JJ,Q1,TEMP,CN2H4)
      INTEGER PRINT
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
     1          SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,
     1          WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2
     2          ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,
      COMMON /MUVST/VISVST(30)
      COMMON /FLAGS/MFLAG,KFLAG,PRINT
      WRITE(6,100)
  100 FORMAT(109H1          ******************************      ENTERING L
     1IQUID-VAPOR REGION        ******************************    //)
```

```
      DERIV(JJ)=Q
      DHDZ(JJ)=Q1
      Z(JJ)=ZLV
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)
      C4=CN2H4*((H4-HF+HL)/(H4+HF-HL))
      WFV=0.
      JJ=JJ+1
 3101 CONTINUE
 1820 Z(JJ)=Z(JJ-1)+DZ
      TEMP=TVAP
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)
      CALL UNBAR (ZTBLAP(1),1,Z(JJ),0.,AP,KK)
      CALL UNBAR (ZTBLA(1),1,Z(JJ),0.,A,KK)
      CALL PARAM(TEMP,Z(JJ),1,0.0,0.0,0,G,GMMA,K,DPA,BETA)
      IF(MFLAG.EQ.1)GO TO 7
      CALL SLOPE (C4,GMMA,K,BETA,EN1,DERIV(JJ),DPA,A,DIF4)
      GO TO 6
 7    DIFN=DIF4*((TEMP/492.)**1.823)*14.7/PRES
      CALL UNBAR (VISVST(1),1,TEMP,0.,VIS,KK)
      RHO=PRES*WM4/(R*TEMP)
      AKC=.61*G/RHO*((VIS/(RHO*DIFN))**-.667)*((G/(AP*VIS))**-.41)
      DERIV(JJ)=AKC*C4/DPA
 6    DERIV(JJ)=Q*(1.-WFV)+DERIV(JJ)*WFV
      DHDZ(JJ)=-(H4*DPA*AP*DERIV(JJ)+FC*(H-HF))/G
      DZ=-H4/(ENMX2*DHDZ(JJ))
      IF(H-HV)15,3050,15
 15   H=H+DHDZ(JJ)*DZ
      IF(H-HV)3050,3050,3500
 3050 WFV=(H-HL)/(HV-HL)
      XLV=(HF-H)/H4
      C4=PRES*WM4/(R*TEMP)*((1.-XLV)/(1.+XLV))
 3160 WRITE(6,3000)
 3000 FORMAT(//30X, 3H Z , 11X,5H TEMP 11X, 3H H  12X, 3H WFV)
      WRITE(6,3100)Z(JJ),TEMP,H,WFV
 3100 FORMAT (22X,E14.5,1X,E14.5,1X,E14.5,1X,E14.5////)
      IF(H-HV)16,3150,16
 16   JJ=JJ+1
      GO TO 3101
 3500 DZ=(HV-H)/DHDZ(JJ)+DZ
      H=HV
      JJ=JJ+1
      GO TO 1820
 3150 RETURN
      END
```

```
      SUBROUTINE CONC (C1,C2,C3,C4,ZC,H,T)
C     THIS ROUTINE CALCULATES INITIAL N2H4,NH3,N2,H2 CONCENTRATIONS FOR
C     VAPOR REGION OF THE REACTOR BED
      INTEGER PRINT
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
     1         SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,
     1         WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2
     2         ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,
      COMMON /MUVST/VISVST(30)
```

```
      COMMON /FLAGS/MFLAG,KFLAG,PRINT
      CALL UNBAR (TBLH4(1),1,T,0.,H4,KK)
      XV=-(H-HF)/H4
      C4=((PRES*WM4)/(R*TVAP))*((1.-XV)/(1.+XV))
      C3=((PRES*WM3)/(R*TVAP))*(XV/(1.+XV))
      C2=((PRES*WM2)/(2.*R*TVAP))*(XV/(1.+XV))
      C1=((PRES*WM1)/(2.*R*TVAP))*(XV/(1.+XV))
      RETURN
      END
```

```
      SUBROUTINE PARAM (T,ZA,LOP,CC,HR,LVOP,G,GMMA,K,DPA,BETA)
      REAL KP,K
      INTEGER PRINT
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
     1          SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,
     1          WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2
     2          ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,
      COMMON /MUVST/VISVST(30)
      COMMON /FLAGS/MFLAG,KFLAG,PRINT
      COMMON /IFCEQU/IFC,GATZ0
      IF(ZA-Z0)43,48,48
   43 G=GO+FC*ZA
      GO TO 52
C     Z HAS EXCEEDED HYDRAZINE INJECTOR TUBE LENGTH  - G CONSTANT FROM
C     HERE TO END OF BED
   48 G=GATZ0
      FC=0.
   52 IF(LVOP.EQ.1)GO TO 1004
      GMMA=AGM/T
C     CALCULATE K,DPA FOR N2H4
      K=ALPHA1*EXP(-GMMA)
 1001 DPL=DIF4*(T/492.)**1.832 *(14.7/PRES)*(1.-EXP(-.0672*(PRES*492.)/(
     114.7*T)))
      DPA=DPL
 1002 BETA=-(CC*HR*DPA)/(KP*T)
      GO TO 1003
 1004 GMMA=BGM/T
C     CALCULATE K,DPA FOR NH3
      K=ALPHA2*EXP(-GMMA)/C1**1.6
      DPV=DIF3*(T/492.)**1.832 *(14.7/PRES)*(1.-EXP(-.0672*(PRES*492.)/(
     114.7*T)))
      DPA=DPV
      GO TO 1002
 1003 RETURN
      END
```

```
      SUBROUTINE VAPOR (TEMP,ZV,LL,Q1,Q,H)
      REAL KP,K
      REAL  MBSS
      INTEGER PRINT
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
```

```
     1          SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,
     1          WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2
     2          ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,ZO,
      COMMON /MUVST/VISVST(30)
      COMMON /FLAGS/MFLAG,KFLAG,PRINT
      COMMON /IFCEQU/IFC,GATZ0
      COMMON  /BBBB/DP3,A,KC3,K0,XOA,CPS,CI3,GAMMA,BETA
      COMMON  /CCC/H4TBL(40),H3TBL(40)
      COMMON  /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)
      JZ=LL
      Z(LL)=ZV
      TEMP=TVAP
      PFRC3D=0.
      ZBOUND=ZEND
      KFLAG=0
      JFLAG=0
      KOUNT=0
      INJECT=0
      N=7
      THREE=3.
      WRITE(6,100)
 100  FORMAT(109H1                  ******************************          ENTE
     1RING VAPOR REGION        ******************************  //)
      CALL CONC (C1,C2,C3,C4,Z(LL),H,TEMP)
      SUM=C1/WM1+C2/WM2+C3/WM3+C4/WM4
      FRAC1=C1/(WM1*SUM)
      FRAC2=C2/(WM2*SUM)
      FRAC3=C3/(WM3*SUM)
      FRAC4=C4/(WM4*SUM)
      FRAC3D=(FRAC1/FRAC2-1.)/(3.-FRAC1/FRAC2)
      WRITE(6,4059)
      WRITE (6,4058) Z(LL),TEMP,PRES,H,C1,C2,C3,C4
      WRITE (6,37)
      WRITE (6,38) FRAC1,FRAC2,FRAC3,FRAC4,FRAC3D
 3990 CALL UNBAR (SHTBL1(1),1,TEMP,0.,CP4,KK)
      CALL UNBAR (SHTBL2(1),1,TEMP,0.,CP3,KK)
      CALL UNBAR (SHTBL3(1),1,TEMP,0.,CP2,KK)
      CALL UNBAR (SHTBL4(1),1,TEMP,0.,CP1,KK)
      CAV=(C4*CP4+C3*CP3+C2*CP2+C1*CP1)/(C4+C3+C2+C1)
      WMAV=(C1+C2+C3+C4)/(C1/WM1+C2/WM2+C3/WM3+C4/WM4)
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)
      CALL UNBAR (ZTBLD(1),1,Z(LL),0.,DELA,KK)
      CALL UNBAR (ZTBLAP(1),1,Z(LL),0.,AP,KK)
      CALL UNBAR (ZTBLA(1),1,Z(LL),0.,A,KK)
      CALL PARAM(TEMP,Z(LL),1,C4,H4,0,G,GMMA,K,DPA,BETA)
      IF(C4)7,29,7
 7    DIFN=DIF4*((TEMP/492.)**1.623)*14.7/PRES
      CALL UNBAR (VISVST(1),1,TEMP,0.,VIS,KK)
      RHO=PRES*WMAV/(R*TEMP)
      AKC=.61*G/RHO*((VIS/(RHO*DIFN))**-.667)*((G/(AP*VIS))**-.41)
      DERIV(LL)=AKC*C4/DPA
 6    T4=AP*DPA*DERIV(LL)
      GO TO 31
 29   T4=0.
 31   CALL UNBAR (TBLH3(1),1,TEMP,0.,H3,KK)
      CALL PARAM(TEMP,Z(LL),0,C3,H3,1,G,GMMA,K,DPA,BETA)
      IF(C3)13,30,13
```

```
 13     CALL SGRAD (GRAD,TGRAD)
        DERIV(LL)=GRAD/DPA
        T3=AP*DPA*DERIV(LL)
        GO TO 32
 30     T3=0.
 32     RHOM = ALPHA3*C4*EXP(-CGM/TEMP)
        T1=PRES*WMAV/(R*TEMP*G)
        T2=RHOM*DELA
        DHDZ(LL)=-H4/G*(T2+T4)-H3/G*T3-FC/G*(H-HF)
 C      KFLAG IS SLOPE INDICATOR
 C      =0 --- SLOPE MOVING TOWARDS FIRST PEAK
 C      =1 --- SLOPE HAS REACHED FIRST PEAK
        IF(KFLAG.EQ.1)GO TO 4000
        Z1=-H4/(ENMX3*DHDZ(LL))
        Z2=.05*(ZEND-Z(LL))
        IF(DHDZ(LL)*(1.-Z1/Z2))4060,4060,15
 15     DZ=Z1
 4000   DTDZ=DHDZ(LL)/CAV
        W1=C1/RHO
        W2=C2/RHO
        W3=C3/RHO
        W4=C4/RHO
        S1=1./G
        S5=FC/(G*RHO)
        DW4DZ=S1*(FC-T2-T4)-C4*S5
        DW3DZ=S1*(T2*WM3/WM4+T4*WM3/WM4-T3)-C3*S5
        DW2DZ=S1*(.5*T2*WM2/WM4+.5*T4*WM2/WM4+.5*T3*WM2/WM3)-C2*S5
        DW1DZ=S1*(.5*T2*WM1/WM4+.5*T4*WM1/WM4+1.5*T3*WM1/WM3)-C1*S5
        SUMWM=W1/WM1+W2/WM2+W3/WM3+W4/WM4
        SMDWDZ=DW1DZ/WM1+DW2DZ/WM2+DW3DZ/WM3+DW4DZ/WM4
        DMDZ=-WMAV/SUMWM*SMDWDZ
        DPDZ = (DELA-1.)/DELA**3*(1.75+75.*VIS*(1.-DELA)/(A*G))*G**2/
       X        (64.4*A*RHO)
        DPDZ = DPDZ/144.
        DRDZR = DMDZ/WMAV-DTDZ/TEMP+DPDZ/PRES
        T5=FC/G-DRDZR
        DC4DZ=T1*(FC-T2-T4)-C4*T5
        DC3DZ=T1*(T2*WM3/WM4+T4*WM3/WM4-T3)-C3*T5
        DC2DZ=T1*(.5*T2*WM2/WM4+.5*T4*WM2/WM4+.5*T3*WM2/WM3)-C2*T5
        DC1DZ=T1*(.5*T2*WM1/WM4+.5*T4*WM1/WM4+1.5*T3*WM1/WM3)-C1*T5
        IF(KFLAG.EQ.0)GO TO 16
 C      JFLAG IS DZ INDICATOR FOR NON-ZERO FEED RATE CASES
 C      =0 --- DZ INCREMENT O.K.
 C      =1 --- INCREMENT INITIALLY TOO SMALL
        IF(JFLAG.EQ.1)GO TO 93
 90     IF(KOUNT.EQ.4.OR.KOUNT.EQ.6.OR.KOUNT.EQ.8.OR.KOUNT.EQ.10.OR.KOUNT.
       X        EQ.12.OR.KOUNT.EQ.14)N=N-1
        KOUNT=KOUNT+1
        DZ=DELTAZ/(THREE**N)
        IF(FC)98,98,93
 98     IF(IFC.EQ.0)GO TO 16
 C      IF FEED RATE IS NON-ZERO WE MUST MAKE ADDITIONAL CHECKS ON STEP
 C      SIZE OF Z
 93     IF(ABS(DTDZ)*DZ.GT..01*TEMP)GO TO 19
 C      CHECK IF WE HAVE REACHED THE END OF THE INJECTOR
        IF((1.+DZ/(Z(LL)-Z0)+.01*Z0/ABS(Z(LL)-Z0)).GT.0.)GO TO 16
 19     DZ1=DZ
        CALL REDIVD (DZ1,DTDZ,NINT,JFLAG,I,LL)
        WRITE (6,91) KOUNT,NINT
 91     FORMAT (//7H KOUNT=I2 ,37H --- THIS INTERVAL HAS BEEN REDIVIDEDI4,
```

```
     X6H TIMES)
 16   H=H+DHDZ(LL)*DZ
      IF (H.LT.HV) GO TO 106
4051  TEMP=TEMP+DTDZ*DZ
      PRES = PRES+DPDZ*DZ
      C4=C4+DC4DZ*DZ
      C3=C3+DC3DZ*DZ
      C2=C2+DC2DZ*DZ
      C1=C1+DC1DZ*DZ
 400  SUM=C1/WM1+C2/WM2+C3/WM3+C4/WM4
      IF(C4.LT.0.)SUM=SUM-C4/WM4
      IF(C3.LT.0.)SUM=SUM-C3/WM3
      FRAC1=C1/(WM1*SUM)
      FRAC2=C2/(WM2*SUM)
      FRAC3=C3/(WM3*SUM)
      FRAC4=C4/(WM4*SUM)
      FRAC3D=(FRAC1/FRAC2-1.)/(3.-FRAC1/FRAC2)
      IF(KFLAG.EQ.1)GO TO 500
C     IF RELATIVE DIFFERENCE OF SUCCESSIVE FRAC3D'S IS GREATER THAN 5
C     PERCENT WE RECALCULATE WITH SMALLER DZ INCREMENT
      IF((FRAC3D-PFRC3D).LT..05)GO TO 500
 17   H=H-DHDZ(LL)*DZ
 18   TEMP=TEMP-DTDZ*DZ
      PRES = PRES-DPDZ*DZ
      C4=C4-DC4DZ*DZ
      C3=C3-DC3DZ*DZ
      C2=C2-DC2DZ*DZ
      C1=C1-DC1DZ*DZ
      DZ=DZ/2.
      GO TO 16
 500  PFRC3D=FRAC3D
      IF(C4)70,71,71
 70   C4=0.
      FRAC4=0.
 71   IF(C3)72,73,73
 72   C3=0.
      FRAC3=0.
 73   LL=LL+1
      Z(LL)=Z(LL-1)+DZ
      IF(JFLAG.EQ.1)NINT=NINT-1
      IF(NINT.EQ.0)JFLAG=0
      WRITE (6,4059)
4059  FORMAT (//121H             Z                    TEMP                  PRES
     X    H                  C1                   C2                    C3
     X C4        )
      WRITE (6,4050) Z(LL),TEMP,PRES,H,C1,C2,C3,C4
4050  FORMAT (1X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8,1X,E
     X15.8,1X,E15.8///)
      WRITE (6,37)
 37   FORMAT (98H                                   MFRAC1               MFRAC2
     1  MFRAC3            MFRAC4              FRAC3D     )
      WRITE (6,38) FRAC1,FRAC2,FRAC3,FRAC4,FRAC3D
 38   FORMAT (20X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8 ///)
      IF(Z(LL).GT.ZBOUND)GO TO 1
      IF(KOUNT.GT.15.AND.JFLAG.EQ.0)GO TO 1
      INJECT=0
      GO TO 3990
C     SLOPE HAS TURNED NEGATIVE --- NEXT INCREMENTS ARE (1/3)**7,
C     (1/3)**6,...,(1/3)**1 OF ZEND-Z(LL)
C     15 INCREMENTS IN TOTAL
```

```
4060 DELTAZ=ZEND-Z(LL)
     ZBOUND=ZEND+DELTAZ/3.
     KFLAG=1
     KOUNT=KOUNT+1
     GO TO 4000
   1 IF(IFC.EQ.1)GO TO 22
C    FOR ZERO FEED RATE CASES WE ADD IN 6 ADDITIONAL Z'S FOR USE IN
C    TRANSIENT MODEL
     ZGAP=Z(LL)-Z(LL-2)
     DZZ=ZGAP/8.
     JJ1=LL-1
     JJ8=LL+6
     DO 27 I=JJ1,JJ8
     Z(I)=Z(I-1)+DZZ
  27 CONTINUE
     LL=LL+6
C    PRINT OUT VAPOR REGION Z VALUES FOR USE IN TRANSIENT MODEL
  22 WRITE (6,62)
  62 FORMAT (1H1,54X,22H Z'S FROM VAPOR REGION)
     WRITE (6,63) (Z(I),I=JZ,LL)
  63 FORMAT (1X,10E13.7)
     MASS = (C1+C2+C3+C4)/(C1/WM1+C2/WM2+C3/WM3+C4/WM4)
     WRITE (6,8001) MASS,G
8001 FORMAT (///42X'STEADY STATE VALUES FOR MBAR AND G AT END OF BED'/
    A            47X'MBAR ='E12.5,5X,'G ='E12.5)
     GO TO 999
 106 WRITE (6,107)
 107 FORMAT (////15X'THERE IS A PUDDLE OF COLD HYDRAZINE AT THE LIQUID-
    AVAPOR/VAPOR INTERFACE --- TRY USING A LARGER VALUE FOR G0' )
 999 RETURN
     END
```

```
     SUBROUTINE REDIVD (DZ1,DTDZ,NINT,JFLAG,I,LL)
C    THIS ROUTINE REDIVIDES Z INCREMENTS TO COMPENSATE FOR RADICAL
C    CHANGES IN TEMP,CONCENTRATION,AND OTHER PARAMETERS WHICH OCCUR IN
C    THAT REGION OF THE REACTOR BED FOLLOWING THE TEMPERATURE PEAK
C    THIS ROUTINE IS USED ONLY WHEN INITIAL HYDRAZINE FEED RATE IS NON-
C    ZERO
     INTEGER PRINT
     COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
    1          SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
     COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,G0,
    1          WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2
    2          ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
     COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
     COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,
     COMMON /MUVST/VISVST(30)
     COMMON /FLAGS/MFLAG,KFLAG,PRINT
     COMMON /IFCEQ0/IFC,GATZ0
     I=0
     NESTCT=1
C    IF A REDIVISION OCCURS WITHIN A PREVIOUS REDIVISION,NESTCT IS USED
C    TO OBTAIN A NEW INTERVAL COUNT
     IF(NINT-1)1,1,2
   2 NESTCT=NINT
   1 I=I+1
     XSIZE=2.**I
```

```
      NINT=XSIZE
      DZ=DZ1/XSIZE
      IF(ABS(DTDZ)*DZ.GT..01*TEMP)GO TO 1
      IF((1.+DZ/(Z(LL)-Z0)+.01*Z0/ABS(Z(LL)-Z0)).LT.0.)GO TO 1
      NINT=NINT*NLSTCT
      JFLAG=1
      RETURN
      END
```

```
      SUBROUTINE SLOPE (CG,GMMA,K,BETA,EN12,RATE,DPA,A,DIFF)
      REAL  KP,K
      INTEGER PRINT
      DIMENSION K(1),      GMMA(1),BETA(1),DPA(1),CG(1),S(210),FST(210),
     1SEC(210),D(210),CPA(210),CPB(210),E(210),A(1),TERM1(210),
     2TERM2(210),C(210),XXX(210),XOA(210)
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
     1           SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,
     1           WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2
     2           ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,
      COMMON /MUVST/VISVST(30)
      COMMON /FLAGS/MFLAG,KFLAG,PRINT
      IFLAG=0
      JFLAG = 0
      FRAC=.99
   12 B=0.0
  702 I=1
      NOT=0
      ADIV=100.
      BDIV=100.
      TOL=.01
      STORE=1.0
      KJ=0
      HOLD=0.
      NI=0
   13 MI=0
      IL=0
      IK=0
      MM=0
      IM=0
      F=0.5
   20 MM=MM+1
      DR=B/ADIV
      BDR=(A(I)-B)/BDIV
      JINT=BDIV
      INIT=ADIV
      IF(MM.EQ.1) GO TO 15
      GO TO 16
   15 MMAX=JINT+1
      MAX=MMAX-1
      MINT=0
      GO TO 17
   16 MMAX=INIT+JINT+1
      MINT=INIT+1
      MAX=MMAX-1
```

```
 17  X=0.0
     DO 40 IJ=1,MMAX
     IF(IJ.GT.MINT) GO TO 49
     X=FLOAT(IJ-1)*DR
     GO TO 23
 49  KMJ=IJ-MINT
     X=B+FLOAT(KMJ)*BDR
 23  CP=CG(I)*X/(A(I)-B)-(B/(A(I)-B))*CG(I)
     IF(CP.LT.0.0) CP=0.0
C    THIS IS THE GENERAL EQUATION FOR A LINE WITH NEGATIVE Y-INTERCEPT
 24  FACT1=K(I)*(CG(I))**(1.-EN12)*(CP)**EN12
     FACT2=EXP(GMMA(I)*BETA(I)*(1.-CP/CG(I))/(1.+BETA(I)*(1.-CP/CG(I)))
    1)
     IF(X) 37,40,37
 37  RCP=FACT1*FACT2
 35  S(IJ)=(1./X-1./A(I))*X*X*RCP
 40  CONTINUE
     GO TO 50
 50  SUM=0.0
     SUMA=0.0
     DO 60 IL=2,MAX
     IF(IL.GT.MINT) GO TO 61
     SUM=SUM+S(IL)
     GO TO 60
 61  SUMA=SUMA+S(IL)
 60  CONTINUE
     S(1) =0.
     SGMA=(S(1)+2.0*SUM)*(DR/(2.0*DPA(I)))+(S(MMAX)+2.0*SUMA)*(BDR/(2.
    10*DPA(I)))
     D2=SGMA-FRAC*CG(I)
     TOT=D2+TOL*CG(I)
     IF(MM-1) 110,110,112
112  IF(D2)1,1,2
1    IF(TOT)2,230,230
2    GO TO 115
110  IF(IFLAG.EQ.1)GO TO 115
     IF(D2)150,115,115
115  IF(MM-1) 20,120,140
120  XOLD=B
     IF (PRINT.EQ.1) WRITE(6,125)
125  FORMAT(41H0INITIAL CHOICE THRU ORIGIN IS TOO LARGE )
     D1=D2
C    CHANGE THE EQUATION OF THE LINE
     B=.999999  *A(I)
     GO TO 20
C    USE PREC EDING RESULTS TO ESTIMATE B FOR NEW LINE
140  TUMP=B
     MI=MI+1
     B=B+(D2/(D2-D1))*(XOLD-B)
1741 XOLD=TUMP
     D1=D2
 143 IF(MI-20) 145,145,147
145  GO TO 20
147  IF (JFLAG.EQ.1) GO TO 230
     B - .9*A(I)
     JFLAG = 1
     GO TO 702
C    INITIAL CHOICE THRU ORIGIN IS SATISFACTORY
 150 KJ=1
     IFLAG=1
```

```
      X=0.
C     CALCULATE THE VALUE OF THE TWO INTEGRALS FOR ALL DR (101 POINTS)
      DO 170 II=1,MMAX
      X=FLOAT(II-1)*BDR
      CP=CG(I)*X/(A(I)-B)-(B/(A(I)-B))*CG(I)
      TERM1(II)=K(I)*(CG(I))**(1.-EN12)*(CP)**EN12
      TERM2(II)=EXP(GMMA(I)*BETA(I)*(1.-CP/CG(I))/(1.+BETA(I)*(1.-CP/CG(
     1I))))
      XXX(II)=X
      XOA(II)=XXX(II)/A(I)
      RCP = TERM1(II)*TERM2(II)
      FST(II)=X*X*RCP
      IF(X) 165,170,165
 165  SEC(II)=(1./X-1./A(I))*X*X*RCP
 170  CONTINUE
C     THE TRAPEZOIDAL RULE IS USED TO EVALUATE BOTH INTEGRALS
 172  C(1)=0.
  173 DO 175 JJ=2,MMAX
      IF(JJ.GT.MINT) GO TO 176
      C(JJ)=C(JJ-1)+(FST(JJ)+FST(JJ-1))*(DR/(2.0*DPA(I)))
      GO TO 175
  176 C(JJ)=C(JJ-1)+(FST(JJ)+FST(JJ-1))*(BDR/(2.0*DPA(I)))
 175  CONTINUE
      SEC(1)=0.
      D(1) = 0.
      DO 180 KK=2,MMAX
      IF(KK.GT.MINT) GO TO 179
      D(KK)=D(KK-1)+(SEC(KK-1)+SEC(KK))*(DR/(2.0*DPA(I)))
      GO TO 180
  179 D(KK)=D(KK-1)+(SEC(KK-1)+SEC(KK))*(BDR/(2.0*DPA(I)))
 180  CONTINUE
C     THE VALUE OF CP AT X=0 IS  CG -D(101)
      E(1)=D(MMAX)
  186 CPA(1)=0.0
C     NEGATIVE VALUES OF CPA(1)=CP(0) CANNOT BE USED
C     STORE THE CPA(1) VALUE IN CASE A NEW F FACTOR MUST BE USED
 184  STORE = CPA(1)
      IF(KJ.EQ.1) GO TO 185
      IF(IM.EQ.0) GO TO 185
      IF(NI.EQ.1) GO TO 368
 185  SAM=0.0
      DO 190 LL=2,MMAX
      IF(LL.GT.MINT) GO TO 188
      E(LL)=E(LL-1)-(SEC(LL)+SEC(LL-1))*(DR/(2.*DPA(I)))
      SAM = FLOAT(LL-1)*DR
      GO TO 189
 188  E(LL)=E(LL-1)-(SEC(LL)+SEC(LL-1))*(BDR/(2.0*DPA(I)))
      SAM=SAM+BDR
  189 CPA(LL)=CG(I)-((1./SAM)-(1./A(I)))*C(LL)-E(LL)
      IF(LL.LT.MINT) CPA(LL)=0.0
      IF(CPA(LL).LT.0.0) CPA(LL)=0.0
 190  CONTINUE
      IF(KJ.EQ.1) GO TO 280
      X=0.
      IF(IM.EQ.0) GO TO 250
      IK=1
      GO TO 280
C     THE NEXT ITERATION USES THE VALUES OF CP JUST CALCULATED
 192  DO 200 LI=1,MMAX
      IF(LI.GT.MINT) GO TO 195
```

```
      X=FLOAT(LI-1)*DR
      GO TO 199
  195 KLK=LI-MINT
      X=B+FLOAT(KLK)*BDR
  199 CONTINUE
      TERM1(LI)=K(I)*(CG(I))**(1.-EN12)*(CPA(LI))**EN12
      TERM2(LI)= EXP(GMMA(I)*BETA(I)*(1.-CPA(LI)/CG(I))/(1.+BETA(I)*(1.-
     1CPA(LI)/CG(I))))
      XXX(LI)=X
      XOA(LI)=XXX(LI)/A(I)
      RCP=TERM1(LI)*TERM2(LI)
      FST(LI)=X*X*RCP
      IF(X) 200,200,193
  193 SEC(LI)=(1./X-1./A(I))*X*X*RCP
  200 CONTINUE
      GO TO 172
C     THIS IS FOR THE CASE WHERE THE INITIAL GUESS WAS TOO LARGE
  230 IF (PRINT.EQ.1) WRITE(6,235)MI,B
  235 FORMAT(41H SATISFACTORY STARTING CURVE FOUND AFTER I2,31H TRIALS T
     1HE VALUE OF B (XO) IS  E12.7)
      IF(B.GT..998*A(I))DERIF=2.6*CG(I)/(A(I)-B)
      IF(B.GT..998*A(I)) GO TO 322
C     THE RANGE OF X FROM ZERO TO A IS USED
  237 X=0.
      MI=1
      DO 240 NN=1,MMAX
      IF(NN.GT.MINT) GO TO 246
      X=FLOAT(NN-1)*DR
      GO TO 354
  246 KJK=NN-MINT
      X=B+FLOAT(KJK)*BDR
  354 IF(IM.GE.1) GO TO 353
  238 CPB(NN) = CG(I)*X/(A(I)-B) - (B/(A(I)-B))*CG(I)
      IF(CPB(NN).LT.0.0) CPB(NN)=0.0
  353 TERM1(NN)=K(I)*(CG(I))**(1.-EN12)*(CPB(NN))**EN12
      TERM2(NN)= EXP(GMMA(I)*BETA(I)*(1.-CPB(NN)/CG(I))/(1.+BETA(I)*(1.-
     1CPB(NN)/CG(I))))
      XXX(NN)=X
      XOA(NN)=XXX(NN)/A(I)
      RCP = TERM1(NN)*TERM2(NN)
      FST(NN)=X*X*RCP
      IF(X) 240,240,247
  247 SEC(NN) = (1./X-1./A(I))*X*X*RCP
  240 CONTINUE
      GO TO 172
  368 DO 370 NL=1,MMAX
      CPB(NL)=CPA(NL)
  370 CONTINUE
      GO TO 185
  250 DO 260 IL=1,MMAX
  252 CPA(IL)=F*CPA(IL)+(1.-F)*CPB(IL)
  260 CONTINUE
      IK=0
C   THE VALUES OF X AT A AND NEAREST A ARE USED IN FINDING THE DERIVATIVE
  280 DERIF=(CG(I)-CPA(MAX))/BDR
      IM=IM+1
      IF(IM.GT.99.AND.IFLAG.EQ.1)GO TO 701
      IF(IM.GT.99)GO TO 328
  310 IF(KJ.EQ.1) IK=1
      IF(ABS(DERIF-HOLD)- 0.05*DERIF)3,3,321
```

```
3     IF(IK.EQ.1)GO TO 322
321   HOLD=DERIF
      IF(KJ.EQ.1) GO TO 192
      IF(IK.EQ.1) GO TO 250
      GO TO 192
322   RATE=DERIF
      IF(C4-CG(I))777,4,777
4     IF(H-HL)777,777,5
5     DIFN=DIFF*((TEMP/492.)**1.823)*14.7/PRES
      CALL UNBAR (VISVST(1),1,TEMP,0.,VIS,KK)
      RHO=PRES*WMAV/(R*TEMP)
      AKC=(.61*G)/(RHO)*((VIS/(RHO*DIFN))**-.667)*((G/(AP*VIS))**-.41)
      RAT=AKC*CG(I)/DPA(I)
      IF(RATE-RAT)778,776,6
6     MFLAG=1
      RATE=RAT
      GO TO 777
778   MFLAG=0
777   IF(B.GT..998*A(I))GO TO 888
      IF (PRINT.EQ.1) WRITE(6,182)IM
182   FORMAT (11H ITERATION=,I3)
      IF (PRINT.EQ.1) WRITE(6,336)
336   FORMAT(13X,105H X/A          CPA           X/A          CPA
     1  X/A          CPA          X/A          CPA          )
      IF (PRINT.EQ.1) WRITE(6,183)(XOA(I),CPA(I),I=1,MMAX,4)
183   FORMAT(9X,E12.7,1X,E12.7,1X,E12.7,1X,E12.7,1X,E12.7,1X,E12.7,1X,E1
     12.7,1X,E12.7)
888   IF (PRINT.EQ.1) WRITE(6,323)RATE
323   FORMAT(/24H THE SLOPE CONVERGES TO E12.7)
327   RETURN
328   PERC=(ABS(DERIF-HOLD)/DERIF)*100.
      ALL = 5.
      GO TO 322
C     SIMPLIFIED VERSION DOES NOT ''CONVERGE'' IN 99 ITERATIONS
C     SET B=.000001*A    ,   AND START OVER
701   B=.000001*A(I)
      IF (PRINT.EQ.1) WRITE(6,700)
700   FORMAT (/ 84H INITIAL CHOICE THRU ORIGIN SEEMINGLY OK, BUT RESULTS
     X ROTTEN AFTER 99 ITERATIONS .../48H SET X0=.000001*A AND USE MORE
     AREFINED TECHNIQUE /)
      DR=B/ADIV
      BDR=(A(I)-B)/BDIV
      MMAX=INIT+JINT+1
      MINT=INIT+1
      MAX=MMAX-1
      IM=0
      KJ=0
      GO TO 237
      END
```

```
      SUBROUTINE SGRAD (GRAD,TGRAD)
      REAL  K0,KP,KC3,KC4,MU
      INTEGER PRINT
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
     1          SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,G0,
     1          WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2
```

```
     2           ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,
      COMMON  /BBBB/DP3,A,KC3,K0,X0A,CPS,CI3,GAMMA,BETA
      COMMON  /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)
      COMMON  /MUVST/ VISVST(30)
      COMMON /FLAGS/MFLAG,KFLAG,PRINT
      COMMON  /CCC/H4TBL(40),H3TBL(40)
      DIMENSION  CPOX(101),PCPOX(101),DX(101),CPX(101),RHET(101)
C     DEFINE DP FUNCTION
      DP3F(X,Y,Z) = 14.7*Y/Z*(X/492.)**1.823*(1.-EXP(-.0672*Z*492./(
     X                14.7*X)))
C     DEFINE KC FUNCTION
      KCF(A,B,C,D,E) = .61*A/B*(C/(B*D))**-.667*(A/(E*C))**-.41
C     ANALYTIC INTEGRATION FUNCTIONS FROM INTEGRAL EQUATION
      EVAL1(A,B) = B**3/3.-A**3/3.
      EVAL2(A,B) = B**2/2.-A**2/2.
      WAF1 = .8
      WAF2 = .2
    1 LTFLG=0
      P=PRES
      T=TEMP
      ALPH2=ALPHA2
      CI1=C1
      CI2=C2
      CI3=C3
      CI4=C4
      D03=DIF3
      D04=DIF4
      N=LN1
      NPART = 50
      LP1 = 1
      TPSP = 0.
      RHO = CI1+CI2+CI3+CI4
      DI3 = D03*14.7/P*(T/492.)**1.823
      DI4 = D04*14.7/P*(T/492.)**1.823
      CALL UNBAR (VISVST,1,T,0.,MU,KK)
      CALL UNBAR (CFTBL4,1,T,0.,CF4,KK)
      CALL UNBAR (CFTBL3,1,T,0.,CF3,KK)
      CALL UNBAR (CFTBL2,1,T,0.,CF2,KK)
      CALL UNBAR (CFTBL1,1,T,0.,CF1,KK)
      KC3 = KCF(G,RHO,MU,DI3,AP)
      KC4 = KCF(G,RHO,MU,DI4,AP)
      CFBAR = (CI1*CF1+CI2*CF2+CI3*CF3+CI4*CF4)/RHO
      HC = .74*G*CFBAR*(G/(AP*MU))**-.41
C
C     LOCATE SUITABLE X0
C
      DP3 = DP3F(T,D03,P)
C     CHOOSE STARTING VALUE FOR CPS TO BE = CI3/2.
      CPS = CI3/2.
      CMCPN = CI3-CPS
      DCPDX = KC3/DP3*(CI3-CPS)
C     H4 CONSTANT FOR EACH ENTRY TO THIS ROUTINE
C     H3 VARIES WITH TEMP AT EACH ITERATION
      CALL UNBAR (H4TBL,1,T,0.,H4,KK)
      CALL UNBAR (H3TBL,1,T,0.,H3,KK)
      IF (LP1.EQ.1) GO TO 6
   40 TPSPP = TPSP
      TPSP = TPS
```

```
 6    TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      DP3P = DP3
      H3P = H3
      TMTPN = T-TPS
 61   GAMMA = BGM/TPS
      BETA = -CPS*H3*DP3/(KP*TPS)
      K0 = ALPH2*EXP(-GAMMA)*CI1**EN3
C     LINEAR EXTRAPOLATION USED TO GUESS AT X0
      X0P = X0
      X0 = A-CPS/DCPDX
      XOA = X0/A
      IF (X0) 11,12,12
 11   X0 = 0.
      XOA = 0.
      CPS = CI3/(DP3/(A*KC3)+1.)
      DCPDX = CI3/A
      TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
      WRITE (6,132) LP1,TPS
 132  FORMAT (/,37X,'WE HAVE CALCULATED A NEGATIVE X0 DURING ITERATION
C     INTEGRATE FOR CP EQUATION
 12   CALL TRAPP (XOA,1.,NPART,RIESUM)
C     CALCULATE NEW CPS ...
      CPSP = CPS
      CMCPO = CMCPN
      CPS = CI3-A*RIESUM/KC3
      IF (LTFLG-1) 80,84,30
 80   IF (CPS-(.25*CI3)) 81,81,130
 81   LTFLG=1
      GO TO 22
 84   LTFLG=0
      IF (CPS) 89,130,130
 89   CPS=0.
      GO TO 46
 130  CMCPN = CI3-CPS
C     CALCULATE NEW TP
 13   DCPDX = KC3/DP3*(CI3-CPS)
      GRAD = DCPDX*DP3
      TGRAD = HC*(T-TPS)
      TPSPP = TPSP
      TPSP = TPS
      TMTPO = TMTPN
 51   TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      TMTPN = T-TPS
      GAMMA = BGM/TPS
      BETA = -CPS*H3*DP3/(KP*TPS)
      K0 = ALPH2*EXP(-GAMMA)*CI1**EN3
C     TEST TEMP,CONCENTRATION FOR 5% LIMIT
      IF (ABS(TMTPO-TMTPN)/TMTPN - .05) 41,41,43
 41   IF (ABS(CMCPO-CMCPN)/CMCPN - .05) 70,70,43
C     TEST FOR TEMPERATURE LOOP ... COMPARE LAST 3 TEMPS
 43   IF (AMIN1(TPS,TPSP,TPSPP) - TPSP) 60,71,60
 60   IF (AMAX1(TPS,TPSP,TPSPP) - TPSP) 46,71,46
C     TEMPERATURE HAS FLUCTUATED ... TAKE AVERAGE AND RECALCULATE CPS
```

```
 71   TPSPP = TPSP
      TPSP = TPS
      TMTPO = TMTPN
      TPS = (TPSP+TPSPP)/2.
      CALL UNBAR (H3,BL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      DP3P = DP3
      TMTPN = T-TPS
      DCPDX = (HC*(T-TPS)-H4*KC4*CI4)/(H3*DP3)
      CPSP = CPS
      CMCPO = CMCPN
      CPS = CI3-DP3/KC3*DCPDX
      IF (CPS.LT.0.) CPS=0.
      CMCPN = CI3-CPS
      LP1 = LP1+1
      IF (LP1-50) 61,61,44
C     NO CONVERGENCE YET ... AVERAGE THE CPS'S FOR LAST TWO CALC'S AND REPEAT
 46   CPS = .2*CPS+.8*CPSP
      GO TO 53
 22   X00 = WAF1*X0P+WAF2*X0
      CPS = CI3/(1.+DP3/(KC3*A-KC3*X00))
 53   DCPDX = KC3/DP3P*(CI3-CPS)
      CMCPN = CI3-CPS
      H3 = H3P
 42   LP1 = LP1+1
      IF (LP1-25) 40,40,44
 44   WAF1 = WAF1+.05
      IF (WAF1.GT.0.95) 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   WRITE (6,98)
 98   FORMAT (///20X,'UNABLE TO FIND SUITABLE X0 AFTER  FOUR TRIES OF 25
     X ITERATIONS EACH --- PROGRAM STOP FOLLOWS' )
      CALL EXIT
C     SATISFACTORY X0 HAS BEEN FOUND
 70   IF (PRINT.EQ.1) WRITE(6,16)LP1,X0
 16   FORMAT (/// 46X,27HSATISFACTORY X0 FOUND AFTER,I3,7H TRIES  /
     X          57X,5H X0 =,E12.5 )
C
C     CALCULATE GRADIENT
C
 131  LP2 = 1
      NX = 24
      NX1 = NX+1
      NXM1 = NX-1
 291  X0A = X0/A
      VNU = -KC3/DP3
      INT1 = 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 I=1,NX1
C     CP(X/A) IS A LINEAR PROFILE DURING FIRST APPROXIMATION
```

```
      IF (LP2.GT.1) GO TO 664
      CPX(I) = (XA-XOA)/(1.-XOA)*CPS
  664 RHET(I) = K0*CI3**(1-N)*CPX(I)**N*EXP(GAMMA*BETA*(1.-CPX(I)/CI3)/
     X          (1.+BETA*(1.-CPX(I)/CI3)))
      DX(I) = XA
      XA = XA+DELXOA
  770 CONTINUE
C   TAKE INTERVAL FUNCT'N MIDPTS AS CONSTANT VALUE FOR CP(X/A) AND RHET
      DO 771 I=1,NX
      CPX(I) = (CPX(I)+CPX(I+1))/2.
      RHET(I) = (RHET(I)+RHET(I+1))/2.
  771 CONTINUE
      XA = XOA+DELXOA
      CTRM = (A*VNU+1.)/(A*VNU)
C   INTEGRAL EQUATION FOLLOWS
C   CPOX(1) IS SPECIAL CASE ... X=X0
      DXL = XOA
      DXU = DXL+DELXOA
      RR1 = 0.
      DO 377 I=1,NX
      RR1 = RR1+RHET(I)*(EVAL2(DXL,DXU)-CTRM*EVAL1(DXL,DXU))
      DXL = DXU
      DXU = DXU+DELXOA
  377 CONTINUE
      CPOX(1) = CI3-A*A/DP3*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) = CI3-A*A/DP3*(R1+R2)
      IF (CPOX(K).LT.0.) CPOX(K)=0.
      XOA = X0/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 378 I=1,NX
      RR2 = RR2+RHET(I)*EVAL1(DXL,DXU)
      DXL = DXU
```

```
      DXU = DXU+DELXOA
  378 CONTINUE
      CPOX(NX1) = CI3-A*A/DP3*(1.-CTRM)*RR2
      IF (CPOX(NX1).LT.0.) CPOX(NX1)=0.
C     CALCULATE A NEW TPS
      DCPDX = KC3/DP3*(CI3-CPOX(NX1))
      H3P = H3
      DP3P = DP3
      TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      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 = CI3-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 CPX(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 CPX(I) = .8*CPX(I)+.2*CPOX(I)
      GO TO 56
C  AVERAGE PRESENT AND PAST CALCULATED PROFILES EVERY 5TH PASS TO SMOOTH
   57 CPX(I) = (CPOX(I)+PCPOX(I))/2.
C  STORE PRESENT CALCULATED PROFILE
   56 PCPOX(I) = CPOX(I)
   55 CONTINUE
      CMCPN = CI3-CPX(NX1)
      DCPDX = KC3/DP3P*(CI3-CPX(NX1))
      TPS = T-(H4*KC4*CI4+H3P*DP3P*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      TMTPO = TMTPN
      TMTPN = T-TPS
      LP2 = LP2+1
      IF (LP2-50) 29,29,30
   30 WRITE (6,18) CPOX(NX1)
   18 FORMAT (///31X,52HUNABLE TO CONVERGE ON CPS IN  50 TRIES ... CP(X/
     XA) =,E12.5)
      WRITE (6,522) GRAD,TGRAD
  522 FORMAT (51X,'KC3*(CI3-CPS) =',E12.5 / 54X,'HC*(T-TPS) =',E12.5)
      GO TO 28
   29 GAMMA = BGM/TPS
      BETA = -CPX(NX1)*H3*DP3/(KP*TPS)
      K0 = ALPH2*EXP(-GAMMA)*CI1**EN3
      GO TO 291
   88 IF (PRINT.EQ.1) WRITE(6,19)(DX(I),CPOX(I),I=1,NX1)
   19 FORMAT (///11X,114HX/A        CP(X/A)        X/A        CP(X/A)
     X X/A        CP(X/A)        X/A        CP(X/A)        X/A        CP(X/A)
     X        /(5X,10E12.6))
      IF (PRINT.EQ.1) 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 )
      GRAD = DCPDX*DP3
```

```
      TGRAD = HC*(T-TPS)
      IF (PRINT.EQ.1) WRITE(6,83)GRAD,TGRAD
   83 FORMAT (51X,'KC3*(CI3-CPS) =',E12.5 / 54X,'HC*(T-TPS) =',E12.5)
   28 RETURN
      END
```

```
      SUBROUTINE TRAPP (U,V,NPART,RIESUM)
C     NUMERICAL INTEGRATION USING TRAPEZOIDAL METHOD
      REAL   K0,KC3
      COMMON  /BBBB/DPS,A,KC3,K0,XOA,CPS,CI3,GAMMA,BETA
C     DEFINE RHET FOR VARIABLE CP,CPS,TP
      RHETF(A,B,C,D,E,N) = E*A**(1-N)*B**N*EXP(C*D*(1.-B/A)/(1.+D*(1.-
     X                   B/A)))
C     FUNCTIONS DEFINING INTEGRANDS
      FOXI1(X,R)=X**2*R
C     FUNCTION DEFINING CP(X) FOR RHET FUNCTION
C     CP(X) IS ASSUMED TO VARY LINEARLY WITH X
      CPXF(X,Y,Z)=(X-Y)/(1.-Y)*Z
      N=NPART-1
      PART=NPART
      H=(V-U)/PART
      UPH = U+H
      SUM=0.
      CPX1=CPXF(U,XOA,CPS)
      CPX2=CPXF(V,XOA,CPS)
      RHET1=RHETF(CI3,CPX1,GAMMA,BETA,K0,1)
      RHET2=RHETF(CI3,CPX2,GAMMA,BETA,K0,1)
C     CALCULATE FIRST,LAST TERMS OF RIEMANN SUM FIRST
    4 TRM1=FOXI1(U,RHEY1)/2.
      TRM2=FOXI1(V,RHET2)/2.
    6 DO 8 I=1,N
      CPX=CPXF(UPH,XOA,CPS)
      RHET = RHETF(CI3,CPX,GAMMA,BETA,K0,1)
      SUM=SUM+FOXI1(UPH,RHET)
      UPH = UPH+H
    8 CONTINUE
    9 RIESUM=H*(TRM1+SUM+TRM2)
   99 RETURN
      END
```

```
      SUBROUTINE UNBAR (T,IK,XIN,YIN,ZZ,KK)
      DIMENSION T(1),X(6),Y(6),A(6)
C     ------------------  MARCH 4, 1961  ------------
C     ------------------  MODIFIED 7/62  -----------------
C     ------------------     TO DO QUADRATIC AND LINEAR INTERPOLATION ALSO
C
      II = IK+1
      N = 3
      N2=
         IF (T(II)-3.) 700,701,702
  700    IF (T(II)+0.) 60,701,704
  704    IF (T(II)-2.) 705,706,701
  705 N = 1
         GO TO 707
```

```
706  N = 2
707  N2= 1
701  II = II+1
702  N1 = N +1
          DO 50 L = II,II
          IF ( T(L) + 0. ) 60,60,51
60    KK = -1
      ZZ = 0.
        GO TO 9999
51   NX = T(L)
          IF (T(L+1) + 0. ) 60,52,50
52   NY = 0
          GO TO 53
50   NY = T(L+1)
53      CONTINUE
     KK  = 0
     KY  = 0
     XX  = XIN
     YY  = YIN
     J1  = II+2
     J2  = NX+II+1
     IF(XX-T(J1))301,306,400
400       DO 302 J=J1,J2
          IF (XX-T(J)) 304,304,302
302  CONTINUE
309  KK  = 2
     XX  = T(J2)
308  JX1 = J2-N
          GO TO 305
301  KK  = 1
     XX  = T(J1)
306  JX1 = J1
          GO TO 305
304       IF (J-J1-1) 301,306,307
307       IF (J-J2)   303,308,309
303  JX1 = J-N2
305  CONTINUE
     XINT  = XX
       IF (NY) 1500, 1500, 3000
1500      DO 1599 L=1,N1
           X(L) = T(JX1)
           LY = JX1 + NX
           Y(L) = T(LY)
1599   JX1 = JX1+1
     I = 1
     GO TO 54
3000 J1  = J1+NX
     J2  = J2+NY
     IF(YY-T(J1))311,316,401
401       DO 312 J=J1,J2
          IF (YY-T(J)) 314,314,312
312  CONTINUE
319  KY  = 4
     YY  = T(J2)
318  JY1 = J2-N
          GO TO 315
311  KY  = 3
     YY  = T(J1)
316  JY1 = J1
          GO TO 315
```

```
 314       IF (J-J1-1)  311,316,317
 317       IF (J-J2)    313,318,319
 313  JY1 = J-N2
 315  CONTINUE
      JX2  = JX1
      LY   = JY1 + NY*(JX2-II-1)
      LY1 = LY
           DO 3099 L=1,N1
      X(L) = T(JX2)
      Y(L) = T(LY1)
      LY1  = LY1+NY
 3099 JX2  = JX2+1
      I    = 0
           GO TO 54
 3098  Y(1)  = ZZ
           DO 4400 I=1,N
      LY1 = LY+1
      Y(I+1) = 0.
           DO 4050 MM=1,N1
      Y(I+1) = Y(I+1) + T(LY1)*X(MM)
 4050 LY1 = LY1+NY
 4400  CONTINUE
           DO 4199 L=1,N1
      X(L) = T(JY1)
 4199 JY1  = JY1+1
      XINT = YY
      I=  1
 54   D  = 1.
      X(N+2) = X(1)
      X(N+3) = X(2)
           DO 55 J=1,N1
      A(J+1) = X(J+1) - X(J)
      TPAL1  = XINT - X(J)
       IF ( TPAL1 ) 57,58,57
 58     ZZ = Y (J)
       X(1) = 0.
       X(2) = 0.
       X(3) = 0.
       X(4) = 0.
       X(J) = 1.0
       GO TO 59
 57   D = D * TPAL1
           GO TO (711,712,713) ,N
 711  X(J)  = TPAL1/A(J+1)
           GO TO 55
 712  X(J)  = -TPAL1
           GO TO 55
 713  X(J)  = (X(J+2)-X(J))*TPAL1
 55       CONTINUE
      A(1) = A(N+2)
      ZZ = 0.
         DO 56 J=1,N1
        X(J) = D/(A(J)*A(J+1)*  X(J))
      ZZ = ZZ + Y(J)*  X(J)
 56       CO[illegible]
 59       [illegible] 3098,9999
 9999 KK  [illegible]
          [illegible]
      E[illegible]
```

```
      BLOCK DATA
      COMMON /MUVST/VISVST(30)
C     BLOCK DATA FOR VISCOSITY VS TEMPERATURE
      DATA (VISVST(I),I=1,30) / 0.0,1.,13.,0.0,
     X        360.,540.,720.,900.,1080.,1260.,1440.,1620.,1800.,1980.,
     X        2160.,2340.,2520.,
     X        .048 E-4,.070 E-4,.093 E-4,.117 E-4,.141 E-4,.164 E-4,
     X        .186 E-4,.207 E-4,.228 E-4,.247 E-4,.266 E-4,.285 E-4,
     X        .302 E-4/
      END
```

```
      BLOCK DATA
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),
     1           SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)
C     BLOCK DATA FOR FUNCTIONS OF TEMPERATURE
      DATA  (TBLVP(I),I=1,70)/10.0,1.,33.0,0.0,492.,519.,528.37,529.08,5
     134.60,534.71,538.34,543.91,545.73,560.20,569.98,579.26,579.48,595.
     234,610.13,614.08,618.07,627.49,628.82,645.68,650.76,665.57,674.99,
     3686.13,692.39,697.47,744.,798.,852.,942.,1032.,1122.,1176.,.0520,.
     41479,.2011,.2069,.2398,.2436,.2823,.2920,.3539,.5453,.7367,.9727,.
     59823,1.510,2.204,2.462,2.740,3.407,3.562,5.240,5.971,8.065,9.711,1
     61.91,13.46,14.70,33.80,73,48,147.0,382.1,823.0,1528.,2131./
      DATA  (TBLH4(I),I=1,42 )/0.0,1.,19.0,0.0,0.0,180.,360.,536.4,540.,
     6720.,900.,1080.,1260.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,27
     900.0,2880.,3060.,-1991.34,-1951.02,-1919.50,-1896.04,-1895.70,-188
     X2.55,-1878.12,-1879.46,-1884.63,-1892.38,-1901.94,-1912.88,-1924.6
     X5,-1937.54,-1950.74,-1964.45,-1978.32,-1992.36,-2006.62/
      DATA  (TBLH3(I),I=1,42 )/0.0,1.,19.0,0.0,0.0,180.,360.,536.4,540.,
     X720.,900.,1080.,1260.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,27
     X00.,2880.,3060.,983.07,1055.57,1103.97,1159.35,1160.40,1213.46,125
     X9.64,1298.00,1329.71,1355.28,1375.57,1391.11,1402.52,1410.13,1414.
     X57,1416.37,1416.05,1414.15,1410.56/
      DATA  (SHTBL1(I),I=1,34)/0.0,1.,15.0,0.0,540.,720.,900.,1080.,1260
     1.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,2700.,2880.,3060.,.380
     24,.4601,.5261,.5784,.6212,.6577,.6899,.7185,.7442,.7673,.7879,.806
     33,.8226,.8373,.8503/
      DATA  (SHTBL2(I),I=1,34)/0.0,1.,15.0,0.0,540.,720.,900.,1080.,1260
     5.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,2700.,2880.,3060.,.500
     65,.5424,.5891,.6344,.6773,.7176,.7553,.7905,.8236,.8541,.8823,.907
     75,.9304,.9512,.9697/
      DATA  (SHTBL3(I),I=1,34)/0.0,1.,15.0,0.0,540.,720.,900.,1080.,1260
     9.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,2700.,2880.,3060.,.248
     X5,.2495,.2524,.2569,.2624,.2682,.2738,.2790,.2836,.2878,.2914,.294
     X6,.2974,.2998,.3019/
      DATA  (SHTBL4(I),I=1,34)/0.0,1.,15.0,0.0,540.,720.,900.,1080.,1260
     X.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,2700.,2880.,3060.,3.41
     X94,3.4596,3.4685,3.4765,3.4899,3.5151,3.5454,3.5806,3.6208,3.6654,
     X3.7150,3.7696,3.8291,3.8802,3.9288/
      END
```

```
      BLOCK DATA
```

```
C    BLOCK DATA FOR SPECIFIC HEAT VS TEMPERATURE
      COMMON /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)
      DATA  (CFTBL1(I),I=1,34) /  0., 1., 15., 0.,
C    TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,
     X 1960. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,
C    SPECIFIC HEATS
     X 3.4194, 3.4596, 3.4685, 3.4765, 3.4899, 3.5151, 3.5454, 3.5006,
     X 3.6208, 3.6654, 3.7150, 3.7696, 3.8291, 3.8802, 3.9288 /
      DATA  (CFTBL2(I),I=1,34) /  0., 1., 15.,  0.,
C    TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,
C    SPECIFIC HEATS
     X .2465 , .2495 , .2524 , .2569 , .2624 , .2682 , .2738 , .2790 ,
     X .2836 , .2878 , .2914 , .2946 , .2974 , .2998 , .3019  /
      DATA  (CFTBL3(I),I=1,34) /  0., 1., 15., 0.,
C    TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,
C    SPECIFIC HEATS
     X .5005 , .5424 , .5891 , .6344 , .6773 , .7176 , .7553 , .7905 ,
     X .8236 , .8541 , .8823 , .9075 , .9304 , .9512 , .9697  /
      DATA  (CFTBL4(I),I=1,34) /  0., 1., 15., 0.,
C    TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,
     X 1960. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,
C    SPECIFIC HEATS
     X .3604 , .4601 , .5261 , .5784 , .6212 , .6577 , .6899 , .7185 ,
     X .7442 , .7673 , .7879 , .8063 , .8226 , .8373 , .8503  /
      END
```

```
      BLOCK DATA
C    BLOCK DATA FOR HEAT OF REACTION VS TEMPERATURE
      COMMON /CCC/H4TBL(40),H3TBL(40)
      DATA  (H4TBL(I),I=1,40) /   0., 1., 18., 0.,
C    TEMPERATURES
     X  160.  ,  360.  ,  536.4 ,  540.  ,  720.  ,  900.  , 1080.  ,
     X 1260.  , 1440.  , 1620.  , 1800.  , 1980.  , 2160.  , 2340.  ,
     X 2520.  , 2700.  , 2880.  , 3060.  ,
C    HEATS OF REACTION
     X-1951.02,-1919.50,-1896.04,-1895.70,-1882.55,-1878.12,-1879.46,
     X-1884.63,-1892.38,-1901.94,-1912.88,-1924.85,-1937.54,-1950.74,
     X-1964.45,-1978.32,-1992.36,-2006.62  /
      DATA  (H3TBL(I),I=1,40) /   0., 1., 18., 0.,
C    TEMPERATURES
     X  180.  ,  360.  ,  536.4 ,  540.  ,  720.  ,  900.  , 1080.  ,
     X 1260.  , 1440.  , 1620.  , 1800.  , 1980.  , 2160.  , 2340.  ,
     X 2520.  , 2700.  , 2880.  , 3060.  ,
C    HEATS OF REACTION
     X1055.57 ,1103.97 ,1159.35 ,1160.40 ,1213.46 ,1259.64 ,1298.00 ,
     X1329.71 ,1355.28 ,1375.57 ,1391.11 ,1402.52 ,1410.13 ,1414.57 ,
     X1416.37 ,1416.05 ,1414.15 ,1410.56   /
      END
```

```
      BLOCK DATA
      COMMON /DAVTBL/VPTBL(44)
C     BLOCK DATA TABLE OF VAPOR PRESSURE VS TEMP  (USED TO FIND TVAP)
      DATA (VPTBL(I),I=1,44) /        0. ,    1. ,   20. ,    0. ,
     X        50. ,  100. , 150. , 200. , 250. , 300. , 350. , 400. ,
     X       450. ,  500. , 550. , 600. , 650. , 700. , 750. , 800. ,
     X       850. , 900. , 950. , 1000.,
     X       770. , 820. , 855. , 880. , 905. , 925. , 945. , 965. ,
     X       980. , 995. ,1010. ,1025. ,1035. ,1050. ,1060. ,1070. ,
     X       1080., 1090. ,1100. ,1110. /
      END
```

```
      BLOCK DATA
      COMMON /LIZTBL/DHVST(18),DHLVST(18)
C     BLOCK DATA TABLES FOR DELHV AND DELHL VS TEMP  (USED TO FIND HV)
      DATA  (DHVST(I),I=1,18) / 0., 1., 7., 0.,
     X       180. , 360. , 534.6 , 540. , 720. , 900. , 1080. ,
     X       1390.16 , 1332.82 , 1280.02 , 1279.12 , 1237.79 , 1208.80 ,
     X       1189.76 /
      DATA  (DHLVST(I),I=1,18) / 0., 1., 7., 0.,
     X       180. , 360. , 534.6 , 540. , 720. , 900. , 1080. ,
     X       652.14 , 665.96 , 679.61 , 679.89 , 700.89 , 733.19 , 777.22
     X         /
      END
```

TWO-DIMENSIONAL STEADY-STATE MODEL

```
C   MAIN PROGRAM DOES REACTOR CALCULATIONS FOR LIQUID REGIONS
C ***********************************************************************
C
C
C  DESCRIPTION OF INPUT DATA PUNCH CARDS FOLLOWS ....
C
C                                                                    FORMAT
C  CARD 1      COL'S  1-3   CONTAIN NCASE    (ONLY ONE CARD 1 PER RUN)   (I3)
C
C                                          (CARDS 2 THRU  21   SHOULD
C                                           BE REPEATED FOR EACH CASE)
C
C  CARD 2      COL'S  1-80  TITLE CARD ... ANY ALPHANUMERIC            (14A6)
C                                          INFORMATION DESIRED
C
C  CARD 3      COL'S  1-3   CONTAIN NRINGS ........................... (I3)
C              COL'S  4-6   CONTAIN NOFZ ............................. (I3)
C
C  CARD 4      COL'S  1-8   CONTAIN F(1) ............................. (E8.4)
C                     9-16          F(2) ............................. (E8.4)
C                    17-24          F(3) ............................. (E8.4)
C                    25-32          F(4) ............................. (E8.4)
C                    33-40          F(5) ............................. (E8.4)
C                    41-48          F(6) ............................. (E8.4)
C                    49-56          F(7) ............................. (E8.4)
C                    57-64          F(8) ............................. (E8.4)
C                    65-72          F(9) ............................. (E8.4)
C                    72-80          F(10) ............................ (E8.4)
C               ( WHERE THE SUBSCRIPT INDICATES THE RING NUMBER )
C
C  CARD 5   ... CONTAINS G0'S ... FORMAT EXACTLY AS IN CARD 4
C
C  CARD 6   ... CONTAINS Z0'S ... FORMAT EXACTLY AS IN CARD 5
C
C  CARD 7      COL'S  1-10   CONTAIN ALPHA3 .......................... (E10.5)
C                    11-20          HF ............................... (E10.5)
C                    21-30          R ................................ (E10.5)
C                    31-40          MN2H4 ............................ (E10.5)
C                    41-50          MNH3 ............................. (E10.5)
C                    51-60          MN2 .............................. (E10.5)
C                    61-70          MH2 .............................. (E10.5)
C                    71-80          ALPHA1 ........................... (E10.5)
C
C  CARD 8      COL'S  1-10   CONTAIN ALPHA2 .......................... (E10.5)
C                    11-20          AGM .............................. (E10.5)
C                    21-30          BGM .............................. (E10.5)
C                    31-40          KP ............................... (E10.5)
C                    41-50          TF ............................... (E10.5)
C                    51-60          CF ............................... (E10.5)
C                    61-70          NMAX1 ............................ (E10.5)
C                    71-80          NMAX2 ............................ (E10.5)
C
C
C  CARD 9      COL'S  1-10   CONTAIN P ............................... (E10.5)
C                    11-20          ZEND ............................. (E10.5)
C                    21-30          DON2H4 ........................... (E10.5)
C                    31-40          DONH3 ............................ (E10.5)
```

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```
C                          41-50            COM ................................ (E10.5)
C                          51-60            RADIUS ............................. (E10.5)
C
C                    (THE TABLE FOR CALALYST PARTICLE RADIUS
C                      VS AXIAL POSITION AND RADIAL POSITION FOLLOWS)
C
C   CARD 10       COL'S  1-8      CONTAIN THE NUMBER  0.  ................... (E8.4)
C                        9-16     CONTAIN THE NUMBER  1.  ................... (E8.4)
C                        17-24    CONTAIN NOFZ (FLOATING PT.) ............... (E8.4)
C                        25-32    CONTAIN NRINGS (FLOATING PT.) ............. (E8.4)
C                                 (THESE NUMBERS ARE THE TABLE DESCRIPTORS
C                                 FOR THE INTERPOLATION TABLE USED TO OBTAIN
C                                 THE CAT. PARTICLE RADIUS AS A FUNCTION OF
C                                 AXIAL DISTANCE AND RADIAL DISTANCE ****
C
C   CARDS 11A,11B,...             CONTAIN THE AXIAL STATION Z VALUES
C                                 Z(1),Z(2),...,Z(NOFZ)
C                                 10 PER CARD, COL'S 1-80 ................. (10E8.4)
C
C   CARDS 12A,12B,...             CONTAIN THE RADIAL STATION RAD VALUES
C                                 RAD(1),RAD(2),....,RAD(NRINGS)
C                                 10 PER CARD, COL'S 1-80 ................. (10E8.4)
C
C   CARDS 13A,13B,...             CONTAIN THE CATALYST PARTICLE RADII AS FUNCTIONS
C                                 OF AXIAL AND RADIAL POSITION WITHIN THE REACTOR
C                                 A(1,1),A(1,2),....,A(1,NRINGS)
C                                 A(2,1),A(2,2),....,A(2,NRINGS)
C                                     .        .       .       .
C                                     .        .       .       .
C                                     .        .       .       .
C                                 A(NOFZ,1),A(NOFZ,2),....,A(NOFZ,NRINGS)
C                                 10 PER CARD, COL'S 1-80 ................. (10E8.4)
C
C                    (THE TABLE FOR CATALYST PARTICLE SURFACE AREA
C                      VS AXIAL DISTANCE AND RADIAL DISTANCE FOLLOWS)
C                              TABLE IS IDENTICAL TO THAT FOR PARTICLE RADIUS VS
C                              AXIAL AND RADIAL POSITION EXCEPT THAT THE RADII
C                              ARE REPLACED BY PARTICLE SURFACE AREAS
C
C   CARD 14                    THIS CARD IS IDENTICAL TO CARD 10
C
C   CARDS 15A,15B,....         THESE CARDS ARE IDENTICAL TO CARDS 11A,11B,...
C
C   CARDS 16A,16B,....         THESE CARDS ARE IDENTICAL TO CARDS 12A,12B,...
C
C   CARDS 1"  17B,...          CONTAIN THE CATALYST PARTICLE SURFACE AREAS (AP) AS A
C                              FUNCTION OF AXIAL AND RADIAL POSITION WITHIN THE
C                              REACTOR ... SAME FORMAT AS CARDS 13A,13B,...
C
C
C
C                    (THE TABLE FOR INTERPARTICLE VOID FRACTION OF CATALYST
C                     PARTICLES VS AXIAL AND RADIAL POSITION FOLLOWS)
C                              TABLE IS IDENTICAL TO THAT FOR PARTICLE RADIUS VS
C                              AXIAL AND RADIAL POSITION EXCEPT THAT THE RADII
C                              ARE REPLACED BY INTERPARTICLE VOID FRACTIONS
C
C   CARD 18                    THIS CARD IS IDENTICAL TO CARD 10
C
C   CARDS 19A,19B,...          THESE CARDS ARE IDENTICAL TO CARDS 11A,11B,...
C
```

```
C  CARDS 20A,20B,...      THESE CARDS ARE IDENTICAL TO CARDS 12A,12B,...
C
C  CARDS 21A,21B,...      CONTAIN THE INTERPARTICLE VOID FRACTION (DELTA) AS A
C                         FUNCTION OF AXIAL AND RADIAL POSITION WITHIN THE
C                         REACTOR ... SAME FORMAT AS CARDS 13A,13B,...
C
C
C ***********************************************************************
      REAL   MH2,MN2,MNH3,MN2H4,NMAX1,NMAX2,K,KP
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZ0(25),G0(25),Z0(25)
      COMMON /BLOK2/A,AP,DELTA,DR,DFA,DON2H4,DONH3,R,CGM,RADIUS,NMAX1,
     X          NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS
      COMMON /BVTBLS/AVSZ(234),APVSZ(234),BELVSZ(234)
      COMMON /AAA/VISVST(30),TBLVP(68)
      COMMON /CCC/H4TBL(40),H3TBL(40)
      COMMON /LIZTBL/DHVST(18),DHLVST(18)
      COMMON /DAVTBL/VPTBL(44)
      COMMON /MMM/MI
      DIMENSION ZL(25),TL(25),ZLV(25),TLV(25),JZ(25),ZZ(25,75),TT(25,75)
      DIMENSION TITLE(14)
      READ (5,702) NCASE
  702 FORMAT (I3)
      KOUNT = 1
  705 READ (5,608) TITLE
  608 FORMAT (14A6)
      WRITE (6,609) TITLE
  609 FORMAT ('1',28X,14A6//)
C     READ INPUT CONSTANTS
      READ (5,810) NRINGS,NOFZ
      READ (5,811) (F(I),I=1,NRINGS)
      READ (5,811) (G0(I),I=1,NRINGS)
      READ (5,811) (Z0(I),I=1,NRINGS)
  810 FORMAT (2I3)
  811 FORMAT (10E8.4)
C   THE SUBSCRIPT 'I' REFERS TO THE ANNULAR REGIONS
C   REGIONS ARE NUMBERED 1,2,...,NRINGS FROM THE CENTER OUTWARD
      I = 0
      READ (5,800) ALPHA3,HF,R,MN2H4,MNH3,MN2,MH2,ALPHA1,ALPHA2,AGM,BGM,
     X     KP,TF,CF,NMAX1,NMAX2,P,ZEND,DON2H4,DONH3,CGM,RADIUS
  800 FORMAT (8E10.5)
      WRITE (6,36) (J,F(J),G0(J),Z0(J),J=1,NRINGS)
   36 FORMAT (////61X,'PROGRAM INPUT' /46X,'RING',11X,'F',11X,'G0',10X,'
     XZ0' /(47X,I2,5X,3E12.5))
      WRITE (6,37) ALPHA3,HF,R,MN2H4,MNH3,MN2,MH2,ALPHA1,ALPHA2,AGM,BGM,
     X     KP,TF,CF,NMAX1,NMAX2,P,ZEND,DON2H4,DONH3,CGM,RADIUS
   37 FORMAT (//5X,'ALPHA3 ='E10.4,3X,'HF ='E10.4,3X,'R ='E10.4,3X,'MN2H
     X4 ='E10.4,3X,'MNH3 ='E10.4,3X,'MN2 ='E10.4,3X,'MH2 ='E10.4 //
     X     3X,'ALPHA1 ='E10.4,3X,'ALPHA2 ='E10.4,3X,'AGM ='E10.4,3X,
     X     'BGM ='E10.4,3X,'KP ='E10.4,3X,'TF ='E10.4,3X,'CF ='E10.4 //
     X     5X,'NMAX1 ='E10.4,3X,'NMAX2 ='E10.4,3X,'P ='E10.4,3X,
     X     'ZEND ='E10.4,3X,'D04 ='E10.4,3X,'D03 ='E10.4,3X,'CGM ='E10.
     X4    4,3X,'RADIUS ='E10.4 /)
      NZTBL = NOFZ+NRINGS+NOFZ*NRINGS+4
      NOFZ4 = NOFZ+4
      NOFZ5 = NOFZ4+1
      NOFZ6 = NOFZ4+NRINGS
C   READ IN A,AP,DELTA AS Z TABLES (BIVARIATE)
      READ (5,40) (AVSZ(I),I=1,4)
   40 FORMAT (4E8.4)
```

```
      READ (5,41) (AVSZ(I),I=5,NOFZ4)
41    FORMAT (10E8.4)
      READ (5,41) (AVSZ(I),I=NOFZ5,NOFZ6)
      I1 = NOFZ6+1
      I2 = NOFZ6+NRINGS
      DO 42 J=1,NOFZ
      READ (5,41) (AVSZ(I),I=I1,I2)
      I1 = I2+1
      I2 = I1+NRINGS-1
42    CONTINUE
      READ (5,40) (APVSZ(I),I=1,4)
      READ (5,41) (APVSZ(I),I=5,NOFZ4)
      READ (5,41) (APVSZ(I),I=NOFZ5,NOFZ6)
      I1 = NOFZ6+1
      I2 = NOFZ6+NRINGS
      DO 43 J=1,NOFZ
      READ (5,41) (APVSZ(I),I=I1,I2)
      I1 = I2+1
      I2 = I1+NRINGS-1
43    CONTINUE
      READ (5,40) (DELVSZ(I),I=1,4)
      READ (5,41) (DELVSZ(I),I=5,NOFZ4)
      READ (5,41) (DELVSZ(I),I=NOFZ5,NOFZ6)
      I1 = NOFZ6+1
      I2 = NOFZ6+NRINGS
      DO 44 J=1,NOFZ
      READ (5,41) (DELVSZ(I),I=I1,I2)
      I1 = I2+1
      I2 = I1+NRINGS-1
44    CONTINUE
      WRITE (6,604)
604   FORMAT (///59X,13H A VS Z TABLE)
      WRITE (6,45) (AVSZ(I),I=1,4)
      WRITE (6,50)
50    FORMAT ( / )
      WRITE (6,46) (AVSZ(I),I=5,NOFZ4)
      WRITE (6,50)
      WRITE (6,46) (AVSZ(I),I=NOFZ5,NOFZ6)
      WRITE (6,50)
45    FORMAT (39X,4E13.5)
46    FORMAT (10E13.5)
      I1 = NOFZ6+1
      I2 = NOFZ6+NRINGS
      DO 47 J=1,NOFZ
      WRITE (6,46) (AVSZ(I),I=I1,I2)
      I1 = I2+1
      I2 = I1+NRINGS-1
47    CONTINUE
      WRITE (6,606)
606   FORMAT (///59X,13HAP VS Z TABLE)
      WRITE (6,45) (APVSZ(I),I=1,4)
      WRITE (6,50)
      WRITE (6,46) (APVSZ(I),I=5,NOFZ4)
      WRITE (6,50)
      WRITE (6,46) (APVSZ(I),I=NOFZ5,NOFZ6)
      WRITE (6,50)
      I1 = NOFZ6+1
      I2 = NOFZ6+NRINGS
      DO 48 J=1,NOFZ
      WRITE (6,46) (APVSZ(I),I=I1,I2)
```

```
      I1 = I2+1
      I2 = I1+NRINGS-1
 48   CONTINUE
      WRITE (6,607)
 607  FORMAT (///57X,17H DELTA VS Z TABLE)
      WRITE (6,45) (DELVSZ(I),I=1,4)
      WRITE (6,50)
      WRITE (6,46) (DELVSZ(I),I=5,NOFZ4)
      WRITE (6,50)
      WRITE (6,46) (DELVSZ(I),I=NOFZ5,NOFZ6)
      WRITE (6,50)
      I1 = NOFZ6+1
      I2 = NOFZ6+NRINGS
      DO 49 J=1,NOFZ
      WRITE (6,46) (DELVSZ(I),I=I1,I2)
      I1 = I2+1
      I2 = I1+NRINGS-1
 49   CONTINUE
      WRITE (6,27)
 27   FORMAT ('1',22X,'POSITIONS AND TEMPERATURES AT EACH AXIAL STATION
     X ---  LIQUID AND LIQUID-VAPOR REGIONS')
      DR = RADIUS/FLOAT(NRINGS)
C     OBTAIN MIDPOINTS OF ANNULAR RINGS
      RAD(1) = DR/2.
      DO 101 J=2,NRINGS
      RAD(J) = RAD(J-1)+DR
 101  CONTINUE
      CALL UNBAR (VPTBL,1,P,0.,TVAP,KK)
      CALL UNBAR (DHVST,1,TVAP,0.,DELHV,KK)
      CALL UNBAR (DHLVST,1,TVAP,0.,DELHL,KK)
      HL = (TVAP-TF)*CF
      HV = HL+DELHV-DELHL
 875  I = I+1
      LIQVP = 0
      J = 0
      Z = 0.
      DZ = 0.
      DERIV = 0.
      H(I) = HF
      GATZ0(I) = G0(I)+F(I)*Z0(I)
 879  Z = Z+DZ
      J = J+1
C     STORE CURRENT Z IN OUTPUT BLOCK
      ZZ(I,J) = Z
C     CHECK IF WE HAVE REACHED THE END OF THE INJECTOR FOR THIS RING
      IF (Z-Z0(I)) 34,34,35
 34   G = G0(I)+F(I)*Z
      GO TO 78
 35   G = GATZ0(I)
      F(I) = 0.
 78   T = TF+(H(I)-HF)/CF
C     STORE CURRENT TEMP IN OUTPUT BLOCK
      TT(I,J) = T
C     CHECK IF WE HAVE REACHED LIQUID-LIQUID VAPOR INTERFACE
      IF (LIQVP.EQ.1) GO TO 102
      CALL UNBAR (TBLVP,1,T,0.,VPR,KK)
      CALL UNBAR (H4TBL,1,T,0.,H4,KK)
      CALL UNBAR (AVSZ,1,Z,RAD(I),A,KK)
      CALL UNBAR (APVSZ,1,Z,RAD(I),AP,KK)
      C4 = VPR*MN2H4/(R*T)
```

```
      GAMMA = AGM/T
      K = ALPHA1*EXP(-GAMMA)
      DPA = DON2H4*(T/492.)**1.832*14.7/P*(1.-EXP(-.067*P*492./
     X      (14.7*T)))
      BETA = -C4*H4*DPA/(KP*T)
      DERIVO = DERIV
      CALL SLOPE (DERIV)
      IF (MI.GT.20) DERIV=DERIVO
      DHDZ = -(H4*DPA*AP*DERIV+F(I)*(H(I)-HF))/G
      DZ = -H4/(NMAX1*DHDZ)
      H(I) = H(I)+DHDZ*DZ
      IF (H(I)-HL) 879,877,878
C   WE HAVE EXCEEDED LIQUID-LIQUID VAPOR INTERFACE FOR THIS RING ---
C   BACKSTEP TO L-LV BOUNDARY
 878  DZ = (HL-H(I))/DHDZ
      H(I) = HL
C   SET FLAG TO INDICATE INTERFACE HAS BEEN REACHED
 877  LIQVP = 1
      GO TO 879
C   WE HAVE REACHED THE LIQUID-LIQUID VAPOR INTERFACE FOR THIS RING
 102  TL(I) = T
      ZL(I) = Z
      CALL LQVP (I,J,DERIV,T,Q,Z,ZZ,TT,DZ)
      TLV(I) = T
      ZLV(I) = Z
      JZ(I) = J
C   CHECK IF ALL RINGS HAVE BEEN PROCESSED
      IF (I-NRINGS) 675,870,870
 870  DO 25 I=1,NRINGS
      JN = JZ(I)
      WRITE (6,28) I
      WRITE (6,26) (ZZ(I,J),TT(I,J),J=1,JN)
 25   CONTINUE
 26   FORMAT (9X,'Z',12X,'T',4(12X,'Z',12X,'T') / (1X,10E13.5) )
 28   FORMAT (//65X,'RING',I3)
      WRITE (6,613)
 613  FORMAT (1H1,27X,75H*************************         LIQUID REGION
     X   ************************* )
      LAST = NRINGS-1
C   IF THERE IS LESS THAN A ONE PERCENT DIFFERENCE IN INTERFACE Z VALUES
C   FOR ANY TWO RINGS , THEN SET THESE INTERFACE VALUES EQUAL
      DO 700 I=1,LAST
      IF (ABS(ZL(I)-ZL(I+1)).LT..01*ZL(I)) ZL(I+1)=ZL(I)
      IF (ABS(ZLV(I)-ZLV(I+1)).LT..01*ZLV(I)) ZLV(I+1)=ZLV(I)
 700  CONTINUE
      WRITE (6,88) (I,ZL(I),RAD(I),TL(I),I=1,NRINGS)
 88   FORMAT (//23X,'POSITION AND TEMPERATURE AT LIQUID - LIQUID VAPOR I
     XNTERFACE FOR EACH ANNULAR REGION' /
     X      36X,57H RING       AXIAL POSITION   RADIAL POSITION   TEMPERA
     XTURE  /
     X      (38X,I2,6X,E12.5,6X,E12.5,4X,E12.5) )
      WRITE (6,90)
 90   FORMAT (////27X,75H**********************         LIQUID-VAPOR REGION
     X      ********************** )
      WRITE (6,89) (I,ZLV(I),RAD(I),TLV(I),I=1,NRINGS)
 89   FORMAT (//24X,'POSITION AND TEMPERATURE AT LIQUID VAPOR - VAPOR IN
     XTERFACE FOR EACH ANNULAR REGION' /
     X      36X,57H RING       AXIAL POSITION   RADIAL POSITION   TEMPERA
     XTURE  /
     X      (38X,I2,6X,E12.5,6X,E12.5,4X,E12.5) )
```

```
C     PROCEED ON TO VAPOR REGION
      CALL VAPOR (ALPHA3,ZLV,TLV)
      KOUNT = KOUNT+1
      IF (KOUNT.LE.NCASE) GO TO 705
      WRITE (6,107)
  107 FORMAT (////48X,35H******  OPERATIONS COMPLETE  ****** )
      STOP
      END


      SUBROUTINE LGVP (I,J,DERIV,T,G,Z,ZZ,TT,DZ)
C     THIS ROUTINE HANDLES REACTOR CALCULATIONS FOR LIQUID VAPOR REGIONS
C     OF EACH ANNULAR RING
      REAL  NMAX2
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZ0(25),G0(25),Z0(25)
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,DON2H4,DONH3,R,CGM,RADIUS,NMAX1,
     X          NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS
      COMMON /BVTBLS/AVSZ(234),APVSZ(234),DELVSZ(234)
      COMMON /CCC/H4TBL(40),H3TBL(40)
      DIMENSION ZZ(25,75),TT(25,75)
C     ASSUME TEMPERATURE CONSTANT IN LIQUID VAPOR REGION
      CALL UNBAR (H4TBL,1,T,0.,H4,KK)
  182 CALL UNBAR (APVSZ,1,Z,RAD(I),AP,KK)
      DPA = DON2H4*(T/492.)**1.832*14.7/P*(1.-EXP(-.067*P*492./
     X       (14.7*T)))
      DHDZ = -(H4*DPA*AP*DERIV+F(I)*(H(I)-HF))/G
      DZ = -H4/(NMAX2*DHDZ)
      Z = Z+DZ
      J = J+1
C     STORE CURRENT Z IN OUTPUT BLOCK
      ZZ(I,J) = Z
      TT(I,J) = T
C     CHECK IF WE HAVE REACHED THE INJECTOR TIP FOR THIS RING
      IF (Z-Z0(I)) 34,34,35
   34 G = G0(I)+F(I)*Z
      GO TO 78
   35 G = GATZ0(I)
      F(I) = 0.
   78 H(I) = H(I)+DHDZ*DZ
      IF (H(I)-HV) 182,195,184
C     WE HAVE EXCEEDED LIQUID VAPOR-VAPOR INTERFACE FOR THIS RING ---
C     BACKSTEP TO LV-V BOUNDARY
  184 DZ = (HV-H(I))/DHDZ
      Z = Z+DZ
      ZZ(I,J) = Z
      H(I) = HV
  195 RETURN
      END


      SUBROUTINE VAPOR (ALPHA3,ZLV,TLV)
C     THIS ROUTINE HANDLES REACTOR CALCULATIONS FOR VAPOR REGION OF EACH
C     ANNULAR RING
      REAL  LAMDA,NR1,NRR1,NR2,NRR2,NR3,NRR3,NR4,NRR4,KC4,MH2,MN2,MNH3,
     X         MN2H4,MBAR
```

```
      INTEGER VAPOR,VP
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZ0(25),G0(25),Z0(25)
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,DON2H4,DONH3,R,CGM,RADIUS,NMAX1,
     X          NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4
      COMMON /BLOK3/K,KA,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS
      COMMON /BVTBLS/AVSZ(234),APVSZ(234),DELVSZ(234)
      COMMON /AAA/VISVST(30),TBLVP(68)
      COMMON /CCC/H4TBL(40),H3TBL(40)
      COMMON /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)
      DIMENSION  HH4(25),XV(25),TLV(25),CI1(25),CI2(25),CI3(25),CI4(25),
     X           RHO(25),RHOM(25),T(25),ZLV(25),ZVO(25),IFN(25),MIX(10),
     X           G(25),ZZ(25),F1(25),F2(25),F3(25),F4(25),F3D(25)
      DIMENSION  TT(25),C1(25),C2(25),C3(25),C5(25),GR(25),TGR(25),
     X           CK4(25),DPDZ(25),Z00(25),NZ0(25)
      VAPOR = 0
      IFFLG = 0
      VP = VAPOR+1
      M = 2
      N = 1
      NM1 = NRINGS-1
      WRITE (6,598)
  598 FORMAT ('1',29X,'*************************     VAPOR REGION     **
     X************************ ')
C     CALCULATE CONCENTRATIONS AT INTERFACES FOR EACH RING
      DO 37 I=1,NRINGS
      CALL UNBAR (H4TBL,1,TLV(I),0.,HH4(I),KK)
      XV(I) = (HF-H(I))/HH4(I)
      X1 = (1.-XV(I))/(1.+XV(I))
      X2 = XV(I)/(1.+XV(I))
      PRT = P/(R*TLV(I))
      CI1(I) = .5*PRT*MH2*X2
      CI2(I) = .5*PRT*MN2*X2
      CI3(I) = PRT*MNH3*X2
      CI4(I) = PRT*MN2H4*X1
      RHO(I) = CI1(I)+CI2(I)+CI3(I)+CI4(I)
      RHOM(I) = ALPHA3*CI4(I)*EXP(-CGM/TLV(I))
      T(I) = TLV(I)
C     SET INITIAL VAPOR REGION VALUES FOR G
      IF (ZLV(I)-Z0(I)) 590,590,591
  590 G(I) = G0(I)+F(I)*ZLV(I)
      GO TO 37
  591 G(I) = GATZ0(I)
      F(I) = 0.
   37 CONTINUE
      WRITE (6,38) CI4(1),CI3(1),CI2(1),CI1(1)
   38 FORMAT (//43X,'CONCENTRATIONS AT LIQUID VAPOR - VAPOR INTERFACE'/
     X       47X,'N2H4          NH3          N2          H2'/41X,4E12.5 )
      SUM = CI1(1)/MH2+CI2(1)/MN2+CI3(1)/MNH3+CI4(1)/MN2H4
      FRAC1 = CI1(1)/(MH2*SUM)
      FRAC2 = CI2(1)/(MN2*SUM)
      FRAC3 = CI3(1)/(MNH3*SUM)
      FRAC4 = CI4(1)/(MN2H4*SUM)
      FRAC3D = (FRAC1/FRAC2-1.)/(3.-FRAC1/FRAC2)
      WRITE (6,39) FRAC1,FRAC2,FRAC3,FRAC4,FRAC3D
   39 FORMAT (///40X,'MFRAC1', 6X,'MFRAC2' 6X,'MFRAC3' 6X,'MFRAC4' 6X,
     X       'FRAC3D' / 35X,5E12.5 )
      DPBDZ = 0.
C     SUBROUTINE ORDER STORES INTERFACE AXIAL STATIONS IN ASCENDING ORDER
      CALL ORDER (ZLV,ZVO)
      Z = ZVO(1)
```

```
C     GET Z0'S STORED IN ASCENDING ORDER
      CALL ORDER (Z0,Z00)
C     SET N (Z0 INDICATOR) TO IGNORE INJECTOR TIPS IF LESS THAN SMALLEST ZVAP
      IF (Z00(NRINGS).LT.ZVO(1)) N=NRINGS+1
C     FIND AND LABEL ALL DISTINCT INTERFACES
      J = 1
      IFACE = 1
      IFN(1) = 1
      DO 74 I=2,NRINGS
      IF (ZVO(J)-ZVO(I)) 72,73,72
   73 J = I
      GO TO 74
   72 J = I
C     IFACE = TOTAL NUMBER OF DISTINCT INTERFACES
      IFACE = IFACE+1
      IFN(IFACE) = J
   74 CONTINUE
C     FIND AND LABEL ALL DISTINCT Z0'S
      J = 1
      NOZ0 = 1
      NZ0(1) = 1
      DO 227 I=2,NRINGS
      IF (Z00(J)-Z00(I)) 228,229,228
  229 J = I
      GO TO 227
  228 J = I
C     NOZ0 = TOTAL NUMBER OF DISTINCT Z0'S
      NOZ0 = NOZ0+1
      NZ0(NOZ0) = J
  227 CONTINUE
C     IF INTERFACE AXIAL POSITIONS FOR ALL RINGS ARE IDENTICAL (IFACE=1),
C     THEN SET VAPOR=1 TO INDICATE ENTRANCE INTO ALL-VAPOR REGION
   78 IF (IFACE-1) 23,22,23
   22 VAPOR = 1
      VP = VP+1
      CALL DELTAZ (CI1,CI2,CI3,CI4,T,G,RHO,RHOM,CK4,GR,TGR,Z,DZ)
      GO TO 8
C     USE CONSTANT DZ VALUE FOR INITIAL PORTIONS OF VAPOR REGION
   23 DZZ = (ZVO(NRINGS)-ZVO(1))/25.
      DZ = DZZ
    8 ZP = Z
      IF (VAPOR.EQ.1) GO TO 15
      IF (IFFLG-1) 40,42,40
   40 IF (DZ.LT.DZZ) DZ=DZZ
      GO TO 15
   42 DZ = DELZ
      IFFLG = 0
   15 Z = Z+DZ
C     TEST IF WE HAVE REACHED THE END OF THE REACTOR
      IF (Z-ZEND) 43,43,44
   44 Z = ZEND
      DZ = ZEND-ZP
C     TEST IF ALL INTERFACES HAVE BEEN ENCOUNTERED
   43 IF (VAPOR-1) 28,33,28
C     STILL WITHIN REGION OF VARIOUS ANNULAR INTERFACES --- NOW MUST TEST
C     FOR CURRENT Z EXCEEDING NEXT INTERFACE POSITION
   28 MM = IFN(M)
      IF (Z-ZVO(MM)) 30,30,31
C     WE HAVE EXCEEDED NEXT LARGEST INTERFACE Z VALUE --- BACKSTEP TO
C     INTERFACE AND ADJUST DZ FOR NEXT PASS
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```
 31   DELZ = Z-ZVO(MM)
      DZ = ZVO(MM)-ZP
      Z = ZVO(MM)
      IFFLG = 1
      M = M+1
C   WAS ZVO(MM) THE LAST INTERFACE
C       YES --- ALL RINGS ARE VAPOR FROM NOW ON SO SET VAPOR=1
C       NO --- PROCEED
      IF (M-IFACE) 30,30,32
 32   VAPOR = 1
C   SET UP MIXING TERM INDICATOR FOR EACH RING AT THIS AXIAL STATION
 30   DO 10 J=1,NRINGS
C   MIX IS STATUS INDICATOR FOR RING J
C   MIX = 1  ... NO RADIAL MIXING
C   MIX = 2  ... INNER ADJACENT RADIAL MIXING
C   MIX = 3  ... OUTER ADJACENT RADIAL MIXING
C   MIX = 4  ... BOTH INNER & OUTER ADJACENT RADIAL MIXING
      MIX(J) = 1
C   TEST IF WE ARE IN FIRST OR LAST RING
      IF (J-1) 1,11,1
 1    IF (J-NRINGS) 2,12,2
C   IF Z<ZVAP FOR THIS RING THEN WE ARE STILL IN LIQUID AREA
 2    IF (Z-ZLV(J)) 10,10,16
 16   IF (Z-ZLV(J-1)) 3,3,4
 4    MIX(J) = 2
 3    IF (Z-ZLV(J+1)) 10,10,5
 5    IF (MIX(J)-2) 6,7,6
 6    MIX(J) = 3
      GO TO 10
 7    MIX(J) = 4
      GO TO 10
C   FIRST AND LAST RINGS ARE SPECIAL CASES
 11   IF (Z-ZLV(2)) 10,10,13
 13   MIX(J) = 3
      GO TO 10
 12   IF (Z-ZLV(NRINGS-1)) 10,10,14
 14   MIX(J) = 2
 10   CONTINUE
 33   IF (N.GT.NOZ0) GO TO 225
      NN = NZ0(N)
C   IF SMALLEST CURRENT Z0 IS ZERO MOVE ON TO PROGRAM CALC'S
      IF (Z00(NN)) 225,225,230
C   TEST IF CURRENT Z EXCEEDS SMALLEST REMAINING Z0
C   YES --- BACKSTEP TO INJECTOR TIP
 230  IF (Z-Z00(NN)) 225,225,226
 226  DZ = Z-Z00(NN)
      Z = Z00(NN)
      N = N+1
C   SET UP CALCULATIONS FOR TEMP AND CONCENTRATION
 225  DO 20 J=1,NRINGS
C   TEST IF WE ARE PRECISELY AT LAST INTERFACE
      IF (Z-ZVO(NRINGS)) 41,41,77
C         YES --- NOT YET IN ALL-VAPOR REGION
C         NO  --- VP INDICATOR HANDLES CASES WHERE Z IS GREATER
 77   GO TO (27,29,27), VP
C   WE ARE IN THE ALL-VAPOR REGION OF THE REACTOR --- MIX PARAMETER NOW
C   FIXED FOR ALL RINGS
 29   MIX(1) = 3
      MIX(NRINGS) = 2
      DO 9 I=2,NM1
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      MIX(I) = 4
 9    CONTINUE
C   INCREMENT VP TO AVOID REDUNDANT SETTINGS OF 'MIX'
      VP = VP+1
      GO TO 27
C   COMPARE CURRENT Z WITH INTERFACE Z FOR THIS RING
C          Z<ZVAP --- MOVE ON TO NEXT RING
C          Z>ZVAP --- CONTINUE ON WITH CALCULATIONS
 41   IF (Z-ZLV(J)) 96,96,27
C   SET UP PRELIMINARY CALCULATIONS FOR DWDZ TERMS
 27   CALL UNBAR (AVSZ,1,ZP,RAD(J),A,KK)
      CALL UNBAR (APVSZ,1,ZP,RAD(J),AP,KK)
      CALL UNBAR (DELVSZ,1,ZP,RAD(J),DELTA,KK)
      CALL UNBAR (H4TBL,1,T(J),0.,H4,KK)
      CALL UNBAR (CFTBL4,1,T(J),0.,CF4,KK)
      CALL UNBAR (CFTBL3,1,T(J),0.,CF3,KK)
      CALL UNBAR (CFTBL2,1,T(J),0.,CF2,KK)
      CALL UNBAR (CFTBL1,1,T(J),0.,CF1,KK)
C   TEST IF Z HAS EXCEEDED INJECTOR TIP FOR THIS RING
      IF (Z-Z0(J)) 34,34,35
 34   G(J) = G0(J)+F(J)*ZP
      GO TO 63
 35   G(J) = GATZ0(J)
      F(J) = 0.
 63   CFBAR = (CF1*CI1(J)+CF2*CI2(J)+CF3*CI3(J)+CF4*CI4(J))/(CI1(J)+
     X        CI2(J)+CI3(J)+CI4(J))
      RHOM(J) = ALPHA3*CI4(J)*EXP(-CGM/T(J))
      EPSLN = -A*G(J)/(5.*RHO(J)*DELTA)
      LAMDA = -A*CFBAR*G(J)/(5.*DELTA)
      MX = MIX(J)
      GO TO (56,57,58,59), MX
C   STATEMENT 56 --- NO MIXING TERMS USED
 56   NR1 = 0.
      NR2 = 0.
      NR3 = 0.
      NR4 = 0.
      QR1 = 0.
      QRN = 0.
      NRR1 = 0.
      NRR2 = 0.
      NRR3 = 0.
      NRR4 = 0.
      QRR1 = 0.
      GO TO 60
C   STATEMENT 57 --- INWARD MIXING ONLY
 57   NR1 = EPSLN*(CI1(J)-CI1P)/DR
      NR2 = EPSLN*(CI2(J)-CI2P)/DR
      NR3 = EPSLN*(CI3(J)-CI3P)/DR
      NR4 = EPSLN*(CI4(J)-CI4P)/DR
      QR1 = LAMDA*(T(J)-TP)/DR
      QRN = (NR1*CF1+NR2*CF2+NR3*CF3+NR4*CF4)*(T(J)-TP)/DR
      NRR1 = 0.
      NRR2 = 0.
      NRR3 = 0.
      NRR4 = 0.
      QRR1 = 0.
      GO TO 60
C   STATEMENT 58 --- OUTWARD MIXING ONLY
 58   NR1 = 0.
      NR2 = 0.
```

```
      NR3 = 0.
      NR4 = 0.
      QR1 = 0.
      QRN = 0.
  220 NRR1 = EPSLN*(CI1(J+1)-CI1(J))/DR
      NRR2 = EPSLN*(CI2(J+1)-CI2(J))/DR
      NRR3 = EPSLN*(CI3(J+1)-CI3(J))/DR
      NRR4 = EPSLN*(CI4(J+1)-CI4(J))/DR
      QRR1 = LAMDA*(T(J+1)-T(J))/DR
      GO TO 60
C     STATEMENT 59 --- BOTH INWARD AND OUTWARD MIXING
   59 NR1 = EPSLN*(CI1(J)-CI1P)/DR
      NR2 = EPSLN*(CI2(J)-CI2P)/DR
      NR3 = EPSLN*(CI3(J)-CI3P)/DR
      NR4 = EPSLN*(CI4(J)-CI4P)/DR
      QR1 = LAMDA*(T(J)-TP)/DR
      QRN = (NR1*CF1+NR2*CF2+NR3*CF3+NR4*CF4)*(T(J)-TP)/DR
  223 NRR1 = EPSLN*(CI1(J+1)-CI1(J))/DR
      NRR2 = EPSLN*(CI2(J+1)-CI2(J))/DR
      NRR3 = EPSLN*(CI3(J+1)-CI3(J))/DR
      NRR4 = EPSLN*(CI4(J+1)-CI4(J))/DR
      QRR1 = LAMDA*(T(J+1)-T(J))/DR
C     CHECK IF WE ARE IN ALL-VAPOR REGION
   60 IF (Z-ZVO(NRINGS)) 61,61,62
C       YES --- SKIP CALL TO SUBROUTINE SGRAD (THIS WAS DONE IN DELTAZ)
C       NO --- CONTINUE AS BEFORE
   61 CALL SGRAD (CI1(J),CI2(J),CI3(J),CI4(J),G(J),T(J),GRAD,TGRAD,J)
      GO TO 64
   62 GRAD = GR(J)
      TGRAD = TGR(J)
      KC4 = CK4(J)
   64 W1 = CI1(J)/RHO(J)
      W2 = CI2(J)/RHO(J)
      W3 = CI3(J)/RHO(J)
      W4 = CI4(J)/RHO(J)
      DW1DZ = (.5*MH2/MN2H4*(RHOM(J)*DELTA+AP*KC4*CI4(J))+1.5*AP*GRAD*
     X       MH2/MNH3+(NR1-NRR1)*DELTA/DR-NRR1*DELTA/RAD(J)-F(J)*W1)/
     X       G(J)
      DW2DZ = (.5*MN2/MN2H4*(RHOM(J)*DELTA+AP*KC4*CI4(J))+.5*AP*GRAD*
     X       MN2/MNH3+(NR2-NRR2)*DELTA/DR-NRR2*DELTA/RAD(J)-F(J)*W2)/
     X       G(J)
      DW3DZ = (MNH3/MN2H4*(RHOM(J)*DELTA+AP*KC4*CI4(J))-AP*GRAD+(NR3-
     X       NRR3)*DELTA/DR-NRR3*DELTA/RAD(J)-F(J)*W3)/G(J)
      DW4DZ = (F(J)-RHOM(J)*DELTA-AP*KC4*CI4(J)+(NR4-NRR4)*DELTA/DR-
     X       NRR4*DELTA/RAD(J)-F(J)*W4)/G(J)
C     READY PROGRAM FOR TEMP,CONCENTRATION CALCULATIONS
      MBAR = (CI1(J)+CI2(J)+CI3(J)+CI4(J))/(CI1(J)/MH2+CI2(J)/MN2+
     X     CI3(J)/MNH3+CI4(J)/MN2H4)
      WMSM = W1/MH2+W2/MN2+W3/MNH3+W4/MN2H4
      DMDZ = -MBAR/WMSM*(DW1DZ/MH2+DW2DZ/MN2+DW3DZ/MNH3+DW4DZ/MN2H4)
      DHDZ = -(F(J)*(H(J)-HF)+AP*TGRAD+DELTA*(H4*RHOM(J)-(QR1-QRR1)/DR)+
     X     QRR1*DELTA/RAD(J)+QRN*DELTA)/G(J)
      DTDZ = DHDZ/CFBAR
      DRODZ = RHO(J)*(DMDZ/MBAR-DTDZ/T(J)+DPBDZ/(144.*P))
      DC1DZ = RHO(J)*DW1DZ+W1*DRODZ
      DC2DZ = RHO(J)*DW2DZ+W2*DRODZ
      DC3DZ = RHO(J)*DW3DZ+W3*DRODZ
      DC4DZ = RHO(J)*DW4DZ+W4*DRODZ
C     STORE TEMP,CONCENTRATIONS FOR INWARD RADIAL MIX CALCS IN NEXT RING
      CI1P = CI1(J)
```

```
      CI2P = CI2(J)
      CI3P = CI3(J)
      CI4P = CI4(J)
      TP = T(J)
      CI1(J) = CI1(J)+DC1DZ*DZ
      CI2(J) = CI2(•)+DC2DZ*DZ
      CI3(J) = CI3(J)+DC3DZ*DZ
      CI4(J) = CI4(J)+DC4DZ*DZ
      IF (CI1(J).LT.0.) CI1(J)=0.
      IF (CI2(J).LT.0.) CI2(J)=0.
      IF (CI3(J).LT.0.) CI3(J)=0.
      IF (CI4(J).LT.0.) CI4(J)=0.
      T(J) = T(J)+DTDZ*DZ
      IF (T(J).LT.0.) GO TO 98
      H(J) = H(J)+DHDZ*DZ
C   STORE Z,TEMP,AND CONCENTRATIONS IN OUTPUT BLOCK
      ZZ(J) = Z
      TT(J) = T(J)
      C1(J) = CI1(J)
      C2(J) = CI2(J)
      C3(J) = CI3(J)
      C5(J) = CI4(J)
      SUM = CI1(J)/MH2+CI2(J)/MN2+CI3(J)/MNH3+CI4(J)/MN2H4
      IF (CI4(J).LT.0.) SUM=SUM-CI4(J)/MN2H4
      IF (CI3(J).LT.0.) SUM=SUM-CI3(J)/MNH3
      FRAC1 = CI1(J)/(MH2*SUM)
      FRAC2 = CI2(J)/(MN2*SUM)
      FRAC3 = CI3(J)/(MNH3*SUM)
      FRAC4 = CI4(J)/(MN2H4*SUM)
      FRAC3D = (FRAC1/FRAC2-1.)/(3.-FRAC1/FRAC2)
      F1(J) = FRAC1
      F2(J) = FRAC2
      F3(J) = FRAC3
      F4(J) = FRAC4
      F3D(J) = FRAC3D
      GO TO 20
C   NO FURTHER CALCULATIONS FOLLOW FOR THIS RING --- ZERO OUT OUTPUT BLOCK
C   AND MOVE ON TO NEXT RING
 96   ZZ(J) = 0.
      TT(J) = 0.
      C1(J) = 0.
      C2(J) = 0.
      C3(J) = 0.
      C5(J) = 0.
      F1(J) = 0.
      F2(J) = 0.
      F3(J) = 0.
      F4(J) = 0.
      F3D(J) = 0.
 20   CONTINUE
      P = P+DPBDZ*DZ/144.
      IF (P.LT.0.) GO TO 94
C   CALCULATE DPDZ FOR PRESSURE CHANGES IN EACH RING
      SUMP = 0.
      DO 75 J=1,NRINGS
      CALL UNBAR (VISVST,1,T(J),0.,VIS,KK)
      CALL UNBAR (AVSZ,1,Z,RAD(J),A,KK)
      CALL UNBAR (DELVSZ,1,Z,RAD(J),DELTA,KK)
      RHO(J) = CI1(J)+CI2(J)+CI3(J)+CI4(J)
      RHOM(J) = ALPHA3*CI4(J)*EXP(-CGM/T(J))
```

```
      DPDZ(J) = -(1.-DELTA)/DELTA**3*(1.75+75.*VIS*(1.-DELTA)/(A*G(J)))*
     X            G(J)**2/(64.4*A*RHO(J))
      SUMP = SUMP+DPDZ(J)*RAD(J)
   75 CONTINUE
      DPBDZ = 2.*DK*SUMP/RADIUS**2
      WRITE (6,599)
  599 FORMAT (  /// 28X,'RING',11X,'Z',10X,'TEMP',8X,'N2H4',9X,'NH3',
     A        5X,'N2',10X,'H2'    )
      WRITE (6,600) (J,ZZ(J),TT(J),C5(J),C3(J),C2(J),C1(J),J=1,NRINGS)
  600 FORMAT (29X,I2,5X,6E12.5)
      WRITE (6,97) P
   97 FORMAT (//54X,'PRESSURE =',E12.5)
      WRITE (6,36) (F1(J),F2(J),F3(J),F4(J),F3D(J),J=1,NRINGS)
   36 FORMAT (//86X,'EQUIVALENT' / 40X,'MFRAC1',6X,'MFRAC2',6X,'MFRAC3',
     X        6X,'MFRAC4',6X,'FRAC3D' / (35X,5E12.5))
      WRITE (6,606)
  606 FORMAT (//25X,'****************************************************
     X********************************')
      DO 108 J=1,NRINGS
      IF (TT(J).LT.TLV(J)) GO TO 106
  108 CONTINUE
C   CHECK IF WE HAVE REACHED THE END OF THE REACTOR
      IF (Z-ZEND) 17,99,99
C   CHECK IF WE HAVE REACHED ALL-VAPOR REGION
   17 IF (Z-ZVO(NRINGS)) 8,21,21
C   YES --- CALL DELTAZ TO CALCULATE A NEW DZ
   21 CALL DELTAZ (CI1,CI2,CI3,CI4,T,G,RHO,RHOM,CK4,GR,TGR,Z,DZ)
      VAPOR = 1
      VP = VP+1
      IF (VP.GT.3) VP=3
      GO TO 8
   94 WRITE (6,95)
   95 FORMAT (//30X,'THE PROGRAM HAS CALCULATED A NEGATIVE PRESSURE ---
     XRETURN AND TERMINATE' )
      GO TO 99
   98 WRITE (6,103) J
  103 FORMAT (//23X,'THE PROGRAM HAS CALCULATED A NEGATIVE TEMPERATURE I
     XN RING',I3,' --- RETURN AND TERMINATE' )
      GO TO 8
  106 WRITE (6,107) J
  107 FORMAT (// 7X,'THERE IS A PUDDLE OF COLD HYDRAZINE AT THE LIQUID-V
     XAPOR/VAPOR INTERFACE IN RING',I3,' --- TRY USING A LARGER VALUE FO
     XR G0')
   99 RETURN
      END
```

```
      SUBROUTINE ORDER (ZV,ZVO)
C   THIS ROUTINE PLACES THE NUMBERS OF THE FIRST ARGUMENT ARRAY IN
C   ASCENDING ORDER AND STORES THEM IN THE SECOND ARGUMENT ARRAY
      COMMON /BLOK3/K,KA,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS
      DIMENSION  ZV(100),ZVO(100)
      LAST = NRINGS-1
      DO 10 I=1,NRINGS
      ZVO(I) = ZV(I)
   10 CONTINUE
      DO 20 J=1,LAST
      DO 15 I=1,LAST
```

```
      IF (ZVO(I)-ZVO(I+1)) 15,15,4
 4    TEMP = ZVO(I)
      ZVO(I) = ZVO(I+1)
      ZVO(I+1) = TEMP
 15   CONTINUE
 20   CONTINUE
      RETURN
      END
```

```
      SUBROUTINE DELTAZ (CI1,CI2,CI3,CI4,T,G,RHO,RHOM,CK4,GR,TGR,Z,DZ)
C   THIS ROUTINE CALCULATES A SUITABLE DZ INCREMENT FOR THE ALL-VAPOR
C   PORTION OF THE REACTOR
      REAL  LAMDA,NR1,NRR1,NR2,NR3,NR4,KC4,MH2,MN2,MNH3,MN2H4
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZO(25),G0(25),Z0(25)
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,D0N2H4,D0NH3,R,CGM,RADIUS,NMAX1,
     X          NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS
      COMMON /BVTBLS/AVSZ(234),APVSZ(234),BELVSZ(234)
      COMMON /CCC/H4TBL(40),H3TBL(40)
      COMMON /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)
      DIMENSION  T(25),CI1(25),CI2(25),CI3(25),CI4(25),G(25),RHO(25),
     X           RHOM(25),DWDZ(25),DWDZ0(25),DTDZ(25),DTDZ0(25),GR(25),
     X           ,GR(25),CK4(25)
      DO 20 J=1,NRINGS
      CALL UNBAR (AVSZ,1,Z,RAD(J),A,KK)
      CALL UNBAR (APVSZ,1,Z,RAD(J),AP,KK)
      CALL UNBAR (DELVSZ,1,Z,RAD(J),DELTA,KK)
      CALL UNBAR (H4TBL,1,T(J),0.,H4,KK)
      CALL UNBAR (CFTBL4,1,T(J),0.,CF4,KK)
      CALL UNBAR (CFTBL3,1,T(J),0.,CF3,KK)
      CALL UNBAR (CFTBL2,1,T(J),0.,CF2,KK)
      CALL UNBAR (CFTBL1,1,T(J),0.,CF1,KK)
C   CHECK CURRENT Z WITH INJECTOR TIP FOR EACH RING
      IF (Z-Z0(J)) 11,12,12
 11   G(J) = G0(J)+F(J)*Z
      GO TO 13
 12   G(J) = GATZ0(J)
      F(J) = 0.
 13   CFBAR = (CF1*CI1(J)+CF2*CI2(J)+CF3*CI3(J)+CF4*CI4(J))/(CI1(J)+
     X         CI2(J)+CI3(J)+CI4(J))
      EPSLN = -A*G(J)/(5.*RHO(J)*DELTA)
      LAMDA = -A*CFBAR*G(J)/(5.*DELTA)
C   FIRST AND LAST RINGS ARE SPECIAL CASES
      IF (J-1) 1,2,1
 1    IF (J-NRINGS) 3,4,3
C   STANDARD MODE --- BOTH INWARD AND OUTWARD MIXING
 3    NR1 = EPSLN*(CI1(J)-CI1(J-1))/DR
      NR2 = EPSLN*(CI2(J)-CI2(J-1))/DR
      NR3 = EPSLN*(CI3(J)-CI3(J-1))/DR
      NR4 = EPSLN*(CI4(J)-CI4(J-1))/DR
      QR1 = LAMDA*(T(J)-T(J-1))/DR
      QRN = (NR1*CF1+NR2*CF2+NR3*CF3+NR4*CF4)*(T(J)-T(J-1))/DR
      NRR1 = EPSLN*(CI1(J+1)-CI1(J))/DR
      QRR1 = LAMDA*(T(J+1)-T(J))/DR
      GO TO 10
C   FIRST RING --- OUTWARD MIXING ONLY
 2    NR1 = 0.
```

```
      NR2 = 0.
      NR3 = 0.
      NR4 = 0.
      QR1 = 0.
      QRN = 0.
      NRR1 = EPSLN*(CI1(J+1)-CI1(J))/DR
      QRR1 = LAMDA*(T(J+1)-T(J))/DR
      GO TO 10
C   LAST RING --- INWARD MIXING ONLY
 4    NR1 = EPSLN*(CI1(J)-CI1(J-1))/DR
      NR2 = EPSLN*(CI2(J)-CI2(J-1))/DR
      NR3 = EPSLN*(CI3(J)-CI3(J-1))/DR
      NR4 = EPSLN*(CI4(J)-CI4(J-1))/DR
      QR1 = LAMDA*(T(J)-T(J-1))/DR
      QRN = (NR1*CF1+NR2*CF2+NR3*CF3+NR4*CF4)*(T(J)-T(J-1))/DR
      NRR1 = 0.
      QRR1 = 0.
 10   CALL SGRAD (CI1(J),CI2(J),CI3(J),CI4(J),G(J),T(J),GR(J),TGR(J),J)
      GRAD = GR(J)
      TGRAD = TGR(J)
      CK4(J) = KC4
      W1 = CI1(J)/RHO(J)
      DWDZ(J) = (.5*MH2/MN2H4*(RHOM(J)*DELTA+AP*KC4*CI4(J))+1.5*AP*GRAD*
     X          MH2/MNH3+(NR1-NRR1)*DELTA/DR-NRR1*DELTA/RAD(J)-F(J)*W1)
     X          /G(J)
      DHDZ = -(F(J)*(H(J)-HF)+AP*TGRAD+DELTA*(H4*RHOM(J)-(QR1-QRR1)/DR)+
     X       QRR1*DELTA/RAD(J)+QRN*DELTA)/G(J)
      DTDZ(J) = ABS(DHDZ)/CFBAR
 20   CONTINUE
C   FIND LARGEST OF DWDZ'S
      CALL ORDER (DWDZ,DWDZ0)
C   FIND LARGEST OF DTDZ'S
      CALL ORDER (DTDZ,DTDZ0)
C   CALCULATE NEW DZ
      DZ1 = .01/DWDZ0(NRINGS)
      DZ2 = 30./DTDZ0(NRINGS)
C   TAKE DELTAZ AS THE SMALLER OF DZ1 AND DZ2
      DZ = AMIN1(DZ1,DZ2)
      RETURN
      END
```

```
      SUBROUTINE SLOPE (RATE)
      REAL  K
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,DON2H4,DONH3,R,CGM,RADIUS,NMAX1,
     X        NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS
      COMMON /MMM/MI
      DIMENSION K(1),     GMMA(1),BETA(1),BPA(1),CG(1),S(210),FST(210),
     1SLC(210),D(210),CPA(210),CPB(210),E(210),A(1),TERM1(210),
     2TERM2(210),C(210),XXX(210),XOA(210)
      CG(1)=C4
      GMMA(1)=GAMMA
      PRES=P
      EN12=1
      DIFF=DON2H4
      IFLAG=0
      JFLAG = 0
```

```
      ALLOW = .05
      FRAC=.99
   12 B=0.0
  702 I=1
      NOT=0
      ADIV=100.
      BDIV=100.
      TOL=.01
      STORE=1.0
      KJ=0
      HOLD=0.
      NI=0
   13 MI=0
      IL=0
      IK=0
      MM=0
      IM=0
      F=0.5
   20 MM=MM+1
      ADR=B/ADIV
      BDR=(A(I)-B)/BDIV
      JINT=BDIV
      INIT=ADIV
      IF(MM.EQ.1) GO TO 15
      GO TO 16
   15 MMAX=JINT+1
      MAX=MMAX-1
      MINT=0
      GO TO 17
   16 MMAX=INIT+JINT+1
      MINT=INIT+1
      MAX=MMAX-1
   17 X=0.0
      DO 40 IJ=1,MMAX
      IF(IJ.GT.MINT) GO TO 49
      X=FLOAT(IJ-1)*ADR
      GO TO 23
   49 KMJ=IJ-MINT
      X=B+FLOAT(KMJ)*BDR
   23 CP=CG(I)*X/(A(I)-B)-(B/(A(I)-B))*CG(I)
      IF(CP.LT.0.0) CP=0.0
C     THIS IS THE GENERAL EQUATION FOR A LINE WITH NEGATIVE Y-INTERCEPT
   24 FACT1=K(I)*(CG(I))**(1.-EN12)*(CP)**EN12
      EFACT=GMMA(I)*BETA(I)*(1.-CP/CG(I))/(1.+BETA(I)*(1.-CP/CG(I)))
      IF(EFACT.GT.88.)EFACT=88.
      FACT2=EXP(EFACT)
      IF(X) 37,40,37
   37 RCP=FACT1*FACT2
   35 S(IJ)=(1./X-1./A(I))*X*X*RCP
   40 CONTINUE
   50 SUM=0.0
      SUMA=0.0
      DO 60 IL=2,MAX
      IF(IL.GT.MINT) GO TO 61
      SUM=SUM+S(IL)
      GO TO 60
   61 SUMA=SUMA+S(IL)
   60 CONTINUE
      S(1) =0.
      SGMA=(S(1)+2.*SUM)*(ADR/(2.*DPA(I)))+(S(MMAX)+2.*SUMA)*(BDR/(2.
```

```
     10*DPA(I)))
      D2=SGMA-FRAC*CG(I)
      TOT=D2+TOL*CG(I)
      IF(MM-1) 110,110,112
 112  IF(D2)1,1,2
 1    IF(TOT)2,230,230
 2    GO TO 115
 110  IF(IFLAG.EQ.1)GO TO 115
      IF(D2)150,115,115
 115  IF(MM-1) 20,120,140
 120  XOLD=B
      D1=D2
C     CHANGE THE EQUATION OF T E LINE
      B=.999999  *A(I)
      GO TO 20
C     USE PRECEDING RESULTS TO ESTIMATE B FOR NEW LINE
 140  TUMP=B
      MI=MI+1
      B=B+(D2/(D2-D1))*(XOLD-B)
 1741 XOLD=TUMP
      D1=D2
 143  IF(MI-20) 145,145,147
 145  GO TO 20
 147  IF (JFLAG.EQ.1) GO TO 230
      B = .9*A(I)
      JFLAG = 1
      GO TO 702
C     INITIAL CHOICE THRU ORIGIN IS SATISFACTORY
 150  KJ=1
      IFLAG=1
      X=0.
C     CALCULATE THE VALUE OF THE TWO INTEGRALS FOR ALL DR (101 POINTS)
      DO 170 II=1,MMAX
      X=FLOAT(II-1)*BDR
      CP=CG(I)*X/(A(I)-B)-(B/(A(I)-B))*CG(I)
      TERM1(II)=K(I)*(CG(I))**(1.-EN12)*(CP)**EN12
      TERM2(II)=EXP(GMMA(I)*BETA(I)*(1.-CP/CG(I))/(1.+BETA(I)*(1.-CP/CG(
     1I))))
      XXX(II)=X
      XOA(II)=XXX(II)/A(I)
      RCP = TERM1(II)*TERM2(II)
      FST(II)=X*X*RCP
      IF(X) 165,170,165
 165  SEC(II)=(1./X-1./A(I))*X*X*RCP
 170  CONTINUE
C     THE TRAPEZOIDAL RULE IS USED TO EVALUATE BOTH INTEGRALS
 172  C(1)=0.
 173  DO 175 JJ=2,MMAX
      IF(JJ.GT.MINT) GO TO 176
      C(JJ)=C(JJ-1)+(FST(JJ)+FST(JJ-1))*(ADR/(2.*DPA(I)))
      GO TO 175
 176  C(JJ)=C(JJ-1)+(FST(JJ)+FST(JJ-1))*(BDR/(2.0*DPA(I)))
 175  CONTINUE
      SEC(1)=0.
      D(1) = 0.
      DO 180 KK=2,MMAX
      IF(KK.GT.MINT) GO TO 179
      D(KK)=D(KK-1)+(SEC(KK-1)+SEC(KK))*(ADR/(2.*DPA(I)))
      GO TO 180
 179  D(KK)=D(KK-1)+(SEC(KK-1)+SEC(KK))*(BDR/(2.0*DPA(I)))
```

```
  180   CONTINUE
 C      THE VALUE OF CP AT X=0 IS  CG -D(101)
        E(1)=D(MMAX)
   186  CPA(1)=0.0
 C      NEGATIVE VALUES OF CPA(1)=CP(0) CANNOT BE USED
 C      STORE THE CPA(1) VALUE IN CASE A NEW F FACTOR MUST BE USED
  184   STORE = CPA(1)
        IF(KJ.EQ.1) GO TO 185
        IF(IM.EQ.0) GO TO 185
        IF(NI.EQ.1) GO TO 368
   185  SAM=0.0
        DO 190 LL=2,MMAX
        IF(LL.GT.MINT) GO TO 188
        E(LL)=E(LL-1)-(SEC(LL)+SEC(LL-1))*(DR/(2.*DPA(I)))
        SAM=FLOAT(LL-1)*ADR
        GO TO 189
   188  E(LL)=E(LL-1)-(SEC(LL)+SEC(LL-1))*(BDR/(2.0*DPA(I)))
        SAM=SAM+BDR
   189  CPA(LL)=CG(I)-((1./SAM)-(1./A(I)))*C(LL)-E(LL)
        IF(LL.LT.MINT) CPA(LL)=0.0
        IF(CPA(LL).LT.0.0) CPA(LL)=0.0
  190   CONTINUE
        IF(KJ.EQ.1) GO TO 200
        X=0.
        IF(IM.EQ.0) GO TO 250
        IK=1
        GO TO 280
 C      THE NEXT ITERATION USES THE VALUES OF CP JUST CALCULATED
   192  DO 200 LI=1,MMAX
        IF(LI.GT.MINT) GO TO 195
        X=FLOAT(LI-1)*ADR
        GO TO 199
   195  KLK=LI-MINT
        X=B+FLOAT(KLK)*BDR
   199  CONTINUE
        TERM1(LI)=K(I)*(CG(I))**(1.-EN12)*(CPA(LI))**EN12
        TERM2(LI)= EXP(GMMA(I)*BETA(I)*(1.-CPA(LI)/CG(I))/(1.+BETA(I)*(1.-
       1CPA(LI)/CG(I))))
        XXX(LI)=X
        XOA(LI)=XXX(LI)/A(I)
        RCP=TERM1(LI)*TERM2(LI)
        FST(LI)=X*X*RCP
        IF(X) 200,200,193
  193   SEC(LI)=(1./X-1./A(I))*X*X*RCP
  200   CONTINUE
        GO TO 172
 C      THIS IS FOR THE CASE WHERE THE INITIAL GUESS WAS TOO LARGE
  230   IF(B.GT..995*A(I))DERIF=2.6*CG(I)/(A(I)-B)
        IF(B.GT..998*A(I)) GO TO 322
 C      THE RANGE OF X FROM ZERO TO A IS USED
  237   X=0.
        NI=1
        DO 240 NN=1,MMAX
        IF(NN.GT.MINT) GO TO 246
        X=FLOAT(NN-1)*ADR
        GO TO 354
   246  KJK=NN-MINT
        X=B+FLOAT(KJK)*BDR
   354  IF(IM.GE.1) GO TO 353
  238   CPB(NN) = CG(I)*X/(A(I)-B) - (B/(A(I)-B))*CG(I)
```

```
      IF(CPB(NN).LT.0.0) CPB(NN)=0.0
  353 TERM1(NN)=K(I)*(CG(I))**(1.-EN12)*(CPB(NN))**EN12
      TERM2(NN)= EXP(GMMA(I)*BETA(I)*(1.-CPB(NN)/CG(I))/(1.+BETA(I)*(1.-
     1CPB(NN)/CG(I))))
      XXX(NN)=X
      XOA(NN)=XXX(NN)/A(I)
      RCP = TERM1(NN)*TERM2(NN)
      FST(NN)=X*X*RCP
      IF(X) 240,240,247
  247 SEC(NN) = (1./X-1./A(I))*X*X*RCP
  240 CONTINUE
      GO TO 172
  366 DO 370 NL=1,MMAX
      CPB(NL)=CPA(NL)
  370 CONTINUE
      GO TO 165
  250 DO 260 IL=1,MMAX
  252 CPA(IL)=.5*CPA(IL)+.5*CPB(IL)
  260 CONTINUE
      IK=0
C   THE VALUES OF X AT A AND NEAREST A ARE USED IN FINDING THE DERIVATIVE
  280 DERIF=(CG(I)-CPA(MAX))/BDR
      IM=IM+1
      IF(IM.GT.99.AND.IFLAG.EQ.1)GO TO 701
      IF(IM.GT.99)GO TO 328
  310 IF(KJ.EQ.1) IK=1
      IF(ABS(DERIF-HOLD)-ALLOW*DERIF)3,3,321
  3   IF(IK.EQ.1)GO TO 322
  321 HOLD=DERIF
      IF(KJ.EQ.1) GO TO 192
      IF(IK.EQ.1) GO TO 250
      GO TO 192
  322 RATE=DERIF
  777 IF (B.GT..998*A(I)) GO TO 327
  327 RETURN
  328 PERC=(ABS(DERIF-HOLD)/DERIF)*100.
      ALL=100.*ALLOW
      GO TO 322
C     SIMPLIFIED VERSION DOES NOT ''CONVERGE'' IN 99 ITERATIONS
C     SET B=.000001*A     ,    AND START OVER
  701 B=.000001*A(I)
      WRITE (6,700)
  700 FORMAT (/ 84H INITIAL CHOICE THRU ORIGIN SEEMINGLY OK, BUT RESULTS
     X ROTTEN AFTER 99 ITERATIONS .../48H SET X0=.000001*A AND USE MORE
     XREFINED TECHNIQUE /)
      ADR=B/ADIV
      BDR=(A(I)-B)/BDIV
      MMAX=INIT+JINT+1
      MINT=INIT+1
      MAX=MMAX-1
      IM=0
      KJ=0
      GO TO 237
      END

      SUBROUTINE SGRAD (CI1,CI2,CI3,CI4,G,T,GRAD,TGRAD,JRING)
C   THIS ROUTINE CALCULATES THE CONCENTRATION GRADIENT AT THE SURFACE
```

```
C     OF THE LOCAL CATALYST PARTICLES
      REAL  K0,KP,KC3,KC4,MU
      COMMON /AAAA/DP3,X0,XOA,CPS
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZ0(25),G0(25),Z0(25)
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,D0N2H4,D0NH3,R,CGM,RADIUS,NMAX1,
     X         NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS
      COMMON /AAA/VISVST(30),TBLVP(68)
      COMMON /CCC/H4TBL(40),H3TBL(40)
      DIMENSION  CPOX(101),PCPOX(101),DX(101),CPX(101),RHET(101)
      DIMENSION  XOBLOK(100)
C     DEFINE DP FUNCTION
      DP3F(X,Y,Z) = 14.7*Y/Z*(X/492.)**1.823*(1.-EXP(-.0072*Z*492./(
     X              14.7*X)))
C     DEFINE KC FUNCTION
      KCF(A,B,C,D,E) = .61*A/B*(C/(B*D))**-.667*(A/(E*C))**-.41
C     ANALYTIC INTEGRATION FUNCTIONS FROM INTEGRAL EQUATION
      EVAL1(A,B) = B**3/3.-A**3/3.
      EVAL2(A,B) = B**2/2.-A**2/2.
      L = 1
      X0 = 0.
      WAF1 = .8
      WAF2 = .2
    1 LTFLG = 0
      ALPH2 = ALPHA2
      D03 = D0NH3
      D04 = D0N2H4
      TPSP = 0.
      N = 1
      NPART = 50
      LP1 = 1
      RHO = CI1+CI2+CI3+CI4
      DI3 = D03*14.7/P*(T/492.)**1.823
      DI4 = D04*14.7/P*(T/492.)**1.823
      CALL UNBAR (VISVST,1,T,0.,MU,KK)
      KC3 = KCF(G,RHO,MU,DI3,AP)
      KC4 = KCF(G,RHO,MU,DI4,AP)
      HC = .74*G*CFBAR*(G/(AP*MU))**-.41
C
C     LOCATE SUITABLE X0
C
      DP3 = DP3F(T,D03,P)
C     CHOOSE STARTING VALUE FOR CPS TO BE = CI3/2.
      CPS = CI3/2.
      CMCPN = CI3-CPS
      DCPDX = KC3/DP3*(CI3-CPS)
C     H4 CONSTANT FOR EACH ENTRY TO THIS ROUTINE
C     H3 VARIES WITH TEMP AT EACH ITERATION
      CALL UNBAR (H4TBL,1,T,0.,H4,KK)
      CALL UNBAR (H3TBL,1,T,0.,H3,KK)
      IF (LP1.EQ.1) GO TO 6
   40 TPSPP = TPSP
      TPSP = TPS
    6 TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
    8 CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      DP3P = DP3
      H3P = H3
      TMTPN = T-TPS
```

```
 61   GAMMA = BGM/TPS
      BETA = -CPS*H3*DP3/(KP*TPS)
      K0 = ALPH2*EXP(-GAMMA)/CI1**1.6
C   LINEAR EXTRAPOLATION USED TO GUESS AT X0
      X0P = X0
      X0 = A-CPS/DCPDX
      X0BLOK(L) = X0
      X0A = X0/A
      IF (X0) 11,12,12
 11   X0 = 0.
      X0A = 0.
      CPS = CI3/(DP3/(A*KC3)+1.)
      DCPDX = CI3/A
      TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      DP3P = DP3
      H3P = H3
      TMTPN = T-TPS
      GAMMA = BGM/TPS
      BETA = -CPS*H3*DP3/(KP*TPS)
      K0 = ALPH2*EXP(-GAMMA)/CI1**1.6
      WRITE (6,132) LP1,TPS
 132  FORMAT (///37X,'WE HAVE CALCULATED A NEGATIVE X0 DURING ITERATION
     X NO',I3,/39X,'SET X0 = 0. , CALCULATE TPS =',E11.6,' , AND CONTINUE
     X ')
      GO TO 131
C   INTEGRATE FOR CP EQUATION
 12   CALL TRAPP (X0A,1.,NPART,RIESUM,CI3)
C   CALCULATE NEW CPS ...
      CPSP = CPS
      CMCP0 = CMCPN
      CPS = CI3-A*RIESUM/KC3
      IF (LTFLG-1) 80,84,80
 80   IF (CPS-(.25*CI3)) 81,81,87
 81   LTFLG = 1
      GO TO 22
 84   LTFLG = 0
      IF (CPS) 89,87,87
 89   CPS = 0.
      GO TO 46
 87   CMCPN = CI3-CPS
C   CALCULATE NEW TP
 13   DCPDX = KC3/DP3*(CI3-CPS)
      GRAD = DCPDX*DP3
      TGRAD = HC*(T-TPS)
      TPSPP = TPSP
      TPSP = TPS
      TMTP0 = TMTPN
 51   TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
 2    CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      TMTPN = T-TPS
      GAMMA = BGM/TPS
      BETA = -CPS*H3*DP3/(KP*TPS)
      K0 = ALPH2*EXP(-GAMMA)/CI1**1.6
C   TEST TEMP,CONCENTRATION FOR 5% LIMIT
      IF (ABS(TMTP0-TMTPN)/TMTPN - .05) 41,41,43
```

```
 41   IF (ABS(CMCPO-CMCPN)/CMCPN - .05) 131,131,43
C   TEST FOR TEMPERATURE LOOP ... COMPARE LAST 3 TEMPS
 43   IF (AMIN1(TPS,TPSP,TPSPP) - TPSP) 60,71,60
 60   IF (AMAX1(TPS,TPSP,TPSPP) - TPSP) 46,71,46
C   TEMPERATURE HAS FLUCTUATED ... TAKE AVERAGE AND RECALCULATE CPS
 71   TPSPP = TPSP
      TPSP = TPS
      TMTPO = TMTPN
      TPS = (TPSP+TPSPP)/2.
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      DP3P = DP3
      TMTPN = T-TPS
      DCPDX = (HC*(T-TPS)-H4*KC4*CI4)/(H3*DP3)
      CPSP = CPS
      CMCPO = CMCPN
      CPS = CI3-DP3/KC3*DCPDX
      IF (CPS.LT.0.) CPS=0.
      CMCPN = CI3-CPS
      LP1 = LP1+1
      L = L+1
      IF (LP1-25) 61,61,44
C   NO CONVERGENCE YET ... AVERAGE THE CPS'S FOR LAST TWO CALC'S AND REPEAT
      CPS = .2*CPS+.8*CPSP
      GO TO 53
C   CALCULATE WEIGHTED AVERAGE OF PRESENT AND PREVIOUS X0
 22   X00 = WAF1*X0P+WAF2*X0
      CPS = CI3/(1.+DP3/(KC3*A-KC3*X00))
 53   DCPDX = KC3/DP3P*(CI3-CPS)
      CMCPN = CI3-CPS
      H3 = H3P
 42   LP1 = LP1+1
      L = L+1
      IF (LP1-25) 40,40,44
 44   WAF1 = WAF1+.05
      IF (WAF1.GT..95) GO TO 99
      WAF2 = 1.-WAF1
C   NO CONVERGENCE WITH PRESENT WEIGHTED AVERAGE FACTORS FOR X0 ---
C   REPEAT ITERATION PROCEDURE WITH NEW
      GO TO 1
 99   LM1 = L-1
      WRITE (6,98)
 98   FORMAT (///20X,'UNABLE TO FIND SUITAB      ER FOUR TRIES OF 25
     XITERATIONS EACH --- PROGRAM STOP FOLLU
      WRITE (6,96) (X0BLOK(I),I=1,LM1)
 96   FORMAT (//52X,'X0 VALUES CALCULATED IN SGRAD' / (10E13.5))
      CALL DUMP
C
C   SATISFACTORY X0 HAS BEEN FOUND
C   CALCULATE GRADIENT
C
131   LP2 = 1
      NX = 24
      NX1 = NX+1
      NXM1 = NX-1
291   X0A = X0/A
      VNU = -KC3/DP3
      INT1 = 1
      L = 2
      R1 = 0.
```

```
      R2 = 0.
      PS1 = 0.
      PS2 = 0.
      DELXOA = (1.-XOA)/FLOAT(NX)
    CALCULATE PROFILE CURVES FOR INTEGRAND FUNCTIONS
      XA = XOA
      DO 770 I=1,NX1
    CP(X/A) IS A LINEAR PROFILE DURING FIRST APPROXIMATION
      IF (LP2.GT.1) GO TO 664
      CPX(I) = (XA-XOA)/(1.-XOA)*CPS
 64   RHET(I) = K0*CI3**(1-N)*CPX(I)**N*EXP(GAMMA*BETA*(1.-CPX(I)/CI3)/
     X          (1.+BETA*(1.-CPX(I)/CI3)))
      DX(I) = XA
      XA = XA+DELXOA
 70   CONTINUE
    TAKE INTERVAL FUNCT'N MIDPTS AS CONSTANT VALUE FOR CP(X/A) AND RHET
      DO 771 I=1,NX
      CPX(I) = (CPX(I)+CPX(I+1))/2.
      RHET(I) = (RHET(I)+RHET(I+1))/2.
 71   CONTINUE
      XA = XOA+DELXOA
      CTRM = (A*VNU+1.)/(A*VNU)
    INTEGRAL EQUATION FOLLOWS
    CPOX(1) IS SPECIAL CASE ... X=X0
      DXL = XOA
      DXU = DXL+DELXOA
      RR1 = 0.
      DO 377 I=1,NX
      RR1 = RR1+RHET(I)*(EVAL2(DXL,DXU)-CTRM*EVAL1(DXL,DXU))
      DXL = DXU
      DXU = DXU+DELXOA
377   CONTINUE
      CPOX(1) = CI3-A*A/DP3*RR1
      IF (CPOX(1).LT.0.) CPOX(1)=0.
    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(L) = CI3-A*A/DP3*(R1+R2)
      IF (CPOX(L).LT.0.) CPOX(L)=0.
      XOA = X0/A
      XA = XOA+DELXOA
      L = L+1
      R1 = 0.
      R2 = 0.
      PS1 = 0.
      PS2 = 0.
```

```
      IF (L.LE.NX) GO TO 769
C   CPOX(NX1) IS SPECIAL CASE ... X=A
      DXL = XOA
      DXU = DXL+DELXOA
      RR2 = 0.
      DO 378 I=1,NX
      RR2 = RR2+RHET(I)*EVAL1(DXL,DXU)
      DXL = DXU
      DXU = DXU+DELXOA
  378 CONTINUE
      CPOX(NX1) = CI3-A*A/DP3*(1.-CTRM)*RR2
      IF (CPOX(NX1).LT.0.) CPOX(NX1)=0.
C   CALCULATE A NEW TPS
      DCPDX = KC3/DP3*(CI3-CPOX(NX1))
      H3P = H3
      DP3P = DP3
      TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      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 = CI3-CPOX(NX1)
      IF (ABS(TMTPO-TMTPN)/TMTPN - .05) 26,26,27
  26  IF (ABS(CMCPO-CMCPN)/CMCPN - .05) 49,49,27
C  CALCULATE NEW CPX(I) PROFILE FOR NEXT PASS
  27  DO 55 I=1,NX1
      IF (MOD(LP2,5)) 34,57,34
C  CALCULATE WEIGHTED AVERAGE OF OLD AVERAGED AND CALCULATED PROFILES
  34  CPX(I) = .8*CPX(I)+.2*CPOX(I)
      GO TO 56
C  AVERAGE PRESENT AND PAST CALCULATED PROFILES EVERY 5TH PASS TO SMOOTH
  57  CPX(I) = (CPOX(I)+PCPOX(I))/2.
C  STORE PRESENT CALCULATED PROFILE
  56  PCPOX(I) = CPOX(I)
  55  CONTINUE
      CMCPN = CI3-CPX(NX1)
      DCPDX = KC3/DP3P*(CI3-CPX(NX1))
      TPS = T-(H4*KC4*CI4+H3P*DP3P*DCPDX)/HC
      IF (TPS.LT.0.) TPS=1.
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)
      DP3 = DP3F(TPS,D03,P)
      TMTPO = TMTPN
      TMTPN = T-TPS
      LP2 = LP2+1
      IF (LP2-50) 29,29,30
  30  WRITE (6,18) CPOX(NX1)
  18  FORMAT (///31X,52HUNABLE TO CONVERGE ON CPS IN  50 TRIES ... CP(X/
     XA) =,E12.5)
      WRITE (6,522) GRAD,TGRAD
 522  FORMAT (51X,'KC3*(CI3-CPS) =',E12.5 / 54X,'HC*(T-TPS) =',E12.5)
      GO TO 28
  29  GAMMA = BGM/TPS
      BETA = -CPX(NX1)*H3*DP3/(KP*TPS)
      K0 = ALPH2*EXP(-GAMMA)/CI1**1.6
      GO TO 291
  49  GRAD = DCPDX*DP3
```

```
      TGRAD = HC*(T-TPS)
 28   RETURN
      END
```

```
      SUBROUTINE TRAPP (U,W,NPART,RIESUM,CI3)
C     NUMERICAL INTEGRATION USING TRAPEZOIDAL METHOD
      REAL    K0,KC3
      COMMON /AAAA/DP3,X0,X0A,CPS
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,DON2H4,DONH3,R,CGM,RADIUS,NMAX1,
     X          NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS
C     DEFINE RHET FOR VARIABLE CP,CPS,TP
      RHETF(A,B,C,D,E,N) = E*A**(1-N)*B**N*EXP(C*D*(1.-B/A)/(1.+D*(1.-
     X                    B/A)))
C     FUNCTIONS DEFINING INTEGRANDS
      FOXI1(X,R)=X**2*R
C     FUNCTION DEFINING CP(X) FOR RHET FUNCTION
C     CP(X) IS ASSUMED TO VARY LINEARLY WITH X
      CPXF(X,Y,Z)=(X-Y)/(1.-Y)*Z
      N=NPART-1
      PART=NPART
      D=(W-U)/PART
      UPH=U+D
      SUM=0.
      CPX1=CPXF(U,X0A,CPS)
      CPX2=CPXF(W,X0A,CPS)
      RHET1=RHETF(CI3,CPX1,GAMMA,BETA,K0,1)
      RHET2=RHETF(CI3,CPX2,GAMMA,BETA,K0,1)
C     CALCULATE FIRST,LAST TERMS OF RIEMANN SUM FIRST
  4   TRM1=FOXI1(U,RHET1)/2.
      TRM2=FOXI1(W,RHET2)/2.
  6   DO 8 I=1,N
      CPX=CPXF(UPH,X0A,CPS)
      RHET = RHETF(CI3,CPX,GAMMA,BETA,K0,1)
      SUM=SUM+FOXI1(UPH,RHET)
      UPH=UPH+D
  8   CONTINUE
  9   RIESUM=D*(TRM1+SUM+TRM2)
 99   RETURN
      END
```

```
      SUBROUTINE  UNBAR(T,IK,XIN,YIN,ZZ,KK)
      DIMENSION T(1),X(6),Y(6),A(6)
C
C     -------------------  MARCH 4, 1961 -------------
C     -------------------  MODIFIED 7/62  ------------------
C     -------------------        TO DO QUADRATIC AND LINEAR INTERPOLATION ALSO
C
      II = IK+1
      N = 3
      N2= 2
           IF (T(II)-3.) 700,701,702
 700       IF (T(II)+0.) 60,701,704
 704       IF (T(II)-2.) 705,706,701
```

```
705   N = 1
            GO TO 707
706   N = 2
707   N2= 1
701   II = II+1
702   N1 = N +1
            DO 50 L = II,II
            IF ( T(L) + 0. ) 60,60,51
60     KK = -1
       ZZ = 0.
          GO TO 9999
51    NX = T(L)
            IF (T(L+1) + 0. ) 60,52,50
52    NY = 0
            GO TO 53
50    NY = T(L+1)
53          CONTINUE
      KK  = 0
      KY  = 0
      XX  = XIN
      YY  = YIN
      J1  = II+2
      J2  = NX+II+1
      IF(XX-T(J1))301,306,400
400         DO 302 J=J1,J2
            IF (XX-T(J)) 304,304,302
302   CONTINUE
309   KK  = 2
      XX  = T(J2)
308   JX1 = J2-N
            GO TO 305
301   KK  = 1
      XX  = T(J1)
306   JX1 = J1
            GO TO 305
304         IF (J-J1-1) 301,306,307
307         IF (J-J2)    303,308,309
303   JX1 = J-N2
305   CONTINUE
      XINT  = XX
        IF (NY) 1500, 1500, 3000
1500        DO 1599 L=1,N1
            X(L) = T(JX1)
             LY = JX1 + NX
             Y(L) = T(LY)
1599   JX1 = JX1+1
      I = 1
      GO TO 54
3000  J1  = J1+NX
      J2  = J2+NY
      IF(YY-T(J1))311,316,401
401         DO 312 J=J1,J2
            IF (YY-T(J)) 314,314,312
312   CONTINUE
319   KY  = 6
      YY  = T(J2)
318   JY1 = J2-N
            GO TO 315
311   KY  = 3
      YY  = T(J1)
```

```
316  JY1 = J1
        GO TO 315
314     IF (J-J1-1) 311,316,317
317     IF (J-J2)   313,318,319
313  JY1 = J-N2
315  CONTINUE
     JX2  = JX1
     LY   = JY1 + NY*(JX2-II-1)
     LY1 = LY
        DO 3099 L=1,N1
     X(L) = T(JX2)
     Y(L) = T(LY1)
     LY1  = LY1+NY
3099 JX2  = JX2+1
     I    = 0
        GO TO 54
3098 Y(I)  = ZZ
        DO 4400 I=1,N
     LY1 = LY+I
     Y(I+1) = 0.
        DO 4050 MM=1,N1
     Y(I+1) = Y(I+1) + T(LY1)*X(MM)
4050 LY1 = LY1+NY
4400  CONTINUE
        DO 4199 L=1,N1
     X(L) = T(JY1)
4199 JY1  = JY1+1
     XINT = YY
     I=  1
54   D  = 1.
     X(N+2) = X(1)
     X(N+3) = X(2)
        DO 55 J=1,N1
     A(J+1) = X(J+1) - X(J)
     TPAL1  = XINT - X(J)
      IF ( TPAL1 ) 57,58,57
 58    ZZ = Y (J)
      X(1) = 0.
      X(2) = 0.
      X(3) = 0.
      X(4) = 0.
      X(J) = 1.0
      GO TO 59
 57  D = D * TPAL1
        GO TO (711,712,713) ,N
711  X(J)  = TPAL1/A(J+1)
        GO TO 55
712  X(J)  = -TPAL1
        GO TO 55
713  X(J)  = (X(J+2)-X(J))*TPAL1
55     CONTINUE
     A(1) = A(N+2)
     ZZ = 0.
       DO 56 J=1,N1
      X(J) = D/(A(J)*A(J+1)*  X(J))
     ZZ = ZZ + Y(J)*  X(J)
56     CONTINUE
 59     IF (I) 3098,3098,9999
9999 KK  = KK+KY
        RETURN
```

```
      END
```

```
      BLOCK DATA
C     BLOCK DATA FOR VISCOSITY VS TEMPERATURE
      COMMON /AAA/VISVST(30),TBLVP(68)
      DATA  (VISVST(I),I=1,30) /  0., 1., 13., 0.,
C     TEMPERATURES
     X 360.  , 540.  , 720.  , 900.  , 1080.  , 1260.  , 1440.  ,
     X 1620.  , 1800.  , 1980.  , 2160.  , 2340.  , 2520.  ,
C     VISCOSITIES
     X.048 E-4,.070 E-4,.093 E-4,.117 E-4,.141 E-4,.164 E-4,.186 E-4,
     X.207 E-4,.228 E-4,.247 E-4,.266 E-4,.285 E-4,.302 E-4 /
C     BLOCK DATA FOR VAPOR PRESSURE AS FUNCTION OF TEMPERATURE
      DATA  (TBLVP(I),I=1,68) /  0. ,  1. ,  32. ,  0. ,
C     TEMPERATURES
     X  492. ,  519. ,  528.4,  529.1,  534.6,  534.7,  538.8,  543.9,
     X  545.7,  560.2,  570.0,  579.3,  579.5,  595.3,  610.1,  614.1,
     X  618.1,  627.5,  628.8,  645.7,  650.8,  665.6,  675.0,  692.4,
     X  697.5,  744.0,  798.0,  852.0,  942.0, 1032.0, 1122.0, 1176.0,
C     VAPOR PRESSURES
     X .052  , .148  , .201  , .207  , .240  , .282  , .292  , .354  ,
     X .545  , .737  , .973  , .982  , 1.51  , 2.20  , 2.46  , 2.74  ,
     X 3.41  , 3.56  , 5.24  , 5.97  , 8.07  , 9.71  , 11.91 , 13.46 ,
     X 14.70 , 33.80 , 73.48 , 147.  , 382.  , 823.  , 1528. , 2131.  /
      END
```

```
      BLOCK DATA
C     BLOCK DATA FOR SPECIFIC HEAT VS TEMPERATURE
      COMMON /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)
      DATA  (CFTBL1(I),I=1,34) /  0., 1., 15., 0.,
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,
C     SPECIFIC HEATS
     X 3.4194, 3.4596, 3.4685, 3.4765, 3.4899, 3.5151, 3.5454, 3.5806,
     X 3.6208, 3.6654, 3.7150, 3.7696, 3.8291, 3.8802, 3.9288 /
      DATA  (CFTBL2(I),I=1,34) /  0., 1., 15., 0.,
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,
C     SPECIFIC HEATS
     X .2485 , .2495 , .2524 , .2569 , .2624 , .2682 , .2738 , .2790 ,
     X .2836 , .2878 , .2914 , .2946 , .2974 , .2998 , .3019  /
      DATA  (CFTBL3(I),I=1,34) /  0., 1., 15., 0.,
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,
C     SPECIFIC HEATS
     X .5085 , .5424 , .5891 , .6344 , .6773 , .7176 , .7553 , .7905 ,
     X .8236 , .8541 , .8823 , .9075 , .9304 , .9512 , .9697  /
      DATA  (CFTBL4(I),I=1,34) /  0., 1., 15., 0.,
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,
```

```
 SPECIFIC HEATS
  X .3804 , .4601 , .5261 , .5784 , .6212 , .6577 , .6899 , .7185 ,
  X .7442 , .7673 , .7879 , .8063 , .8226 , .8373 , .8503  /
   END


   BLOCK DATA
 BLOCK DATA FOR HEAT OF REACTION VS TEMPERATURE
   COMMON /CCC/H4TBL(40),H3TBL(40)
   DATA  (H4TBL(I),I=1,40) /   0., 1., 18., 0.,
 TEMPERATURES
  X  180.   ,  360.   ,  536.4 ,  540.   ,  720.   ,  900.   , 1080.   ,
  X 1260.   , 1440.   , 1620.   , 1800.   , 1980.   , 2160.   , 2340.   ,
  X 2520.   , 2700.   , 2880.   , 3060.   ,
 HEATS OF REACTION
  X-1951.02,-1919.50,-1896.04,-1895.70,-1882.55,-1878.12,-1879.46,
  X-1884.63,-1892.38,-1901.94,-1912.88,-1924.85,-1937.54,-1950.74,
  X-1964.45,-1978.32,-1992.36,-2006.62  /
   DATA  (H3TBL(I),I=1,40) /   0., 1., 18., 0.,
 TEMPERATURES
  X  180.   ,  360.   ,  536.4 ,  540.   ,  720.   ,  900.   , 1080.   ,
  X 1260.   , 1440.   , 1620.   , 1800.   , 1980.   , 2160.   , 2340.   ,
  X 2520.   , 2700.   , 2880.   , 3060.   ,
 HEATS OF REACTION
  X1055.57 ,1103.97 ,1159.35 ,1160.40 ,1213.46 ,1259.64 ,1298.00 ,
  X1329.71 ,1355.28 ,1375.57 ,1391.11 ,1402.52 ,1410.13 ,1414.57 ,
  X1416.37 ,1416.05 ,1414.15 ,1410.56   /
   END


   BLOCK DATA
   COMMON /DAVTBL/VPTBL(44)
C  BLOCK DATA TABLE OF VAPOR PRESSURE VS TEMP  (USED TO FIND TVAP)
   DATA (VPTBL(I),I=1,44) /      0. ,    1. ,   20. ,    0. ,
  X      50.  ,  100. , 150. , 200. , 250. , 300. , 350. , 400. ,
  X     450.  ,  500. , 550. , 600. , 650. , 700. , 750. , 800. ,
  X     850.  , 900.  , 950. , 1000.,
  X     770. , 820. , 855. , 880. , 905. , 925. , 945. , 965. ,
  X     980. , 995. ,1010. ,1025. ,1035. ,1050. ,1060. ,1070. ,
  X     1080., 1090. ,1100. ,1110. /
   END


   BLOCK DATA
   COMMON /LIZTBL/DHVST(18),DHLVST(18)
C  BLOCK DATA TABLES FOR DELHV AND DELHL VS TEMP  (USED TO FIND HV)
   DATA  (DHVST(I),I=1,18) / 0., 1., 7., 0.,
  X     180. , 360. , 534.6 , 540. , 720. , 900. , 1080. ,
  X     1390.16 , 1332.82 , 1280.02 , 1279.12 , 1237.79 , 1208.80 ,
  X     1189.76 /
   DATA  (DHLVST(I),I=1,18) / 0., 1., 7., 0.,
  X     180. , 360. , 534.6 , 540. , 720. , 900. , 1080. ,
  X     652.14 , 665.96 , 679.61 , 679.89 , 700.89 , 733.19 , 777.22
  X      /
   END
```