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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

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AUGUST, 1968

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United Aircraft Research Laboratories

UNITED AIRCRAFT CORPORATION

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ABSTRACT

Two machine computational programs have been developed under NASA Contract NAS 7-456 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

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

$$\text{for } h_i \leq h_i^V$$

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

$$\frac{dh_i}{dz} = -\frac{1}{G}\left\{F(h_i - h_F) + A_P h_C \left[T_i - (T_P)_S\right] + H^{N_2H_4} r_{hom}^{N_2H_4} \delta\right\} \qquad (4)$$

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

$$\frac{dw_i^{N_2H_4}}{dz} = \frac{i}{G}\left\{F - r_{hom}^{N_2H_4}\delta - A_P (k_C c_i)^{N_2H_4} - F\left(\frac{c_i}{\rho_i}\right)^{N_2H_4}\right\} \qquad (5)$$

*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)

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

and

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

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

$$\frac{dC_i^J}{dz} = \rho_i\,\frac{dw_i}{dz} \qquad \frac{\rho_i}{dz} \tag{11}$$

where

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

and

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

and

$$\frac{dP}{dz} = - \left(\frac{1-\delta}{\delta^3} \right) \left(175 + \frac{150(1-\delta)}{2aG/\mu} \right) \left(\frac{G^2}{2a\rho_i g_c} \right) \tag{14}$$

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

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

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, $c_i^{NH_3}$. 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

$$T_p - (T_p)_s = \frac{H D_p}{K_p} \left[(c_p)_s - c_p \right] \qquad (20)$$

The use of this relationship enables the reaction rate, $r_{het}^{NH_3}$, tc 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

$$c_p(x)^{NH_3} = c_i^{NH_3} - \left[\frac{1}{x} - \frac{a k_c^{NH_3} - D_p^{NH_3}}{a^2 k_c^{NH_3}}\right] \int_0^x \xi^2 \frac{r_{het}^{NH_3}(c_p)}{D_p^{NH_3}} \, d\xi \qquad (21)$$

$$- \int_x^a \left[\frac{1}{\xi} - \frac{a k_c^{NH_3} - D_p^{NH_3}}{a^2 k_c^{NH_3}}\right] \xi^2 \frac{r_{het}^{NH_3}(c_p)}{D_p^{NH_3}} \, d\xi$$

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 conver-

gence 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

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

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.

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

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

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

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

where

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

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

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

$$k_c^J = \left[\frac{0.61G}{\rho_i}\right] \left[\frac{\mu}{A D_i^J}\right]^{-0.667} \left[\frac{G}{A_p \mu}\right]^{-0.41} \tag{31}$$

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

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

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.

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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 one 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. $1 \leq NCASE \leq 999$.

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 ≠ 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 enthelpy of liquid hydrazine entering the bed in Btu/lb.

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

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 PRINT NØFZ	- - -	Liq.-Vap. Indicator Print Indicator No. of Z's in Input Tables
4	1	8E10.5	1-10 11-20 21-30 31-40 41-50 51-60 61-70 71-80	ZO GO FC ALPHA3 HF R WM4 WM3	Z_o G_o F α_{hom} h_F R $M_{N_2H_4}$ M_{NH_3}	Axial distance to injector end Inlet mass flow rate Distributed feed rate Preexponential factor Enthalpy of feed Gas constant Molecular wt. of N_2H_4 Molecular wt. of NH_3
5	1	8E10.5	1-10 11-20 21-30 31-40 41-50 51-60 61-70 71-80	WM2 WM1 ALPHA1 ALPHA2 AGM BGM KP CGM	M_{N_2} M_{H_2} $\alpha_{N_2H_4}$ α_{NH_3} $Q_{hot_{N_2H_4}}/R$ $Q_{hot_{NH_3}}/R$ K_T $Q_{hom_{N_2H_4}}/R$	Molecular wt. of N_2 Molecular wt. of H_2 Preexponential factor Preexponential factor Activation energy, deg R Activation energy, deg R Thermal conductivity Activation energy, deg R
6	1	8E10.5	1-10 11-20 21-30 31-40 41-50 51-60 61-70 71-80	TF CFL ENMX1 ENMX2 ENMX3 DIF3 DIF4 PRES	T_F C_f - - - $D_{o_{NH_3}}$ $D_{o_{N_2H_4}}$ P	Feed temperature Specific heat of liquid N_2H_4 Determines step size in liquid region Determines step size in liq-vapor region Determines step size in vapor region Diffusion coef. of NH_3 Diffusion coef. of N_2H_4 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 11-20 21-30 31-40	ZEND EN1 EN2 EN3	- n n n	Bed length Order of decomposition reaction Order of decomposition reaction Order of decomposition reaction
8	1	4E8.5	1-8 9-16 17-24 25-32	0. 1. NØFZ. 0.		Table descriptor Table descriptor Table descriptor Table descriptor
9*	*	10E8.5	1-18 9-16 17-24 ↓ 73-80	Z(I)	z	Axial station
10**	**	10E8.5	1-8 9-16 17-24 ↓ 73-80	A(I)	a	Catalyst Particle Radius
11	1	4E8.5	1-8 9-16 17-24 25-32	0. 1. NØFZ. 0.		Table descriptor Table descriptor Table descriptor 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)

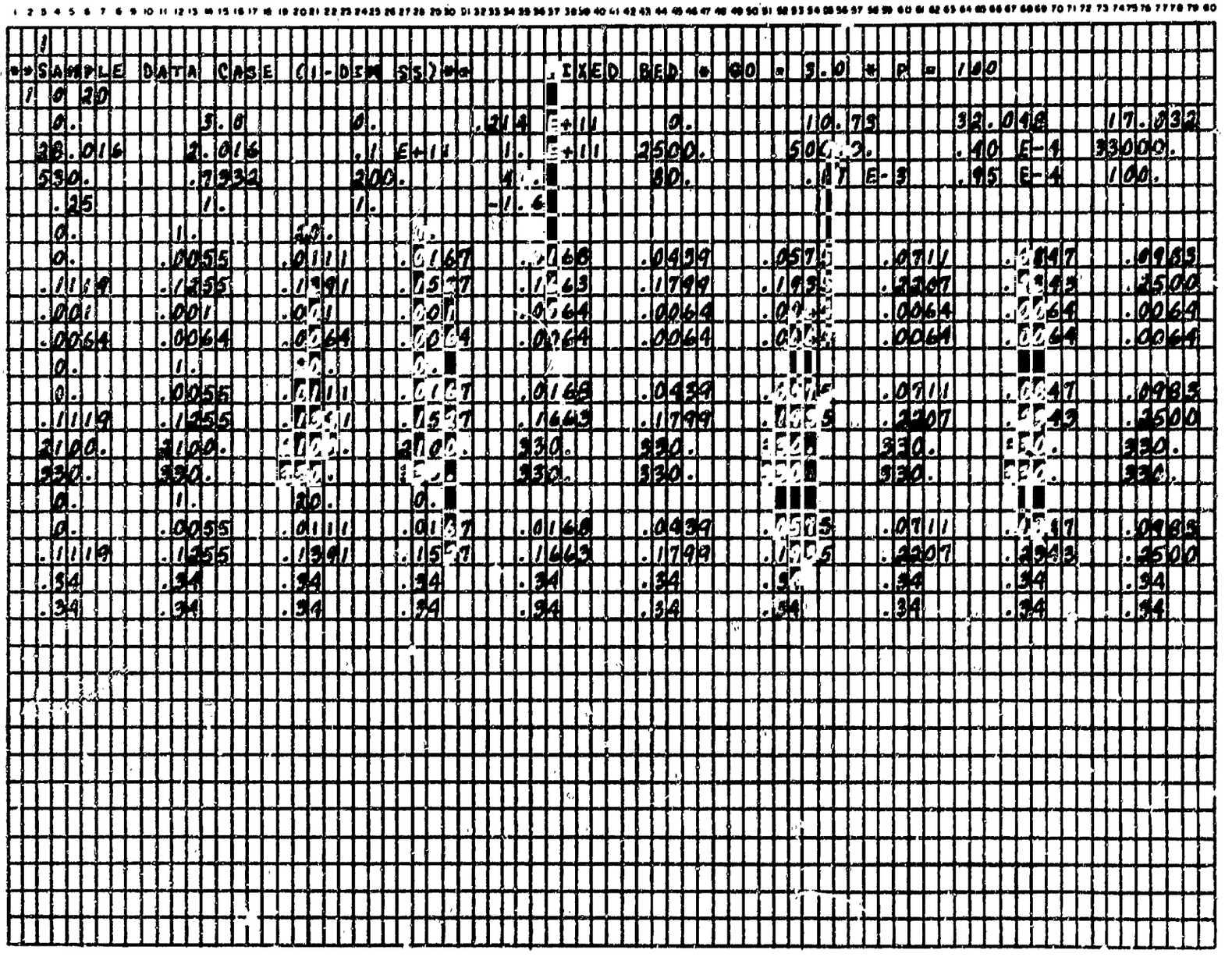
CARD NUMBER	NUMBER OF CARDS	FORTRAN IV FORMAT	COLUMNS USED	SYMBOL OR DESCRIPTION	CORRESPONDING SYMBOL USED IN EQUATIONS	NOMENCLATURE
12*	*	10E8.5	1-8 9-16 17-24 ↓ 73-80	Z(I)	z	Axial station
13**	**	10E8.5	1-8 9-16 17-24 ↓ 73-80	AP(I)	A_p	Total external catalyst particle surface area per unit vol. of 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.

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

CODING OF A SAMPLE DATA CASE

One-Dimensional Steady-State Model



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FIG. 2

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 st ady-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 .XXXXXX ± 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 SLOPE CONVERGES TO .XXXXX ± 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) "CONCENTRATION GRADIENT FOUND 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.

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

FIG. 3a

```
**SAMPLE DATA CASE (1-DIM SS)**    MIXED RED # 60 = 3.0 * P = 100.

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

      R           ALPHA3      C6M         DIF3        DIF4        WM4         WM3         WM2         WM1         ZEND
   .107300+02  .214000+11  .338000+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       ZO
   .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

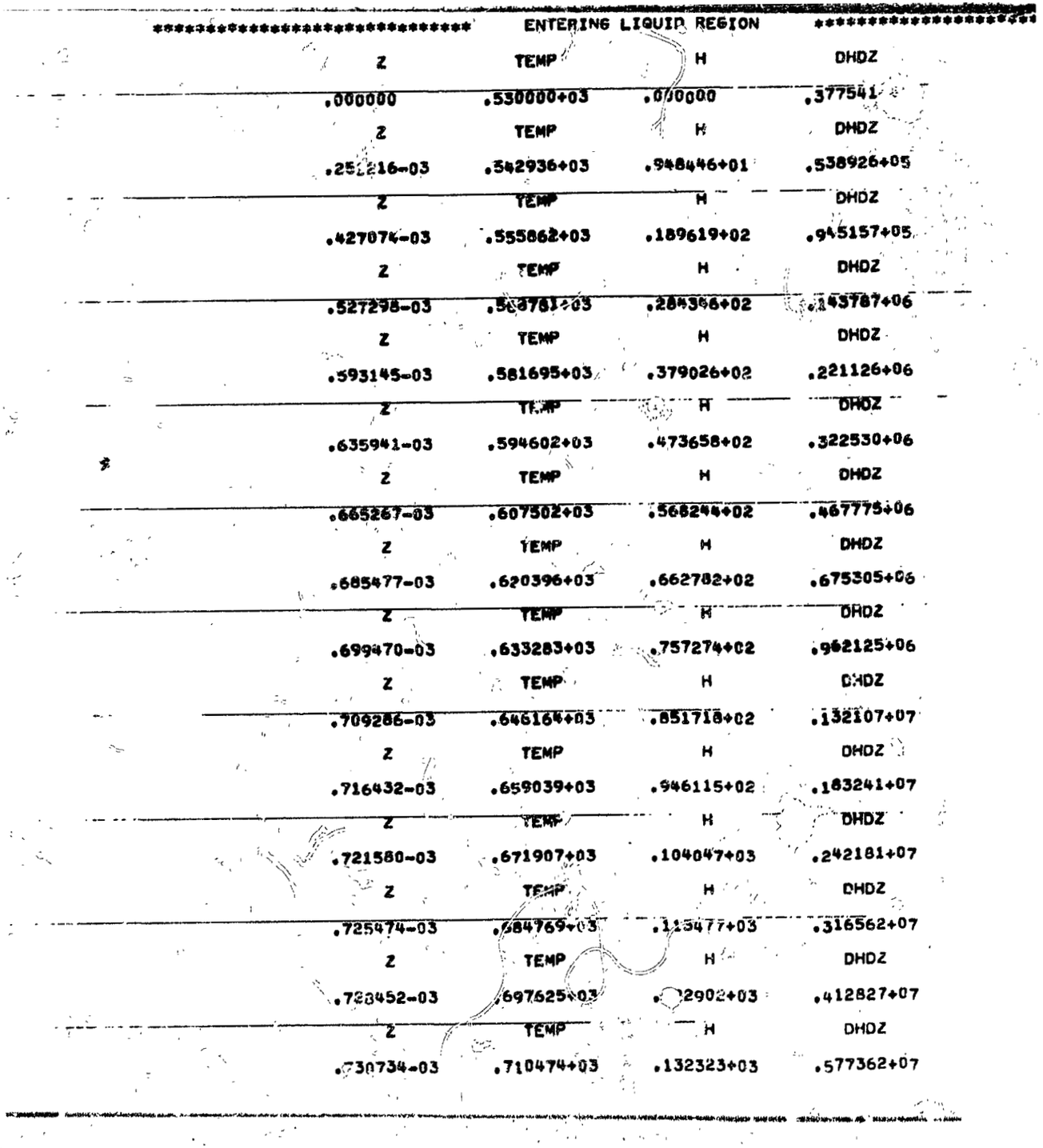
.000000	.000000	.100000+01	.210000+02	.000000						
.000000	.550000-02	.111000-01	.167000-01	.168000-01	.439000-01	.575000-01	.711000-01	.847000-01	.983000-01	
.111900+00	.125500-00	.139100-00	.152700-00	.166300-00	.179900-00	.193500-00	.207100-00	.220700-00	.234300-00	
.250000-00										
.100000-02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

Z VS AP TABLE

.000000	.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	.330000+03
.330000+03										

Z VS DELTA TABLE

.000000	.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	.340000-00
.340000-00										



**********	ENTERING LIQUID REGION		**********
Z	TEMP	H	DHDZ
.000000	.530000+03	.000000	.377541
Z	TEMP	H	DHDZ
.251216-03	.542936+03	.948446+01	.538926+05
Z	TEMP	H	DHDZ
.427074-03	.555862+03	.189619+02	.945157+05
Z	TEMP	H	DHDZ
.527298-03	.563781+03	.284366+02	.143787+06
Z	TEMP	H	DHDZ
.593145-03	.581695+03	.379026+02	.221126+06
Z	TEMP	H	DHDZ
.635941-03	.594602+03	.473658+02	.322530+06
Z	TEMP	H	DHDZ
.665267-03	.607502+03	.568244+02	.467775+06
Z	TEMP	H	DHDZ
.685477-03	.620396+03	.662782+02	.675305+06
Z	TEMP	H	DHDZ
.699470-03	.633283+03	.757274+02	.962125+06
Z	TEMP	H	DHDZ
.709286-03	.646164+03	.851718+02	.132107+07
Z	TEMP	H	DHDZ
.716432-03	.659039+03	.946115+02	.183241+07
Z	TEMP	H	DHDZ
.721580-03	.671907+03	.104047+03	.242181+07
Z	TEMP	H	DHDZ
.725474-03	.684769+03	.113477+03	.316562+07
Z	TEMP	H	DHDZ
.728452-03	.697625+03	.122902+03	.412827+07
Z	TEMP	H	DHDZ
.730734-03	.710474+03	.132323+03	.577362+07

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FIG. 3b

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	.187839+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	.583323+08

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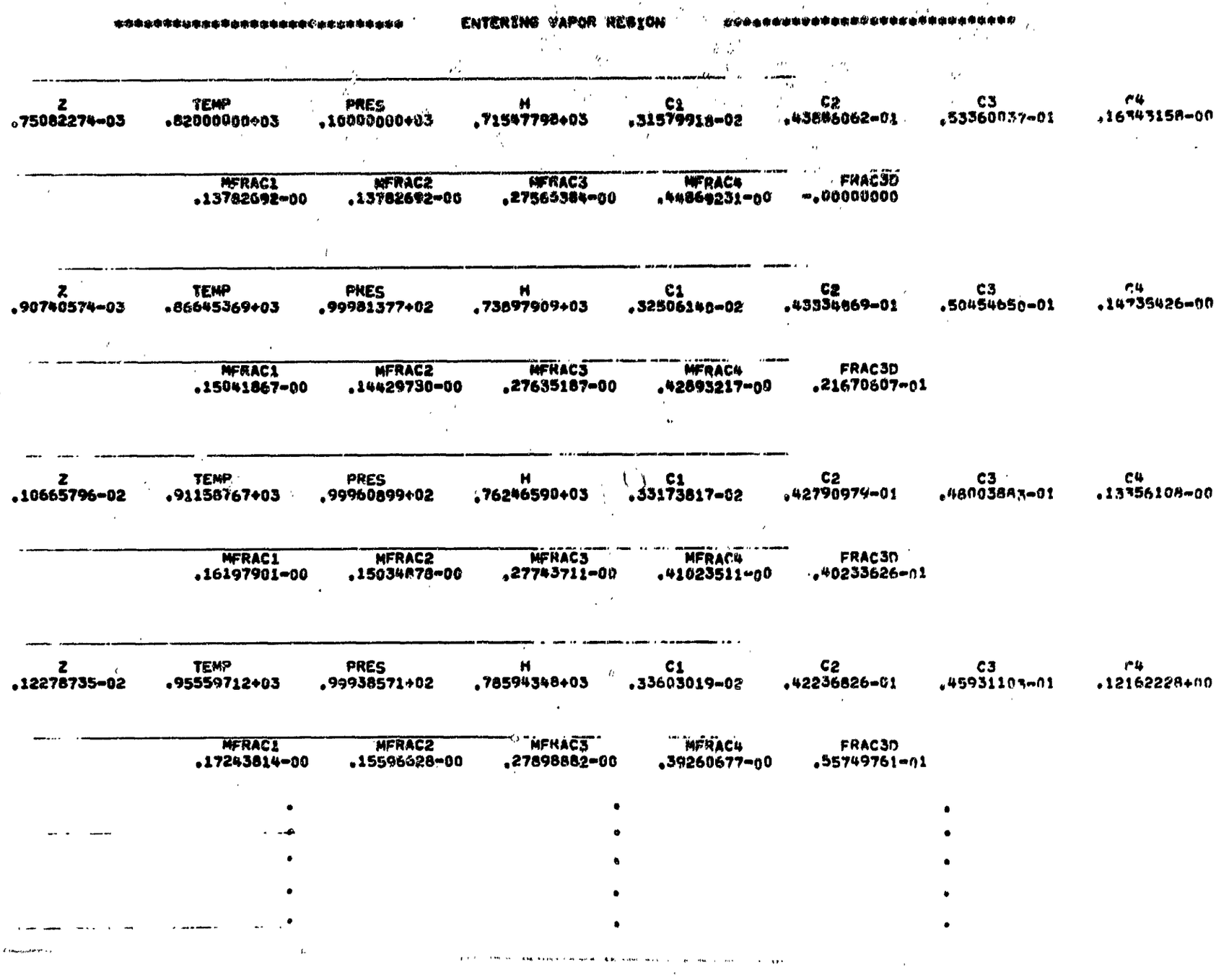
FIG. 3c

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FIG. 3d


```
**********  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
```



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FIG. 3e

Z	TEMP	PRES	H	C1	C2	C3	C4
.17155202-00	.19507243+04	.78863929+02	.14092872+04	.39661221-02	.31522408-01	.96798352-02	.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
.2459068-02	.2655209-02	.2858234-02	.3068889-02	.3287984-02	.3516443-02	.3755323-02	.4005866-02	.4269497-02	.4547898-02
.4843068-02	.5157416-02	.5493988-02	.5856422-02	.6249363-02	.6678468-02	.7151910-02	.7680163-02	.8278725-02	.8971330-02
.9797482-02	.1083580-01	.1225605-01	.1465606-01	.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	.2303880-00	.2500000-00					

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

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

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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. $1 \leq NCASE \leq 999$.

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 0.95×10^{-4} ft^2/sec.

DONH3 is the diffusion coefficient of ammonia in the gas phase at STP. It equals 0.17×10^{-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.

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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	ALPHA1	$\alpha^{N_2H_4}$	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	**	10F8.4	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

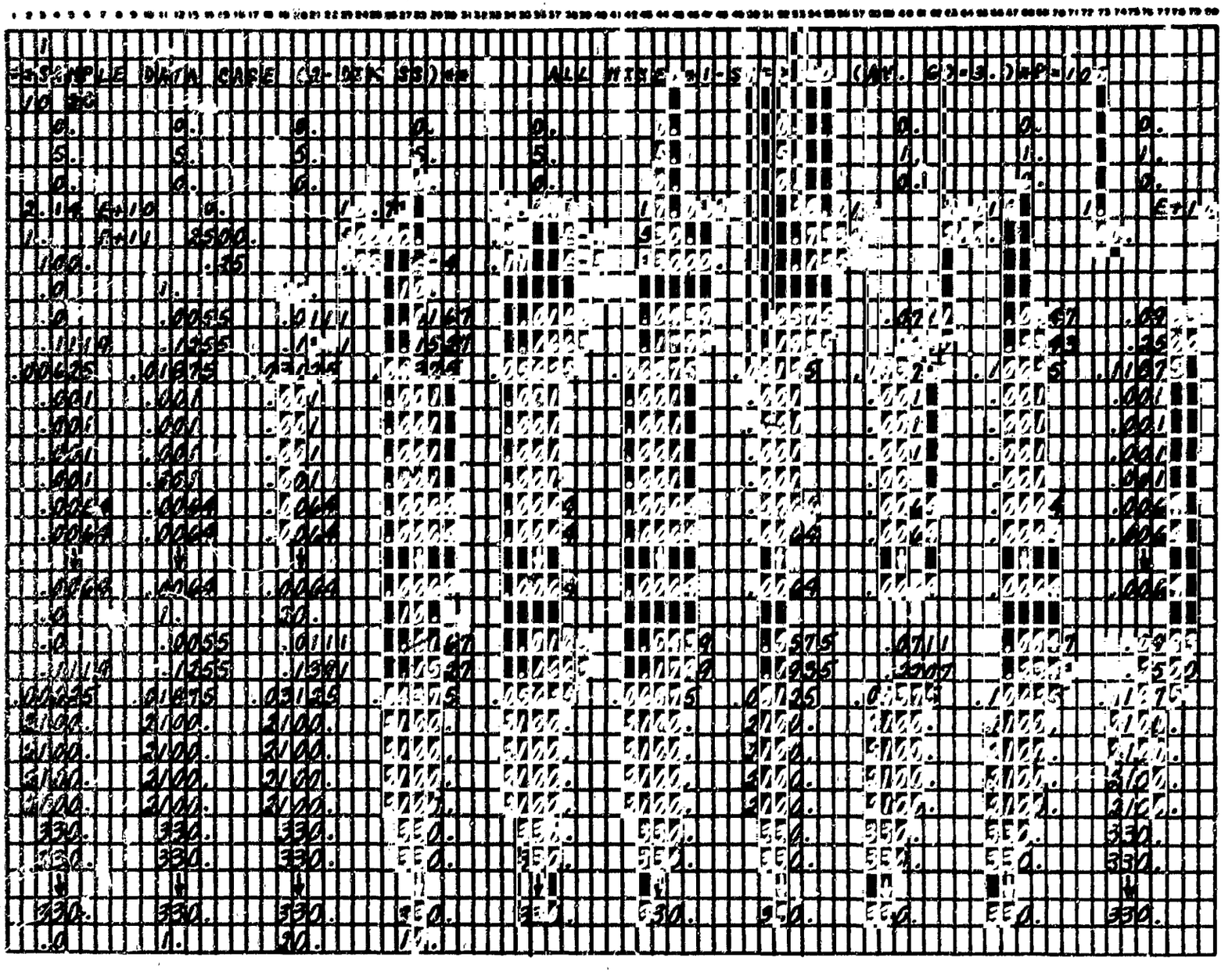
*Enough cards should be used to contain (NØFZ) values of z at the rate of ten per card.
**Enough cards should be used to contain (NRINGS) values of RAD at the rate of ten per card.
***Enough cards should be used to contain (NRINGS) values of A and AP for each z at the rate of ten per card (see detailed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



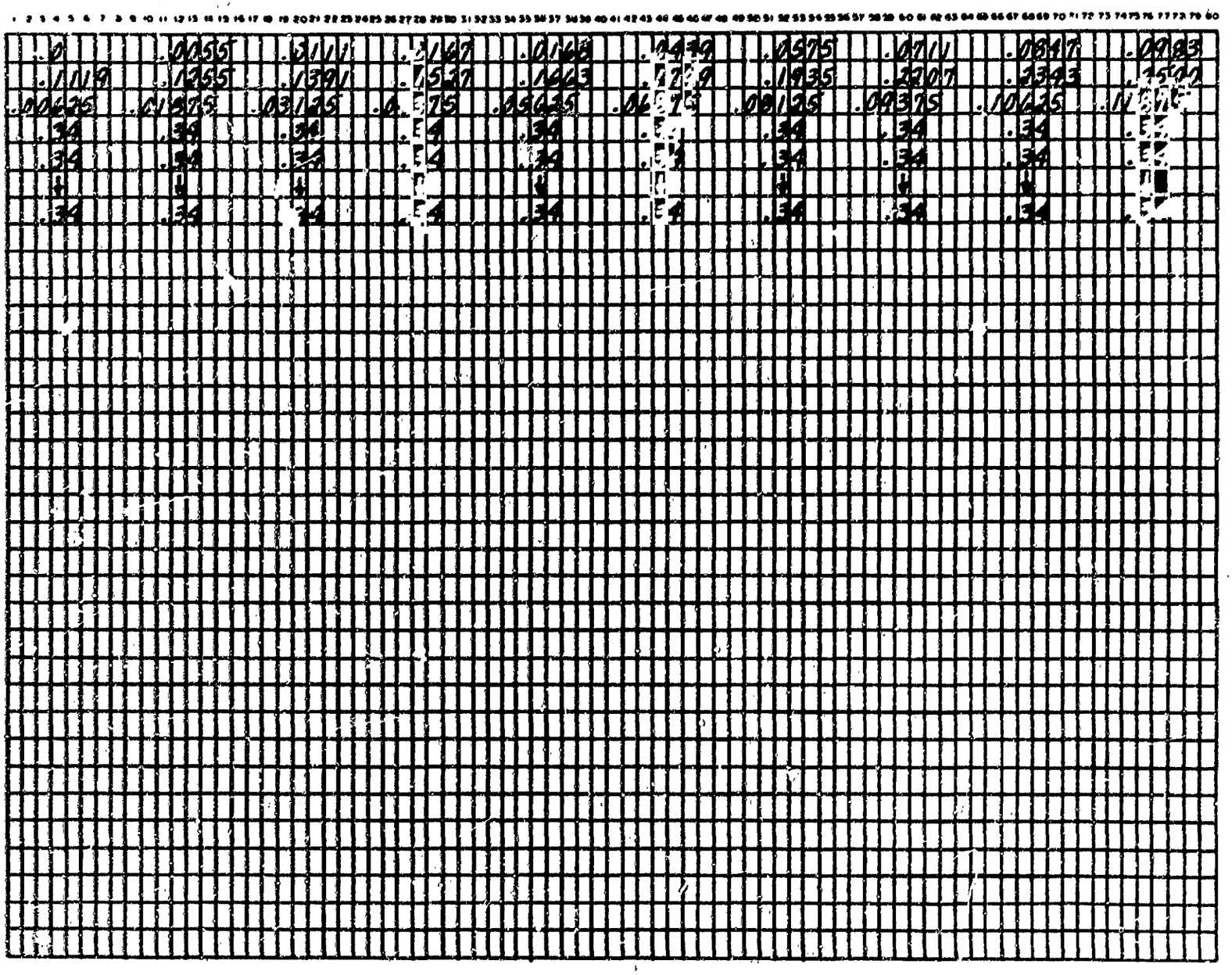
Card No.
1
2
3
4
5
6
7
8
9
10
11a
11b
12
13a
13b
13c
13d
13e
13f
↓
13t
14
15a
15b
↓
17a
17b
17c
17d
17e
17f
↓
17t
18
(CONT.)

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FIG. 4a

CODING OF A SAMPLE DATA CASE (CONTINUED)

TWO - DIMENSIONAL STEADY - STATE MODEL



Card No.

21b

21t

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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. G0=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

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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.		330.	330.	330.	330.	330.	330.	330.	330.	17g
3		330.	330.	330.	330.	330.	330.	330.	330.	17h
		330.	330.	330.	330.	330.	330.	330.	330.	17i
		330.	330.	330.	330.	330.	330.	330.	330.	17j
		330.	330.	330.	330.	330.	330.	330.	330.	17k
		330.	330.	330.	330.	330.	330.	330.	330.	17l
		330.	330.	330.	330.	330.	330.	330.	330.	17m
		330.	330.	330.	330.	330.	330.	330.	330.	17n
		330.	330.	330.	330.	330.	330.	330.	330.	17o
330.		330.	330.	330.	330.	330.	330.	330.	330.	17p
33		330.	330.	330.	330.	330.	330.	330.	330.	17q
330.		330.	330.	330.	330.	330.	330.	330.	330.	17r
330.		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	.0167	.0168	.0439	.0575	.0711	.0847	.0983	19a
.1119	.1255	.1391	.1527	.1663	.1799	.1935	.2207	.2343	.2500	19b
.0062	.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

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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, (N_2H_4), ammonia, (NH_3), nitrogen, (N_2), and hydrogen, (H_2), 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-STEP GO (AV. GI=1.)*P=100

PROGRAM INPUT

KINd	F	Gg	Zu
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 = .2500+01 HF = .0000 R = .1873+02 MN2d4 = .4205+02 MdH3 = .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

KAUXUS = .4250+05

A VS Z TABLE

			.04000	.10000+01	.20000+02	.19000+02			
.00000	.05000-02	.11100-01	.16700-01	.16800-01	.43900-01	.57500-01	.71100-01	.84700-01	.98300-01
.11940+00	.12550+00	.13910-00	.15270-00	.16630-00	.17990-00	.19350-00	.22070-00	.23430-00	.25000-00
.02500-02	.13750-01	.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

AP VS Z TABLE

.00000	.55000-02	.11100-01	.16700-01	.16800-01	.43900-01	.57500-01	.71100-01	.84700-01	.98300-01
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
.62500-02	.18750-01	.31250-01	.43750-01	.56250-01	.68750-01	.81250-01	.93750-01	.10625+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
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04	.21000+04
.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
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
.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
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
.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	.55000-02	.11100-01	.16700-01	.16800-01	.43900-01	.57500-01	.71100-01	.84700-01	.98700-01
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
.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
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
.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
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
.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
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
.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

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	.59400+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 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	.59400+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 3

Z	T	Z	T	Z	T	Z	T	Z	T
.00000	.53000+03	.41918-03	.54294+03	.66785-03	.55586+03	.78787-03	.56878+03	.87087-03	.58169+03
.91777-03	.59400+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	.78748+03	.10530-02	.80031+03	.10536-02	.81313+03	.10535-02	.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	.87086-03	.58169+03
.91775-03	.59400+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 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	.59400+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 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	.59400+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 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
.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	.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

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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

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FIG. 6e

********** 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	.25034-03	.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 = .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
.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	.31893-05	.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

MFRAC1	MFRAC2	MFRAC3	MFRAC4	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	.16161-04	.74414-00
.59266-00	.31853-00	.88614-01	.00000	.75529-00

FIG. 6h

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RING	Z	TEMP	N2H4	NH3	N2	H2
1	.25000-00	.19944+04	.30099-05	.69183-02	.21362-01	.26649-02
2	.25000-00	.19939+04	.28178-05	.69062-02	.21372-01	.26671-02
3	.25000-00	.19919+04	.29399-05	.68667-02	.21408-01	.26746-02
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

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****** 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_1 [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_1.

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
a	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.

One-Dimensional Model

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):

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

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_o.

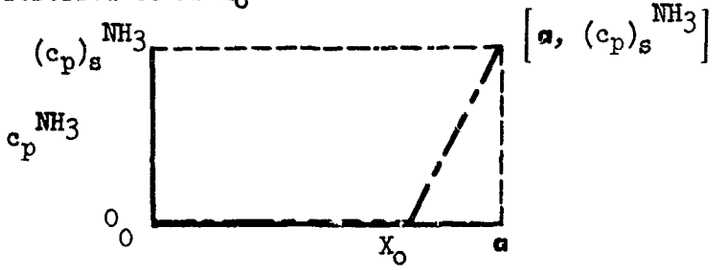


Fig. (I-9)

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: $(c_p)_s^{NH3} = c_i^{NH3}/2$.

2. Using this value, a value is found for the slope of the concentration profile at the surface, $\left[dc_p^{NH3}/dx\right]_{x=a}$.

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

where k_c^{NH3} is calculated from an equation given in Ref. 1 and D_p^{NH3} is calculated from Eq. (I-3).

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

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

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

where T_i and c_i^{N2H4} are input to the subroutine, H^{N2H4} and H^{NH3} are taken from tables in the computer program, and h_c and k_c^{N2H4} are calculated according to the equations in Ref. 1.

4. Using the point $\left[a, (c_p)_s^{NH3}\right]$ and the slope $\left[dc_p^{NH3}/dx\right]_{x=a}$, a line is established and extrapolated to the $c_p^{NH3} = 0$ axis line, intersecting the axis line at X_o (as in Fig. I-9).

5. The value for X_o is calculated from

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

Since the region of primary interest is the particle surface, it is at this point that convergence on a value for $c_p^{NH3}(x)$ is tested. To test for convergence, a new $(c_p)_s^{NH3}$ is calculated and compared to the previous $(c_p)_s^{NH3}$. The new value for $(c_p)_s^{NH3}$ 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

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

As can be seen in Fig. (I-9) in distributions of this type all values of $c_p^{NH3}(x)$ 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

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

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

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

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

6. A new value for $(c_p)_s^{NH3}$ is calculated using Eq. (I-7) where the integral is evaluated numerically using the trapezoidal method.

7. A new value for $\left[dc_p^{NH3}/dx\right]_{x=a}$ is calculated from Eq. (I-3) using the newly calculated $(c_p)_s^{NH3}$.

8. New values are calculated for $(T_p)_s$, D_p^{NH3}, γ, β, k_o.

9. The following convergence tests are made:

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

and

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

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 $(c_p)_s^{NH3}$ 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 $X_o/a \leq x/a \leq 1$ 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

$$
\begin{aligned}
c_p^{NH_3}(x/a) = c_i^{NH_3} - \frac{a}{D_p^{NH_3}}\left[\frac{1}{x/a} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right]\Bigg\{ & r_{het}^{1}\int_{X_o/a}^{X_o/a + \Delta X/a} \xi\, d\xi \\
& + r_{het}^{2}\int_{X_o/a + \Delta X/a}^{X_o/a + 2\Delta X/a} \xi\, d\xi \quad + \cdots + r_{het}^{24}\int_{X_o/a + (k-1)\Delta X/a}^{X_o/a + k\Delta X/a} \xi\, d\xi \Bigg\} \\
& - \frac{a^2}{D_p^{NH_3}}\Bigg\{ r_{het}^{1}\int_{X_o/a + k\Delta X/a}^{X_o/a + (k+1)\Delta X/a}\left[\frac{1}{\xi} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right]\xi^2\, d\xi \\
& + r_{het}^{2}\int_{X_o/a + (k+1)\Delta X/a}^{X_o/a + (k+2)\Delta X/a}\left[\frac{1}{\xi} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right]\xi^2 d\xi + \cdots \\
& + r_{het}^{24}\int_{X_o/a + 23\Delta X/a}^{X_o/a + 24\Delta X/a}\left[\frac{1}{\xi} - \frac{ak_c^{NH_3} - D_p^{NH_3}}{ak_c^{NH_3}}\right]\xi^2 d\xi
\end{aligned}
\qquad \text{(I-13)}
$$

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

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

viz $$\int_a^b \xi\, d\xi = \frac{\xi^2}{2}\Bigg|_a^b = \frac{b^2}{2} - \frac{a^2}{2}$$

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

(d) rearranging and integrating term by term in Eq. (I-13) yields the finite sum approximation for $c_p^{NH3}(x/a)$ at each subdivision of the interval from X_o/a to 1:

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

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

(e) the values for $c_p^{NH3}(x/a)\big|_{x=X_o}$ and $c_p^{NH3}(x/a)\big|_{x=a}$ 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 $\left[dc_p^{NH3}/dx\right]_{x=a}$ is calculated from Eq. (I-3) using the newly calculated $(c_p)_s^{NH3}$.

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.

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

$$TGRAD = h_c \left[T_i - (T_p)_s \right] \qquad \text{(I-16)}$$

(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)

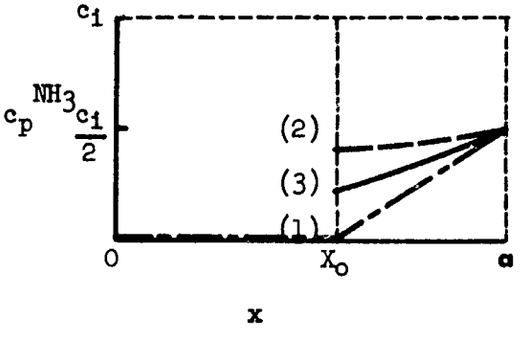


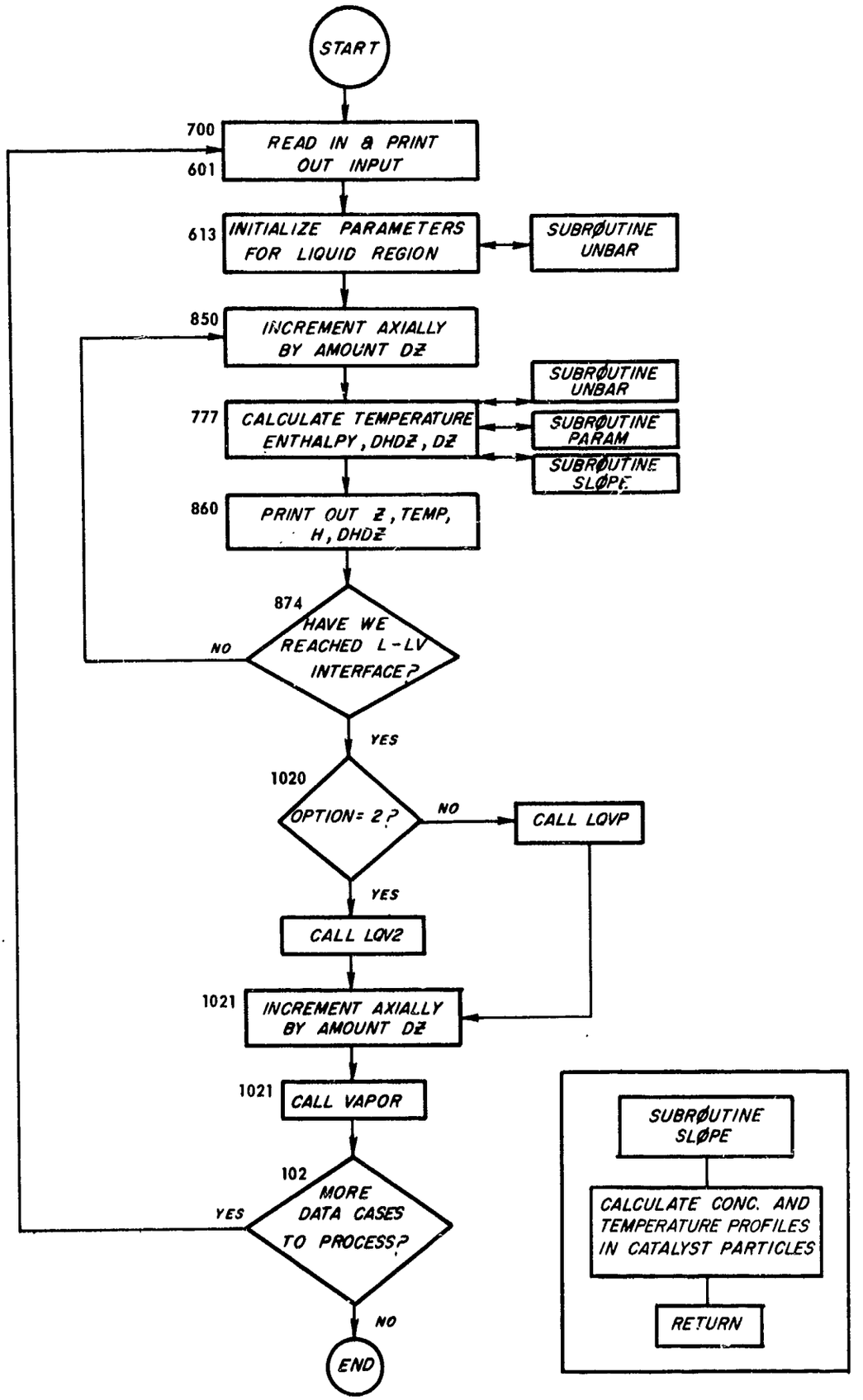
Fig. (I-10)

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FIG. I-1

ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

MAIN PROGRAM and SUBRØUTINE SLØPE: Flow Diagrams

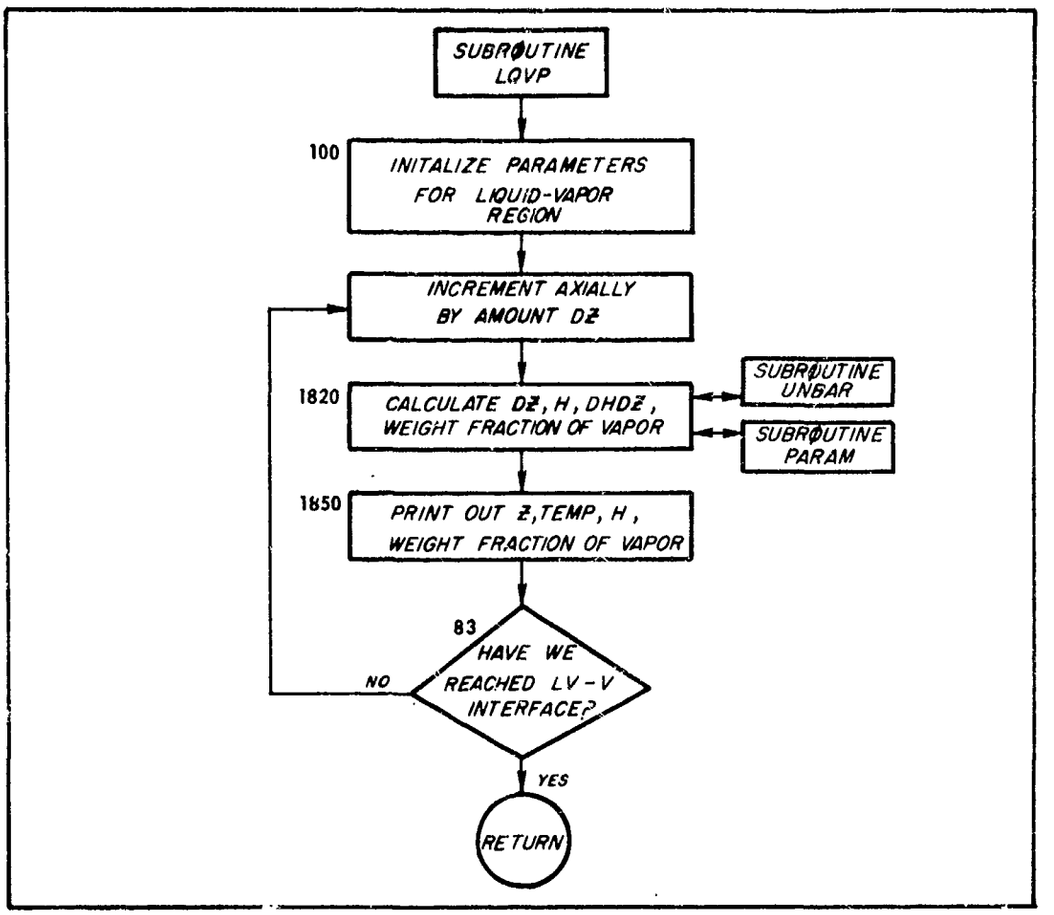


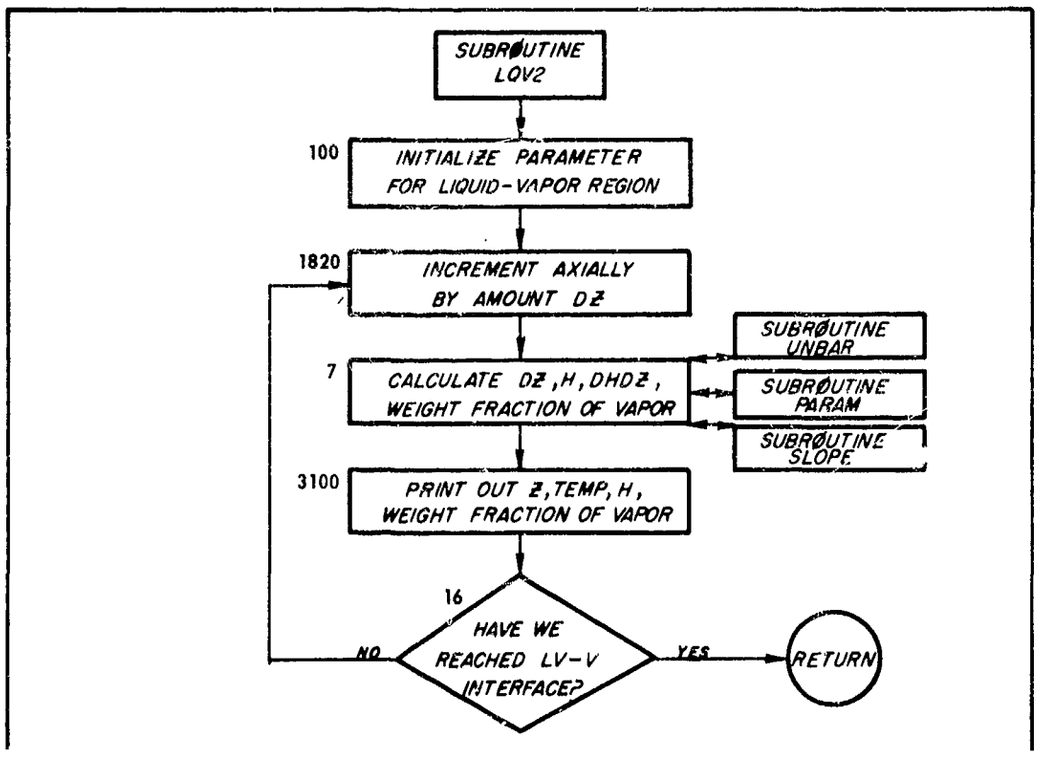
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ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

FIG. I-2

SUBROUTINES LQVP and LQV2 : Flow Diagrams



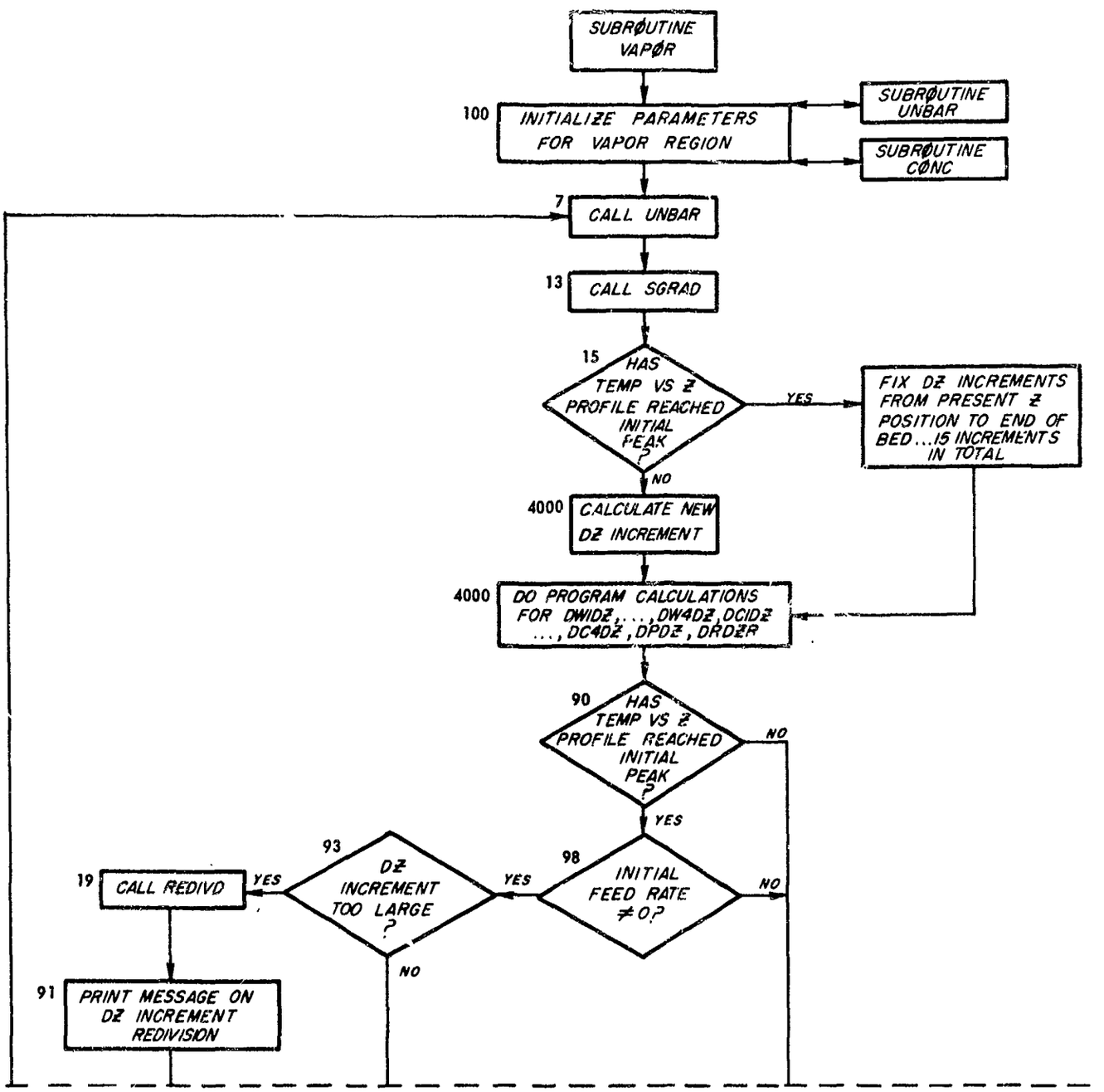


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FIG. I-3

ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

SUBRØUTINE VAPØR : Flow Diagram



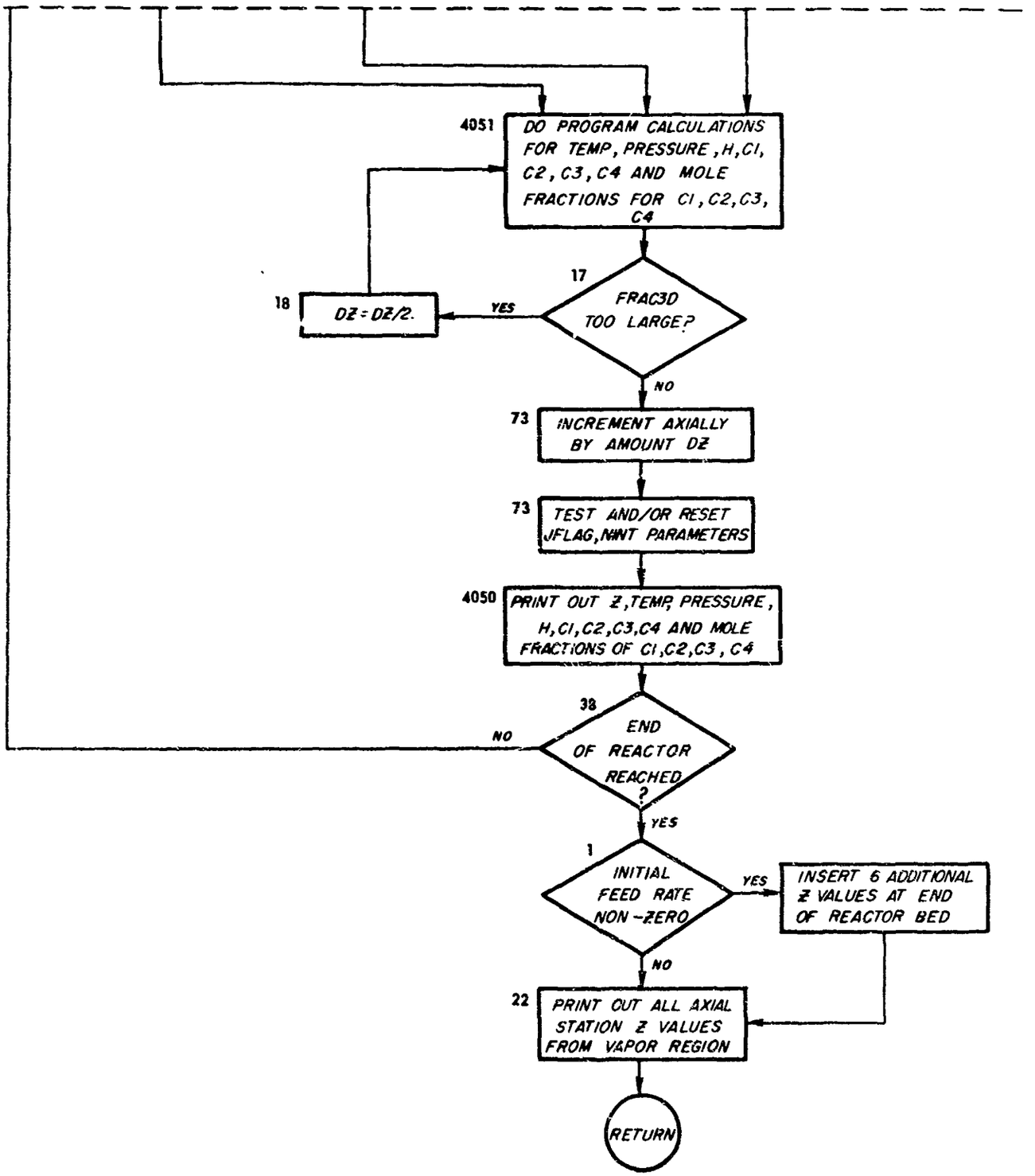
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ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

SUBROUTINE VAPOR (cont.)

FIG. I-4

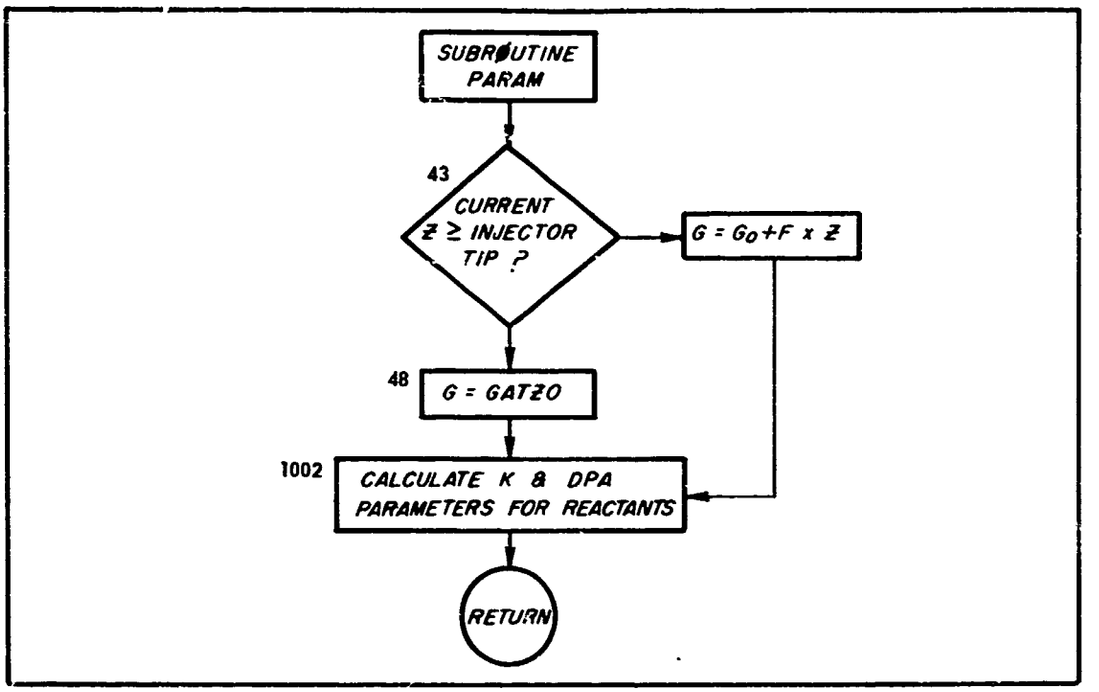


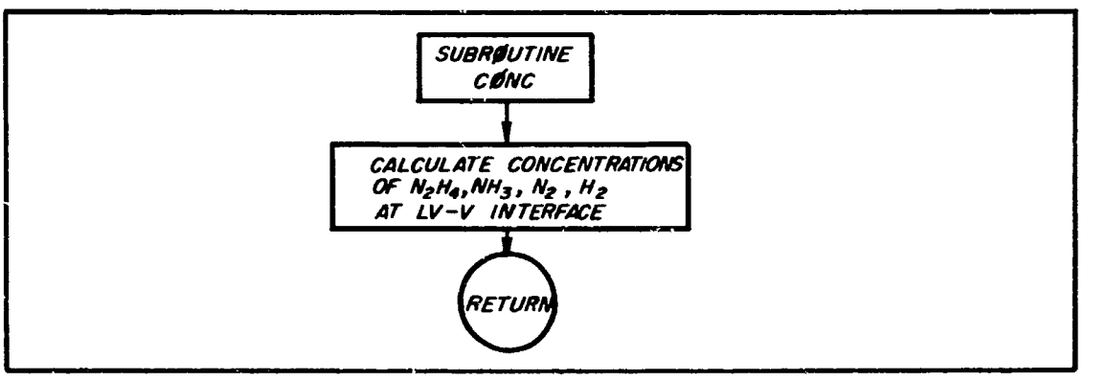
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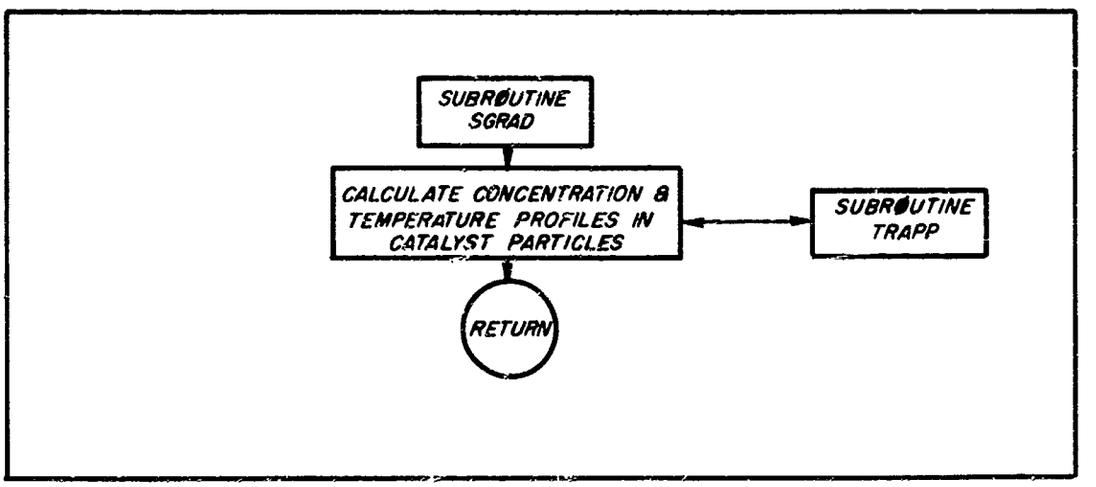
ONE-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

FIG. I-5

SUBRØUTINES PARAM, CØNC, and SGRAD: Flow Diagrams







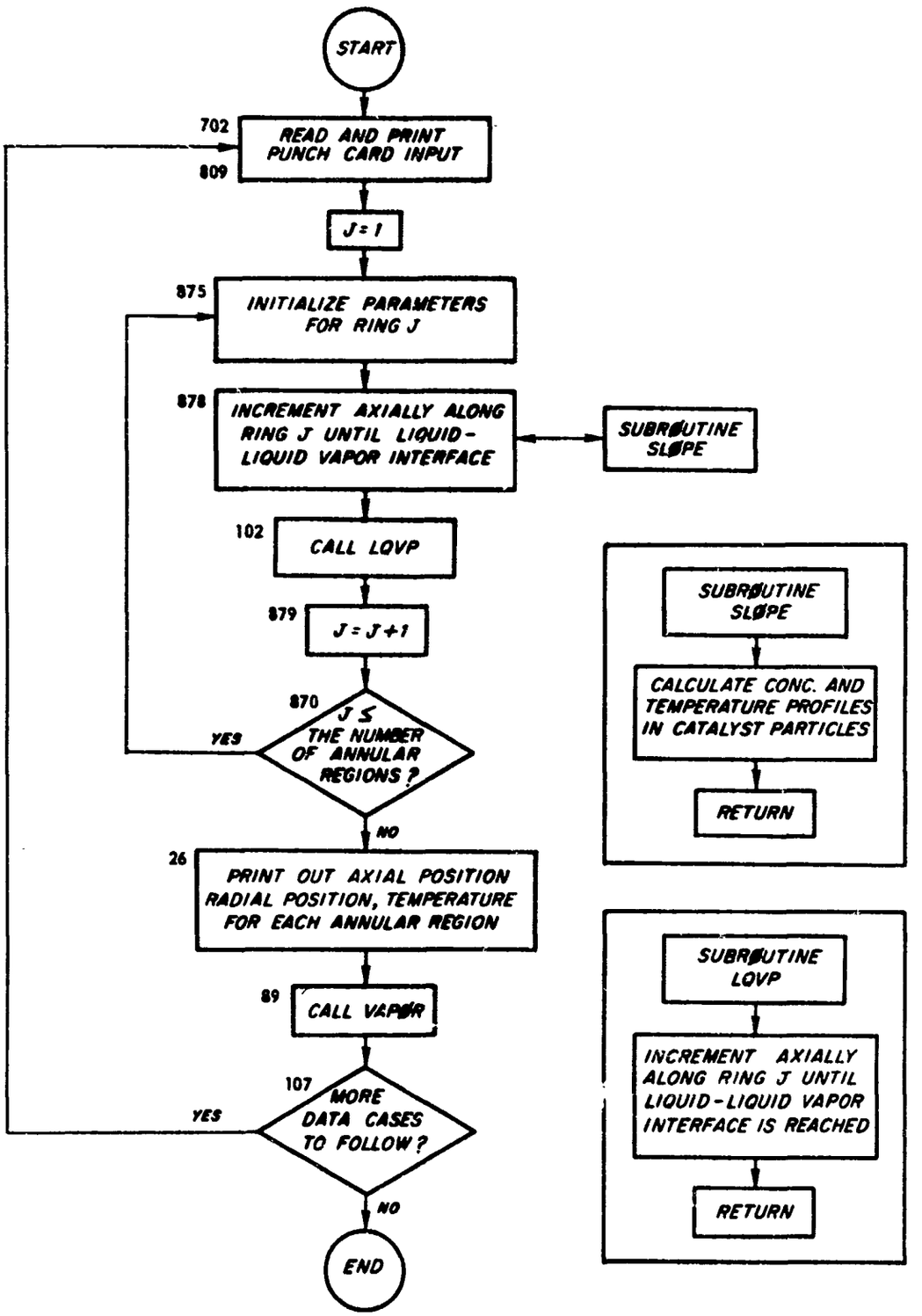
G910461-30

FIG. I-6

TWO-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

MAIN PROGRAM

FLOW DIAGRAM

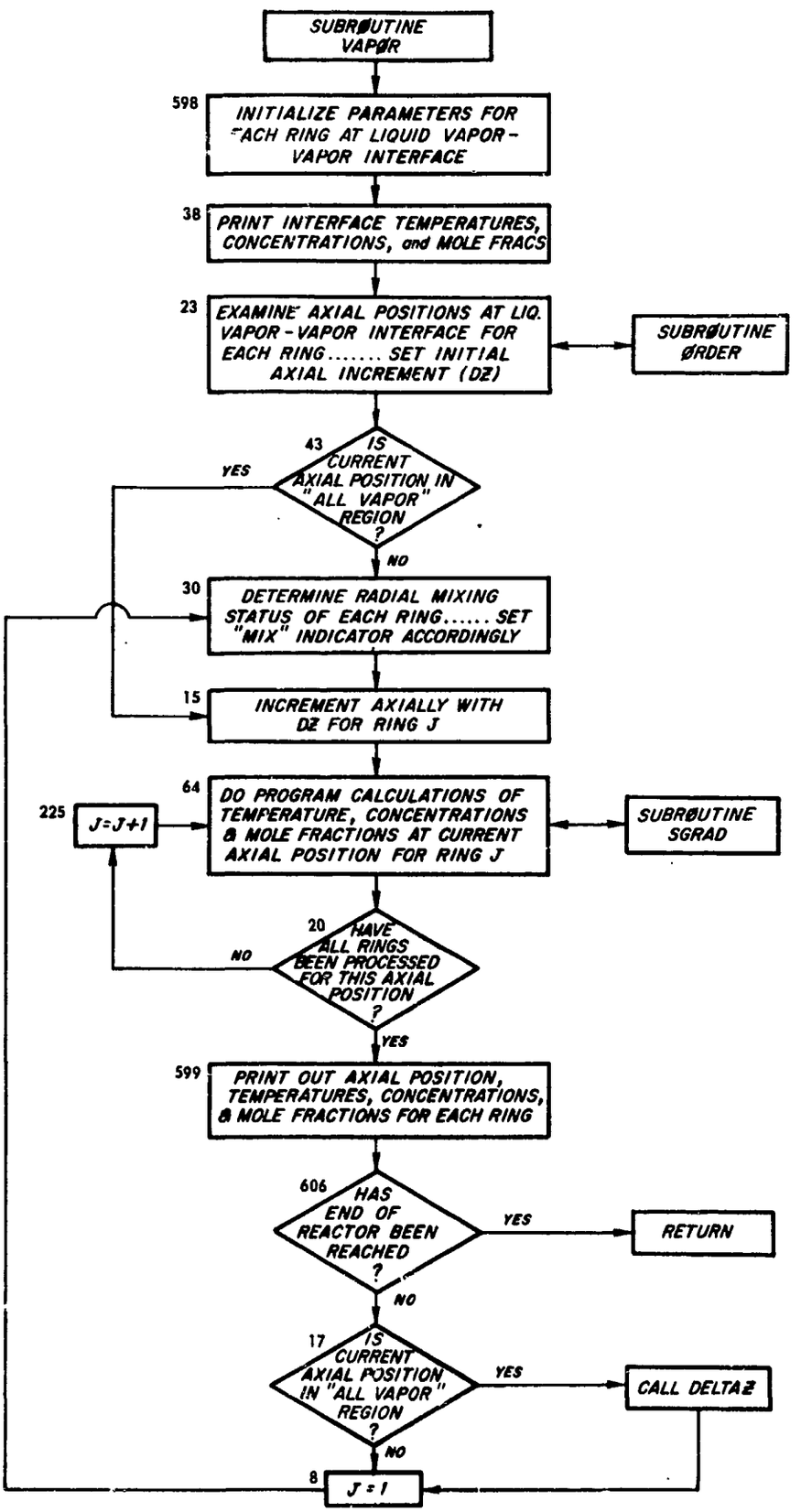


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FIG. I-7

TWO-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

SUBRØUTINE VAPØR : Flow Diagram



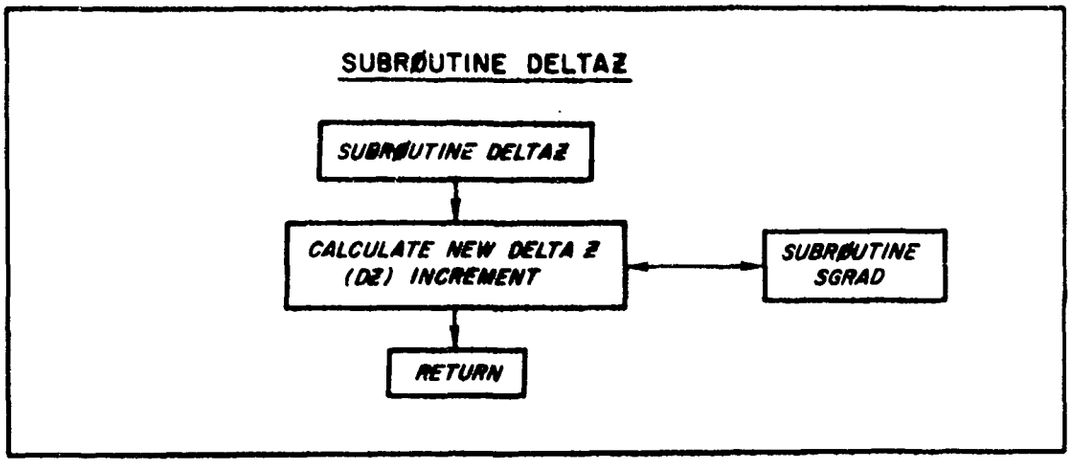
G910461-30

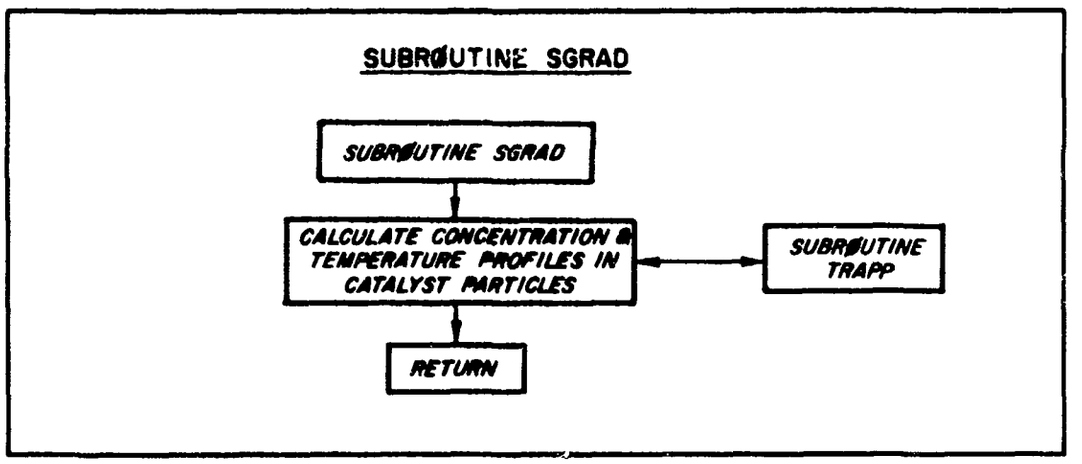
FIG. I-8

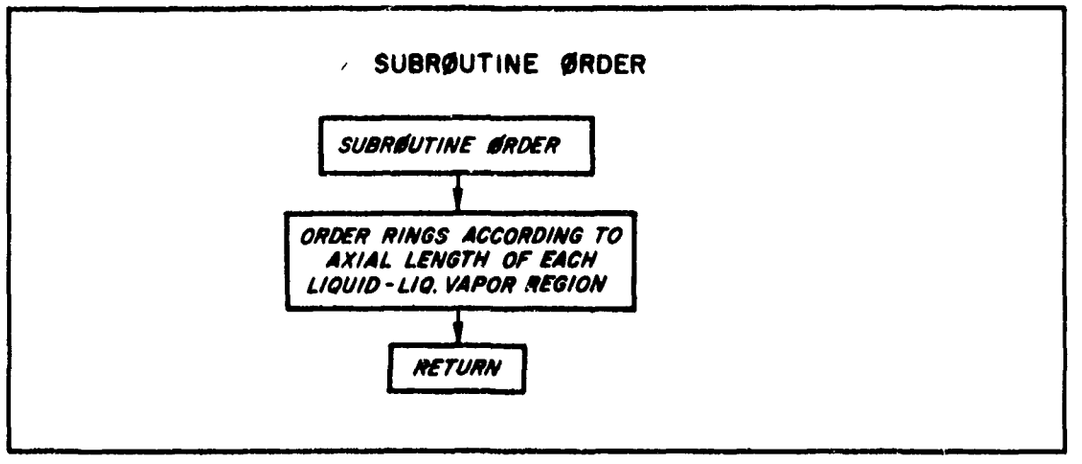
TWO-DIMENSIONAL STEADY-STATE COMPUTER PROGRAM

SUBRØUTINES DELTAZ, SGRAD, and ØRDER

Flow Diagrams







APPENDIX II

LISTING OF COMPUTER PROGRAMS

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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 9,10,...          CONTAIN THE AXIAL STATION Z VALUES
```

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```
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                                                              0
      INTEGER OPTION,PRINT                                                  10
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),      20
     1        SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)          30
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,        40
     1        WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2     50
     2        ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI                             60
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)                               70
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,           80
      COMMON /MUVST/VISVST(30)                                              90
      COMMON /FLAGS/MFLAG,KFLAG,PRINT                                      100
      COMMON /IFGEQ0/IFC,SATZ0                                             110
      COMMON /LIZTBL/DHVST(18),DHLVST(18)                                  120
      COMMON /DAVTBL/VPTBL(44)                                             130
      DIMENSION  TITLE(14)                                                 140
      READ (5,700) NCASE                                                   150
  700 FORMAT (I3)                                                          160
      KOUNT=1                                                              170
  705 READ (5,608) TITLE                                                   180
  608 FORMAT (14A6)                                                        190
      WRITE (6,609) TITLE                                                  200
  609 FORMAT (1H1,14A6//)                                                  210
      IFC=1                                                                220
      READ (5,809) OPTION,PRINT,NOFZ                                       230
  809 FORMAT (2I2,I3)                                                      240
```

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```
      READ (5,800) Z0,GO,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 (6E10.5)
      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=GO+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
     X       HV
     X       TF          TVAP          CFL          PRESSURE          KP
     X       F
     X       GO )
      WRITE (6,601) HF,HL,HV,TF,TVAP,CFL,PRES,KP,FC,GO
  601 FORMAT (3X,10E11.6//)
      WRITE (6,602)
  602 FORMAT (7X,11HR          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) (ZTBLJ(I),I=1,4)
      READ (5,21) (ZTBLJ(I),I=5,NOFZ4)
      READ (5,21) (ZTBLJ(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)
```

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```
      WRITE (6,607)                                                          850
  607 FORMAT (52X,17H Z Vs DELTA TABLE )                                     860
      WRITE (6,22) (ZTBLD(I),I=1,4)                                          870
      WRITE (6,23) (ZTBLD(I),I=5,NOFZ4)                                      880
      WRITE (6,25)                                                           890
      WRITE (6,23) (ZTBLD(I),I=NOFZ5,NZTBL)                                  900
      WRITE (6,613)                                                          910
  613 FORMAT ('1'18X,'*********************************      ENTERING LIQUID  920
     A REGION      *********************************' )                      930
      NPEAC=0                                                                940
      DZ=0.0                                                                 950
      Z(1)=0.0                                                               960
      H=HF                                                                   970
      II=2                                                                   980
  850 Z(II)=Z(II-1)+DZ                                                       990
      TEMP=TF+(H-HF)/CPL                                                    1000
      CALL UNBAR (TBLVP(1),1,TEMP,0.,VP,KK)                                 1010
      CN2H4=(VP*YN4)/(R*TEMP)                                               1020
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)                                 1030
      CALL UNBAR (ZTBLAP(1),1,Z(II),0.,AP,KK)                               1040
      CALL UNBAR (ZTBLA(1),1,Z(II),0.,A,KK)                                 1050
      CALL PARAM(TEMP,Z(II),1,CN2H4,H4,0,G,GMMA,K,DPA,BETA)                 1060
      CALL SLOPE (CN2H4,GMMA,K,BETA,EN1,DERIV(II),DPA,A,DIF4)               1070
      IF(H-HL)777,776,777                                                   1080
  776 IF(H1.GT.20)DERIV(II)=DERIV(II-1)                                     1090
  777 DHDZ(II)=-(H4*DPA*AP*DERIV(II)+FC*(H-HF))/G                           1100
      DZ=-H4/(EMMX1*DHDZ(II))                                               1110
      WRITE(6,820)                                                          1120
  820 FORMAT (/39X,4HZ              TEMP              H              DHDZ )   1130
      WRITE (6,860) Z(II),TEMP,H,DHDZ(II)                                   1140
  860 FORMAT (/30X,4E15.6)                                                  1150
      IF(H-HL)874,1020,874                                                  1160
  874 H=H+DHDZ(II)*DZ                                                       1170
      IF(H-HL)875,1020,1000                                                 1180
  875 II=II+1                                                               1190
      GO TO 850                                                             1200
C     BACKSTEP TO L-L-V-BOUNDARY
 1000 DZ=(HL-H)/DHDZ(II)+DZ                                                 1210
      H=HL                                                                  1220
      II=II+1                                                               1230
      GO TO 850                                                             1240
 1020 IF(OPTION.EQ.2)CALL LQV2(H,Z(II),DERIV(II),II,DHDZ(II),TEMP,CN2H4)    1250
      IF(OPTION.EQ.2)GO TO 1021                                             1260
      CALL LQVP(H,Z(II),DERIV(II),II,DHDZ(II),TEMP)                         1270
C     START VAPOR REGION
 1021 DZ=-H4/(EMMX3*DHDZ(II))                                               1280
      CALL VAPOR(TEMP,Z(II),II,DHDZ(II),DERIV(II),H)                        1290
      KOUNT=KOUNT+1                                                         1300
      IF(KOUNT.LE.NCASE)GO TO 705                                           1310
      WRITE (6,102)                                                         1320
  102 FORMAT (////41X,30H *****   OPERATIONS COMPLETE   *****  )            1330
      STOP                                                                  1340
      END                                                                   1350


      SUBROUTINE LQVP (H,ZLV,Q,JJ,G1,TEMP)                                     0
      REAL KP,K                                                               10
      INTEGER PRINT                                                           20
```

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```
      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
      WRITE(6,100)
  100 FORMAT(109H1          ********************************    ENTERING L
     1IQUID-VAPOR REGION       ********************************   //)
      DERIV(JJ)=Q
      DHDZ(JJ)=01
      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),1,0.0,0.0,0.0,0,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 LQV2 (H,ZLV,G,JJ,01,TEMP,GN2H4)
      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
      WRITE(6,100)
  100 FORMAT(109H1          ********************************    ENTERING L
     1IQUID-VAPOR REGION       ********************************   //)
```

G910461-30

```
      DERIV(JJ)=Q                                                        140
      DHDZ(JJ)=Q1                                                        150
      Z(JJ)=ZLV                                                          160
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)                              170
      C4=CN2H4*((H4-HF+HL)/(H4+HF-HL))                                   180
      WFV=0.                                                             190
      JJ=JJ+1                                                            200
3101  CONTINUE                                                           210
1820  Z(JJ)=Z(JJ-1)+DZ                                                   220
      TEMP=TVAP                                                          230
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)                              240
      CALL UNBAR (ZTBLAP(1),1,Z(JJ),0.,AP,KK)                            250
      CALL UNBAR (ZTBLA(1),1,Z(JJ),0.,A,KK)                              260
      CALL PARAM(TEMP,Z(JJ),1,0.0,0.0,0,G,GMMA,K,DPA,BETA)               270
      IF(MFLAG.EQ.1)GO TO 7                                              280
      CALL SLOPE (C4,GMMA,K,BETA,EN1,DERIV(JJ),DPA,A,DIF4)               290
      GO TO 6                                                            300
7     DIFN=DIF4*((TEMP/492.)**1.823)*14.7/PRES                           310
      CALL UNBAR (VISVST(1),1,TEMP,0.,VIS,KK)                            320
      RHO=PRES*WM4/(R*TEMP)                                              330
      AKC=.61*G/RHO*((VIS/(RHO*DIFN))**-.667)*((G/(AP*VIS))**-.41)       340
      DERIV(JJ)=AKC*C4/DPA                                               350
6     DERIV(JJ)=Q*(1.-WFV)+DERIV(JJ)*WFV                                 360
      DHDZ(JJ)=-(H4*DPA*AP*DERIV(JJ)+FC*(H-HF))/G                        370
      DZ=-H4/(ENMX2*DHDZ(JJ))                                            380
      IF(H-HV)15,3050,15                                                 390
15    H=H+DHDZ(JJ)*DZ                                                    400
      IF(H-HV)3050,3050,3500                                             410
3050  WFV=(H-HL)/(HV-HL)                                                 420
      XLV=(HF-H)/H4                                                      430
      C4=PRES*WM4/(R*TEMP)*((1.-XLV)/(1.+XLV))                           440
3160  WRITE(6,3000)                                                      450
3000  FORMAT(//30X, 3H Z , 11X,5H TEMP 11X, 3H H  12X, 2  FV)            460
      WRITE(6,3100)Z(JJ),TEMP,H,WFV                                      470
3100  FORMAT (22X,E14.5,1X,E14.5,1X,E14.5,1X,E14.5////)                  480
      IF(H-HV)16,3150,16                                                 490
16    JJ=JJ+1                                                            500
      GO TO 3101                                                         510
3500  DZ=(HV-H)/DHDZ(JJ)*DZ                                              520
      H=HV                                                               530
      JJ=JJ+1                                                            540
      GO TO 1820                                                         550
3150  RETURN                                                             560
      END                                                                570
```

```
      SUBROUTINE CONC (C1,C2,C3,C4,ZC,H,T)                                C
C     THIS ROUTINE CALCULATES INITIAL N2H4,NH3,N2,H2 CONCENTRATIONS FOR
C     VAPOR REGION OF THE REACTOR BED
      INTEGER PRINT                                                       10
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),    20
     1        SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)        30
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,      40
     1        WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2  50
     2        ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI                           60
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)                             70
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,         80
      COMMON /MUVST/VISVST(30)                                            90
```

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```
      COMMON /FLAGS/MFLAG,KFLAG,PRINT                                   100
      CALL UNBAR (TBLH4(1),1,T,0.,H4,KK)                                110
      XV=-(H-HF)/H4                                                     120
      C4=((PRES*WM4)/(R*TVAP))*((1.-XV)/(1.+XV))                        130
      C3=((PRES*WM3)/(R*TVAP))*(XV/(1.+XV))                             140
      C2=((PRES*WM2)/(2.*R*TVAP))*(XV/(1.+XV))                          150
      C1=((PRES*WM1)/(2.*R*TVAP))*(XV/(1.+XV))                          160
      RETURN                                                            170
      END                                                               180
```

```
      SUBROUTINE PARAM (T,ZA,LOP,CC,HR,LVOP,G,GMMA,K,DPA,BETA)            0
      REAL KP,K                                                          10
      INTEGER PRINT                                                      20
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),   30
     1        SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)       40
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,     50
     1        WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2  60
     2        ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI                          70
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)                            80
      COMMON /TOL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,         90
      COMMON /MUVST/VISVST(30)                                          100
      COMMON /FLAGS/MFLAG,KFLAG,PRINT                                   110
      COMMON /IFCGO/IFC,GATZ0                                           120
      IF(ZA-Z0)43,48,48                                                 130
   43 G=GO+FC*ZA                                                        140
      GO TO 52                                                          150
C     Z HAS EXCEEDED HYDRAZINE INJECTOR TUBE LENGTH    - G CONSTANT FROM
C     HERE TO END OF REG
   48 G=GATZ0                                                           160
      FC=0.                                                             170
   52 IF(LVOP.EQ.1)GO TO 1004                                           180
      GMMA=AGM/T                                                        190
C     CALCULATE K,DPA FOR N2H4
      K=ALPHA1*EXP(-GMMA)                                               200
 1001 DPL=DIF4*(T/492.)**1.832 *(14.7/PRES)*(1.-EXP(-.0672*(PRES*492.)/(  210
     114.7*T)))                                                         220
      DPA=DPL                                                           230
 1002 BETA=-(CC*HR*DPA)/(KP*T)                                          240
      GO TO 1003                                                        250
 1004 GMMA=BGM/T                                                        260
C     CALCULATE K,DPA FOR NH3
      K=ALPHA2*EXP(-GMMA)/C1**1.5                                       270
      DPV=DIF3*(T/492.)**1.832 *(14.7/PRES)*(1.-EXP(-.0672*(PRES*492.)/(  280
     114.7*T)))                                                         290
      DPA=DPV                                                           300
      GO TO 1002                                                        310
 1003 RETURN                                                            320
      END                                                               330
```

```
      SUBROUTINE VAPOR (TEMP,ZV,LL,Q1,Q,H)                               0
      REAL KP,K                                                          10
      REAL  MBSS                                                         20
      INTEGER PRINT                                                      30
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),   40
```

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```
     1         SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)                50
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,              60
     1         WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2          70
     2         ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI                                  80
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)                                    90
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,               100
      COMMON /MUVST/VISVST(30)                                                  110
      COMMON /FLAGS/MFLAG,KFLAG,PRINT                                           120
      COMMON /IFCEOD/IFC,GAMZ0                                                  130
      COMMON  /BBBB/DP3,A,KC3,K0,X0A,CPS,CI3,GAMMA,BETA                        140
      COMMON  /CCC/HHTBL(40),HITBL(40)                                          150
      COMMON  /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)                  160
      JZ=LL                                                                     170
      Z(LL)=ZV                                                                  180
      TEMP=TVAP                                                                 190
      PERC3D=0.                                                                 200
      ZBOUND=ZEND                                                               210
      KFLAG=0                                                                   220
      JFLAG=0                                                                   230
      KOUNT=0                                                                   240
      INJECT=0                                                                  250
      N=7                                                                       260
      THREE=3.                                                                  270
      WRITE(6,100)                                                              280
  100 FORMAT(109H1                    ********************************        ENTE  290
     1RING VAPOR REGION       ********************************  //)            300
      CALL CONC (C1,C2,C3,C4,Z(LL),H,TEMP)                                      310
      SUM=C1/WM1+C2/WM2+C3/WM3+C4/WM4                                           320
      FRAC1=C1/(WM1*SUM)                                                        330
      FRAC2=C2/(WM2*SUM)                                                        340
      FRAC3=C3/(WM3*SUM)                                                        350
      FRAC4=C4/(WM4*SUM)                                                        360
      FRAC3D=(FRAC1/FRAC2-1.)/(3.-FRAC1/FRAC2)                                  370
      WRITE(6,4059)                                                             380
      WRITE (6,4050) Z(LL),TEMP,PRES,H,C1,C2,C3,C4                              390
      WRITE (6,37)                                                              400
      WRITE (6,38) FRAC1,FRAC2,FRAC3,FRAC4,FRAC3D                               410
 3990 CALL UNBAR (SHTBL1(1),1,TEMP,0.,CP4,KK)                                   420
      CALL UNBAR (SHTBL2(1),1,TEMP,0.,CP3,KK)                                   430
      CALL UNBAR (SHTBL3(1),1,TEMP,0.,CP2,KK)                                   440
      CALL UNBAR (SHTBL4(1),1,TEMP,0.,CP1,KK)                                   450
      CAV=(C4*CP4+C3*CP3+C2*CP2+C1*CP1)/(C4+C3+C2+C1)                           460
      WMAV=(C1+C2+C3+C4)/(C1/WM1+C2/WM2+C3/WM3+C4/WM4)                          470
      CALL UNBAR (TBLH4(1),1,TEMP,0.,H4,KK)                                     480
      CALL UNBAR (ZTBLD(1),1,Z(LL),0.,DELA,KK)                                  490
      CALL UNBAR (ZTBLAP(1),1,Z(LL),0.,AP,KK)                                   500
      CALL UNBAR (ZTBLA(1),1,Z(LL),0.,A,KK)                                     510
      CALL PARAM(TEMP,Z(LL),1,C4,H4,0,G,GMMA,K,DPA,BETA)                        520
      IF(C4)7,29,7                                                              530
    7 DIFN=DIF4*((TEMP/492.)**1.823)*14.7/PRES                                  540
      CALL UNBAR (VISVST(1),1,TEMP,0.,VIS,KK)                                   550
      RHO=PRES*WMAV/(R*TEMP)                                                    560
      AKC=.61*G/RHO*((VIS/(RHO*DIFN))**-.667)*((G/(AP*VIS))**-.41)              570
      DERIV(LL)=AKC*C4/DPA                                                      580
    6 T4=AP*DPA*DERIV(LL)                                                       590
      GO TO 31                                                                  600
   29 T4=0.                                                                     610
   31 CALL UNBAR (TBLH3(1),1,TEMP,0.,H3,KK)                                     620
      CALL PARAM(TEMP,Z(LL),0,C3,H3,1,G,GMMA,K,DPA,BETA)                        630
      IF(C3)13,30,13                                                            640
```

```
  13    CALL SGRAD (GRAD,TGRAD)                                          650
        DERIV(LL)=GRAD/DPA                                               660
        T3=AP*DPA*DERIV(LL)                                              670
        GO TO 32                                                         680
  30    T3=0.                                                            690
  32    RHOM = ALPHA3*C4*EXP(-CGM/TEMP)                                  700
        T1=PRES*WMAV/(R*TEMP*G)                                          710
        T2=RHOM*DELA                                                     720
        DMDZ(LL)=-H4/G*(T2+T4)-H3/6*T3-FC/G*(H-HF)                       730
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                                         740
        Z1=-H4/(ENMX3*DMDZ(LL))                                          750
        Z2=.05*(ZEND-Z(LL))                                              760
        IF(DMDZ(LL)*(1.-Z1/Z2))4060,4060,15                              770
  15    DZ=Z1                                                            780
 4000   DTDZ=DMDZ(LL)/CAV                                                790
        W1=C1/RHO                                                        800
        W2=C2/RHO                                                        810
        W3=C3/RHO                                                        820
        W4=C4/RHO                                                        830
        S1=1./6                                                          840
        S5=FC/(G*RHO)                                                    850
        DW4DZ=S1*(FC-T2-T4)-C4*S5                                        860
        DW3DZ=S1*(T2*WM3/WM4+T4*WM3/WM4-T3)-C3*S5                        870
        DW2DZ=S1*(.5*T2*WM2/WM4+.5*T4*WM2/WM4+.5*T3*WM2/WM3)-C2*S5       880
        DW1DZ=S1*(.5*T2*WM1/WM4+.5*T4*WM1/WM4+1.5*T3*WM1/WM3)-C1*S5      890
        SUMWM=W1/WM1+W2/WM2+W3/WM3+W4/WM4                                900
        SMDWDZ=DW1DZ/WM1+DW2DZ/WM2+DW3DZ/WM3+DW4DZ/WM4                   910
        DMDZ=-WMAV/SUMWM*SMDWDZ                                          920
        DPDZ = (DELA-1.)/DELA**3*(1.75+75.*VIS*(1.-DELA)/(A*G))*G**2/    930
       X       (64.4*A*RHO)                                              940
        DPDZ = DPDZ/144.                                                 950
        DRDZR = DMDZ/WMAV-DTDZ/TEMP+DPDZ/PRES                            960
        T5=FC/G-DRDZR                                                    970
        DC4DZ=T1*(FC-T2-T4)-C4*T5                                        980
        DC3DZ=T1*(T2*WM3/WM4+T4*WM3/WM4-T3)-C3*T5                        990
        DC2DZ=T1*(.5*T2*WM2/WM4+.5*T4*WM2/WM4+.5*T3*WM2/WM3)-C2*T5      1000
        DC1DZ=T1*(.5*T2*WM1/WM4+.5*T4*WM1/WM4+1.5*T3*WM1/WM3)-C1*T5     1010
        IF(KFLAG.EQ.0)GO TO 16                                          1020
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                                          1030
  90    IF(KOUNT.EQ.4.OR.KOUNT.EQ.6.OR.KOUNT.EQ.8.OR.KOUNT.EQ.10.OR.KOUNT.  1040
       X       EQ.12.OR.KOUNT.EQ.14)N=N-1                               1050
        KOUNT=KOUNT+1                                                   1060
        DZ=DELTAZ/(THREE**N)                                            1070
        IF(FC)98,98,93                                                  1080
  98    IF(IFC.EQ.0)GO TO 16                                            1090
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                            1100
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       1110
  19    DZ1=DZ                                                          1120
        CALL REDIVD (DZ1,DTDZ,NINT,JFLAG,I,LL)                          1130
        WRITE (6,91) KOUNT,NINT                                         1140
  91    FORMAT (//7H KOUNT=I2 ,37H --- THIS INTERVAL HAS BEEN REDIVIDEDI4,  1150
```

```
     X6H TIMES)                                                          1160
  16 H=H+DHDZ(LL)*DZ                                                     1170
     IF (H.LT.HV) GO TO 106                                              1180
4051 TEMP=TEMP+DTDZ*DZ                                                  1190
     PRES = PRES+DPDZ*DZ                                                1200
     C4=C4+DC4DZ*DZ                                                     1210
     C3=C3+DC3DZ*DZ                                                     1220
     C2=C2+DC2DZ*DZ                                                     1230
     C1=C1+DC1DZ*DZ                                                     1240
 400 SUM=C1/WM1+C2/WM2+C3/WM3+C4/WM4                                    1250
     IF(C4.LT.0.)SUM=SUM-C4/WM4                                         1260
     IF(C3.LT.0.)SUM=SUM-C3/WM3                                         1270
     FRAC1=C1/(WM1*SUM)                                                 1280
     FRAC2=C2/(WM2*SUM)                                                 1290
     FRAC3=C3/(WM3*SUM)                                                 1300
     FRAC4=C4/(WM4*SUM)                                                 1310
     FRAC3D=(FRAC1/FRAC2-1.)/(3.-FRAC1/FRAC2)                           1320
     IF(KFLAG.EQ.1)GO TO 500                                            1330
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                                1340
  17 H=H-DHDZ(LL)*DZ                                                    1350
  18 TEMP=TEMP-DTDZ*DZ                                                  1360
     PRES = PRES-DPDZ*DZ                                                1370
     C4=C4-DC4DZ*DZ                                                     1380
     C3=C3-DC3DZ*DZ                                                     1390
     C2=C2-DC2DZ*DZ                                                     1400
     C1=C1-DC1DZ*DZ                                                     1410
     DZ=DZ/2.                                                           1420
     GO TO 16                                                           1430
 500 PFRC3D=FRAC3D                                                      1440
     IF(C4)70,71,71                                                     1450
  70 C4=0.                                                              1460
     FRAC4=0.                                                           1470
  71 IF(C3)72,73,73                                                     1480
  72 C3=0.                                                              1490
     FRAC3=0.                                                           1500
  73 LL=LL+1                                                            1510
     Z(LL)=Z(LL-1)+DZ                                                   1520
     IF(JFLAG.EQ.1)NINT=NINT-1                                          1530
     IF(NINT.EQ.0)JFLAG=0                                               1540
     WRITE (6,4059)                                                     1550
4059 FORMAT (//121H          Z              TEMP              PRES       1560
    X     H               C1               C2               C3         1570
    X C4      )                                                         1580
     WRITE (6,4050) Z(LL),TEMP,PRES,H,C1,C2,C3,C4                       1590
4050 FORMAT (1X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8,1X,E 1600
    X15.8,1X,E15.8///)                                                  1610
     WRITE (6,37)                                                       1620
  37 FORMAT (98H                                MFRAC1           MFRAC2  1630
    1   MFRAC3           MFRAC4           FRAC3D    )                   1640
     WRITE (6,38) FRAC1,FRAC2,FRAC3,FRAC4,FRAC3D                        1650
  38 FORMAT (20X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8,1X,E15.8 ///)         1660
     IF(Z(LL).GT.ZBOUND)GO TO 1                                         1670
     IF(KOUNT.GT.15.AND.JFLAG.EQ.0)GO TO 1                              1680
     INJECT=0                                                           1690
     GO TO 3990                                                         1700
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
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```
 4060 DELTAZ=ZEND-Z(LL)                                                 1710
      ZBOUND=ZEND+DELTAZ/3.                                             1720
      KFLAG=1                                                           1730
      KOUNT=KOUNT+1                                                     1740
      GO TO 4000                                                        1750
    1 IF(IFC.EQ.1)GO TO 22                                              1760
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)                                                1770
      DZZ=ZGAP/6.                                                       1780
      JJ1=LL-1                                                          1790
      JJ6=LL+6                                                          1800
      DO 27 I=JJ1,JJ6                                                   1810
      Z(I)=Z(I-1)+DZZ                                                   1820
   27 CONTINUE                                                          1830
      LL=LL+6                                                           1840
C     PRINT OUT VAPOR REGION Z VALUES FOR USE IN TRANSIENT MODEL
   22 WRITE (6,62)                                                      1850
   62 FORMAT (1H1,54X,22H Z'S FROM VAPOR REGION)                        1860
      WRITE (6,63) (Z(I),I=JZ,LL)                                       1870
   63 FORMAT (1X,10E13.7)                                               1880
      MBSS = (C1+C2+C3+C4)/(C1/WM1+C2/WM2+C3/WM3+C4/WM4)                1890
      WRITE (6,8001) MBSS,G                                             1900
 8001 FORMAT (///42X'STEADY STATE VALUES FOR MBAR AND G AT END OF BED'/ 1910
     A           47X'MBAR ='E12.5,5X,'G ='E12.5)                        1920
      GO TO 999                                                         1930
  106 WRITE (6,107)                                                     1940
  107 FORMAT (////13X'THERE IS A PUDDLE OF COLD HYDRAZINE AT THE LIQUID-1950
     XVAPOR/VAPOR INTERFACE --- TRY USING A LARGER VALUE FOR GO' )       1960
  999 RETURN                                                            1970
      END                                                               1980
```

```
      SUBROUTINE REDIVD (DZ1,DTDZ,NINT,JFLAG,I,LL)                      0
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                                                     10
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),  20
     1        SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)      30
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,     40
     1        WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2 50
     2        ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI                         60
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)                           70
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,       80
      COMMON /MUVST/VISVST(30)                                          90
      COMMON /FLAGS/MFLAG,KFLAG,PRINT                                  100
      COMMON /IFCEQU/IFC,GATZ0                                         110
      I=0                                                              120
      NESTCT=1                                                         130
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                                                  140
    2 NESTCT=NINT                                                      150
    1 I=I+1                                                          160
      XSIZE=2.**I                                                      170
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```
      NINT=XSIZE                                                        180
      DZ=DZ1/XSIZE                                                      190
      IF(ABS(DTDZ)*DZ.GT..01*TEMP)GO TO 1                               200
      IF((1.+DZ/(Z(LL)-Z0)+.01*Z0/ABS(Z(LL)-Z0)).LT.0.)GO TO 1          210
      NINT=NINT*NLSTCT                                                  220
      JFLAG=1                                                           230
      RETURN                                                            240
      END                                                               250


      SUBROUTINE SLOPE (CG,GMMA,K,BETA,EN12,RATE,DPA,A,DIFF)              0
      REAL  KP,K                                                         10
      INTEGER PRINT                                                      20
      DIMENSION K(1),     GMMA(1),BETA(1),DPA(1),CG(1),S(210),FST(210),  30
     1SEC(210),D(210),CPA(210),CPB(210),E(210),A(1),TERM1(210),          40
     2TERM2(210),C(210),XXX(210),XOA(210)                                50
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),   60
     1     SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)          70
      COMMON /CO/HL,HV,FC,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,     80
     1     WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2    90
     2     ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI                            100
      COMMON /VAR/DERIV(250),DHDZ(250),Z(250)                           110
      COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,       120
      COMMON /MUVST/VISVST(30)                                          130
      COMMON /FLAGS/MFLAG,KFLAG,PRINT                                   140
      IFLAG=0                                                           150
      JFLAG=0                                                           160
      FRAC=.99                                                          170
   12 B=0.0                                                             180
  702 I=1                                                               190
      NOT=0                                                             200
      ADIV=100.                                                         210
      BDIV=100.                                                         220
      TOL=.01                                                           230
      STORE=1.0                                                         240
      KJ=0                                                              250
      HOLD=0.                                                           260
      NI=0                                                              270
   13 MI=0                                                              280
      IL=0                                                              290
      IK=0                                                              300
      MM=0                                                              310
      IM=0                                                              320
      F=0.5                                                             330
   20 MM=MM+1                                                           340
      DR=B/ADIV                                                         350
      BDR=(A(I)-B)/BDIV                                                 360
      JINT=BDIV                                                         370
      INIT=ADIV                                                         380
      IF(MM.EQ.1) GO TO 15                                              390
      GO TO 16                                                          400
   15 MMAX=JINT+1                                                       410
      MAX=MMAX-1                                                        420
      MINT=0                                                            430
      GO TO 17                                                          440
   16 MMAX=INIT+JINT+1                                                  450
      MINT=INIT+1                                                       460
      MAX=MMAX-1                                                        470
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```
 17   X=0.0                                                                  480
      DO 40 IJ=1,MMAX                                                        490
      IF(IJ.GT.MINT) GO TO 49                                                500
      X=FLOAT(IJ-1)*DR                                                       510
      GO TO 23                                                               520
 49   KMJ=IJ-MINT                                                            530
      X=B+FLOAT(KMJ)*BDR                                                     540
 23   CP=CG(I)*X/(A(I)-B)-(B/(A(I)-B))*CG(I)                                 550
      IF(CP.LT.0.0) CP=0.0                                                   560
C     THIS IS THE GENERAL EQUATION FOR A LINE WITH NEGATIVE Y-INTERCEPT
 24   FACT1=K(I)*(CG(I))**(1.-EN12)*(CP)**EN12                               570
      FACT2=EXP(GMMA(I)*BETA(I)*(1.-CP/CG(I))/(1.+BETA(I)*(1.-CP/CG(I)))     580
     1)                                                                      590
      IF(X) 37,40,37                                                         600
 37   RCP=FACT1*FACT2                                                        610
 35   S(IJ)=(1./X-1./A(I))*X*X*RCP                                           620
 40   CONTINUE                                                               630
      GO TO 50                                                               640
 50   SUM=0.0                                                                650
      SUMA=0.0                                                               660
      DO 60 IL=2,MAX                                                         670
      IF(IL.GT.MINT) GO TO 61                                                680
      SUM=SUM+S(IL)                                                          690
      GO TO 60                                                               700
 61   SUMA=SUMA+S(IL)                                                        710
 60   CONTINUE                                                               720
      S(1) =0.                                                               730
      SGMA=(S(1)+2.0*SUM)*(DR/(2.0*DPA(I)))+(S(MMAX)+2.0*SUMA)*(BDR/(2.      740
     10*DPA(I)))                                                             750
      D2=SGMA-FRAC*CG(I)                                                     760
      TOT=D2+TOL*CG(I)                                                       770
      IF(MM-1) 110,110,112                                                   780
 112  IF(D2)1,1,2                                                            790
 1    IF(TOT)2,230,230                                                       800
 2    GO TO 115                                                              810
 110  IF(IFLAG.EQ.1)GO TO 115                                                820
      IF(D2)150,115,115                                                      830
 115  IF(MM-1) 20,120,140                                                    840
 120  XOLD=B                                                                 850
      IF (PRINT.EQ.1) WRITE(6,125)                                           860
 125  FORMAT(41H0INITIAL CHOICE THRU ORIGIN IS TOO LARGE )                   870
      D1=D2                                                                  880
C     CHANGE THE EQUATION OF THE LINE
      B=.999999  *A(I)                                                       890
      GO TO 20                                                               900
C     USE PREDICTING RESULTS TO ESTIMATE B FOR NEW LINE
 140  TEMP=B                                                                 910
      MI=MI+1                                                                920
      B=B+(D2/(D2-D1))*(XOLD-B)                                              930
 1741 XOLD=TEMP                                                              940
      D1=D2                                                                  950
 143  IF(MI-20) 145,145,147                                                  960
 145  GO TO 20                                                               970
 147  IF (JFLAG.EQ.1) GO TO 230                                              980
      B = .9*A(I)                                                            990
      JFLAG = 1                                                             1000
      GO TO 702                                                             1010
C     INITIAL CHOICE THRU ORIGIN IS SATISFACTORY
 150  KU=1                                                                  1020
      IFLAG=1                                                               1030
```

```
      X=0.                                                              1040
C     CALCULATE THE VALUE OF THE TWO INTEGRALS FOR ALL DR (101 POINTS)
      DO 170 II=1,MMAX                                                  1050
      X=FLOAT(II-1)*BDR                                                 1060
      CP=CG(I)*X/(A(I)-B)-(B/(A(I)-B))*CG(I)                            1070
      TERM1(II)=K(I)*(CG(I))**(1.-EN12)*(CP)**EN12                      1080
      TERM2(II)=EXP(GMMA(I)*BETA(I)*(1.-CP/CG(I))/(1.+BETA(I)*(1.-CP/CG(  1090
     1I))))                                                             1100
      XXX(II)=X                                                         1110
      XOA(II)=XXX(II)/A(I)                                              1120
      RCP = TERM1(II)*TERM2(II)                                         1130
      FST(II)=X*X*RCP                                                   1140
      IF(X) 165,170,165                                                 1150
  165 SEC(II)=(1./X-1./A(I))*X*X*RCP                                    1160
  170 CONTINUE                                                          1170
C     THE TRAPEZOIDAL RULE IS USED TO EVALUATE BOTH INTEGRALS
  172 C(1)=0.                                                           1180
  173 DO 175 JJ=2,MMAX                                                  1190
      IF(JJ.GT.MINT) GO TO 176                                          1200
      C(JJ)=C(JJ-1)+(FST(JJ)+FST(JJ-1))*(DR/(2.0*DPA(I)))               1210
      GO TO 175                                                         1220
  176 C(JJ)=C(JJ-1)+(FST(JJ)+FST(JJ-1))*(BDR/(2.0*DPA(I)))              1230
  175 CONTINUE                                                          1240
      SEC(1)=0.                                                         1250
      D(1) = 0.                                                         1260
      DO 180 KK=2,MMAX                                                  1270
      IF(KK.GT.MINT) GO TO 179                                          1280
      D(KK)=D(KK-1)+(SEC(KK-1)+SEC(KK))*(DR/(2.0*DPA(I)))               1290
      GO TO 180                                                         1300
  179 D(KK)=D(KK-1)+(SEC(KK-1)+SEC(KK))*(BDR/(2.0*DPA(I)))              1310
  180 CONTINUE                                                          1320
C     THE VALUE OF CP AT X=0 IS  CG -D(101)
      E(1)=D(MMAX)                                                      1330
  186 CPA(1)=0.0                                                        1340
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)                                                    1350
      IF(KJ.EQ.1) GO TO 185                                             1360
      IF(IM.EQ.0) GO TO 185                                             1370
      IF(NI.EQ.1) GO TO 368                                             1380
  185 SAM=0.0                                                           1390
      DO 190 LL=2,MMAX                                                  1400
      IF(LL.GT.MINT) GO TO 188                                          1410
      E(LL)=E(LL-1)-(SEC(LL)+SEC(LL-1))*(DR/(2.*DPA(I)))                1420
      SAM = FLOAT(LL-1)*DR                                              1430
      GO TO 189                                                         1440
  188 E(LL)=E(LL-1)-(SEC(LL)+SEC(LL-1))*(BDR/(2.0*DPA(I)))              1450
      SAM=SAM+BDR                                                       1460
  189 CPA(LL)=CG(I)-((1./SAM)-(1./A(I)))*C(LL)-E(LL)                    1470
      IF(LL.LT.MINT) CPA(LL)=0.0                                        1480
      IF(CPA(LL).LT.0.0) CPA(LL)=0.0                                    1490
  190 CONTINUE                                                          1500
      IF(KJ.EQ.1) GO TO 280                                             1510
      X=0.                                                              1520
      IF(IM.EQ.0) GO TO 250                                             1530
      IK=1                                                              1540
      GO TO 280                                                         1550
C     THE NEXT ITERATION USES THE VALUES OF CP JUST CALCULATED
  192 DO 290 LI=1,MMAX                                                  1560
      IF(LI.GT.MINT) GO TO 195                                          1570
```

```
      X=FLOAT(LI-1)*DR                                                  1580
      GO TO 199                                                         1590
  195 KLK=LI-MINT                                                       1600
      X=B+FLOAT(KLK)*BDR                                                1610
  199 CONTINUE                                                          1620
      TERM1(LI)=K(I)*(CG(I))**(1.-EN12)*(CPA(LI))**EN12                 1630
      TERM2(LI)= EXP(GMMA(I)*BETA(I)*(1.-CPA(LI)/CG(I))/(1.+BETA(I)*(1.-1650
     1CPA(LI)/CG(I))))                                                  1650
      XXX(LI)=X                                                         1660
      XOA(LI)=XXX(LI)/A(I)                                              1670
      RCP=TERM1(LI)*TERM2(LI)                                           1680
      FST(LI)=X*X*RCP                                                   1690
      IF(X) 200,200,193                                                 1700
  193 SEC(LI)=(1./X-1./A(I))*X*X*RCP                                    1710
  200 CONTINUE                                                          1720
      GO TO 172                                                         1730
C     THIS IS FOR THE CASE WHERE THE INITIAL GUESS WAS TOO LARGE
  230 IF (PRINT.EQ.1) WRITE(6,235)MI,B                                  1740
  235 FORMAT(41H SATISFACTORY STARTING CURVE FOUND AFTER I2,31H TRIALS T1750
     1HE VALUE OF B (XO) IS  E12.7)                                     1760
      IF(B.GT..998*A(I))DERIF=2.6*CG(I)/(A(I)-B)                        1770
      IF(B.GT..998*A(I)) GO TO 322                                      1780
C     THE RANGE OF X FROM ZERO TO A IS USED
  237 X=0.                                                              1790
      N1=1                                                              1800
      DO 240 NN=1,MMAX                                                  1810
      IF(NN.GT.MINT) GO TO 246                                          1820
      X=FLOAT(NN-1)*DR                                                  1830
      GO TO 354                                                         1840
  246 KJK=NN-MINT                                                       1850
      X=B+FLOAT(KJK)*BDR                                                1860
  354 IF(IM.GE.1) GO TO 353                                             1870
  238 CPB(NN) = CG(I)*X/(A(I)-B) - (B/(A(I)-B))*CG(I)                   1880
      IF(CPB(NN).LT.0.0) CPB(NN)=0.0                                    1890
  353 TERM1(NN)=K(I)*(CG(I))**(1.-EN12)*(CPB(NN))**EN12                 1900
      TERM2(NN)= EXP(GMMA(I)*BETA(I)*(1.-CPB(NN)/CG(I))/(1.+BETA(I)*(1.-1910
     1CPB(NN)/CG(I))))                                                  1920
      XXX(NN)=X                                                         1930
      XOA(NN)=XXX(NN)/A(I)                                              1940
      RCP = TERM1(NN)*TERM2(NN)                                         1950
      FST(NN)=X*X*RCP                                                   1960
      IF(X) 240,240,247                                                 1970
  247 SEC(NN) = (1./X-1./A(I))*X*X*RCP                                  1980
  240 CONTINUE                                                          1990
      GO TO 172                                                         2000
  368 DO 370 NL=1,MMAX                                                  2010
      CPB(NL)=CPA(NL)                                                   2020
  370 CONTINUE                                                          2030
      GO TO 185                                                         2040
  250 DO 260 IL=1,MMAX                                                  2050
  252 CPA(IL)=F*CPA(IL)+(1.-F)*CPB(IL)                                  2060
  260 CONTINUE                                                          2070
      IK=0                                                              2080
C   THE VALUES OF X AT A AND NEAREST A ARE USED IN FINDING THE DERIVATIVE
  280 DERIF=(CG(I)-CPA(MAX))/BDR                                        2090
      IM=IM+1                                                           2100
      IF(IM.GT.99.AND.IFLAG.EQ.1)GO TO 701                              2110
      IF(IM.GT.99)GO TO 328                                             2120
  310 IF(KJ.EQ.1) IK=1                                                  2130
      IF(ABS(DERIF-HOLD)- 0.05*DERIF)3,3,321                            2140
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 3     IF(IK.EQ.1)GO TO 322                                                    2150
 321   HOLD=DERIF                                                              2160
       IF(KJ.EQ.1) GO TO 192                                                   2170
       IF(IK.EQ.1) GO TO 250                                                   2180
       GO TO 192                                                               2190
 322   RATE=DERIF                                                              2200
       IF(CG-CG(I))777,4,777                                                   2210
 4     IF(H-HL)777,777,5                                                       2220
 5     DIFN=DIFF*((TEMP/492.)**1.823)*14.7/PRES                                2230
       CALL UNBAR (VISVST(1),1,TEMP,0.,VIS,KK)                                2240
       RHO=PRES*WMAV/(R*TEMP)                                                  2250
       AKC=(.61*G)/(RHO)*((VIS/(RHO*DIFN))**-.667)*((G/(AP*VIS))**-.41)        2260
       RAT=AKC*CG(I)/DPA(I)                                                    2270
       IF(RATE-RAT)778,776,6                                                   2280
 6     MFLAG=1                                                                 2290
       RATE=RAT                                                                2300
       GO TO 777                                                               2310
 778   MFLAG=0                                                                 2320
 777   IF(B.GT..998*A(I))GO TO 888                                             2330
       IF (PRINT.EQ.1) WRITE(6,182)IM                                          2340
 182   FORMAT (11H ITERATION=,I3)                                              2350
       IF (PRINT.EQ.1) WRITE(6,336)                                            2360
 336   FORMAT(13X,105H X/A          CPA          X/A          CPA              2370
      1  X/A          CPA          X/A          CPA          )                2380
       IF (PRINT.EQ.1) WRITE(6,183)(XOA(I),CPA(I),I=1,MMAX,4)                  2390
 183   FORMAT(9X,E12.7,1X,E12.7,1X,E12.7,1X,E12.7,1X,E12.7,1X,E12.7,1X,E1      2400
      112.7,1X,E12.7)                                                          2410
 888   IF (PRINT.EQ.1) WRITE(6,323)RATE                                        2420
 323   FORMAT(/24H THE SLOPE CONVERGES TO E12.7)                               2430
 327   RETURN                                                                  2440
 328   PERC=(ABS(DERIF-HOLD))/DERIF)*100.                                      2450
       ALL = 5.                                                                2460
       GO TO 322                                                               2470
C      SIMPLIFIED VERSION DOES NOT ''CONVERGE'' IN 99 ITERATIONS
C      SET B=.000001*A     ,     AND START OVER
 701   B=.000001*A(I)                                                          2480
       IF (PRINT.EQ.1) WRITE(6,700)                                            2490
 700   FORMAT (/ 84H INITIAL CHOICE THRU ORIGIN SEEMINGLY OK, BUT RESULTS      2500
      X ROTTEN AFTER 99 ITERATIONS .../48H SET X0=.000001*A AND USE MORE       2510
      XREFINED TECHNIQUE /)                                                    2520
       DR=B/ADIV                                                              2530
       BOR=(A(I)-B)/BDIV                                                      2540
       MMAX=INIT+JINT+1                                                       2550
       MINT=INIT+1                                                            2560
       MAX=MMAX-1                                                             2570
       IM=0                                                                   2580
       KJ=0                                                                   2590
       GO TO 237                                                              2600
       END                                                                    2610
```

```
       SUBROUTINE SGRAD (GRAD,TGRAD)                                           0
       REAL  K0,KP,KC3,KC4,MU                                                 10
       INTEGER PRINT                                                          20
       COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),       30
      1         SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)          40
       COMMON /CO/HL,HV,FG,TF,CFL,CGM,ENMX1,AGM,DIF3,DIF4,KP,PRES,GO,         50
      1         WM4,WM3,WM2,WM1,ALPHA3,R,TVAP,ZEND,BGM,HF,DZ,ALPHA1,ALPHA2    60
```

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     2      ,ENMX2,ENMX3,EN1,EN2,EN3,H,RAT,MI                                  70
       COMMON /VAR/DERIV(250),DHDZ(250),Z(250)                                  80
       COMMON /TOLL/ALIM,OPTION,C1,C2,C3,C4,CAV,G,TEMP,AP,WMAV,Z0,              90
       COMMON  /BBBB/DP3,A,KC3,K0,X0A,CPS,CI3,GAMMA,BETA                       100
       COMMON  /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)                 110
       COMMON  /MUVST/ VISVST(30)                                               120
       COMMON /FLAGS/MFLAG,KFLAG,PRINT                                          130
       COMMON  /CCC/H4TBL(40),H3TBL(40)                                         140
       DIMENSION  CPOX(101),PCPOX(101),DX(101),CPX(101),RHET(101)               150
C    DEFINE DP FUNCTION
       DP3F(X,Y,Z) = 14.7*Y/Z*(X/492.)**1.823*(1.-EXP(-.0672*Z*492./(           160
      X               14.7*X)))                                                 170
C    DEFINE KC FUNCTION
       KCF(A,B,C,D,E) = .61*A/B*(C/(B*D))**-.667*(A/(E*C))**-.41                180
C    ANALYTIC INTEGRATION FUNCTIONS FROM INTEGRAL EQUATION
       EVAL1(A,B) = B**3/3.-A**3/3.                                             190
       EVAL2(A,B) = B**2/2.-A**2/2.                                             200
       WAF1 = .8                                                                210
       WAF2 = .2                                                                220
 1     LTFLG=0                                                                  230
       P=PRES                                                                   240
       T=TEMP                                                                   250
       ALPH2=ALPHA2                                                             260
       CI1=C1                                                                   270
       CI2=C2                                                                   280
       CI3=C3                                                                   290
       CI4=C4                                                                   300
       D03=DIF3                                                                 310
       D04=DIF4                                                                 320
       N=EN1                                                                    330
       NPART = 50                                                               340
       LP1 = 1                                                                  350
       TPSP = 0.                                                                360
       RHO = CI1+CI2+CI3+CI4                                                    370
       DI3 = D03*14.7/P*(T/492.)**1.823                                         380
       DI4 = D04*14.7/P*(T/492.)**1.823                                         390
       CALL UNBAR (VISVST,1,T,0.,MU,KK)                                         400
       CALL UNBAR (CFTBL4,1,T,0.,CF4,KK)                                        410
       CALL UNBAR (CFTBL3,1,T,0.,CF3,KK)                                        420
       CALL UNBAR (CFTBL2,1,T,0.,CF2,KK)                                        430
       CALL UNBAR (CFTBL1,1,T,0.,CF1,KK)                                        440
       KC3 = KCF(G,RHO,MU,DI3,AP)                                               450
       KC4 = KCF(G,RHO,MU,DI4,AP)                                               460
       CFBAR = (CI1*CF1+CI2*CF2+CI3*CF3+CI4*CF4)/RHO                            470
       HC = .74*G*CFBAR*(G/(AP*MU))**-.41                                       480
C
C    LOCATE SUITABLE X0
C
       DP3 = DP3F(T,D03,P)                                                      490
C    CHOOSE STARTING VALUE FOR CPS TO BE = CI3/2.
       CPS = CI3/2.                                                             500
       CMCPN = CI3-CPS                                                          510
       DCPDX = KC3/DP3*(CI3-CPS)                                                520
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)                                          530
       CALL UNBAR (H3TBL,1,T,0.,H3,KK)                                          540
       IF (LP1.EQ.1) GO TO 6                                                    550
 40    TPSPP = TPSP                                                             560
       TPSP = TPS                                                               570
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 6      TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC                              580
        IF (TPS.LT.0.) TPS=1.                                            590
        CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                                600
        DP3 = DP3F(TPS,D03,P)                                            610
        DP3P = DP3                                                       620
        H3P = H3                                                         630
        TMTPN = T-TPS                                                    640
 61     GAMMA = BGM/TPS                                                  650
        BETA = -CPS*H3*DP3/(KP*TPS)                                      660
        K0 = ALPH2*EXP(-GAMMA)*CI1**EN3                                  670
C    LINEAR EXTRAPOLATION USED TO GUESS AT X0
        X0P = X0                                                         680
        X0 = A-CPS/DCPDX                                                 690
        X0A = X0/A                                                       700
        IF (X0) 11,12,12                                                 710
 11     X0 = 0.                                                          720
        X0A = 0.                                                         730
        CPS = CI3/(DP3/(A*KC3)+1.)                                       740
        DCPDX = CI3/A                                                    750
        TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC                             760
        IF (TPS.LT.0.) TPS=1.                                            770
        WRITE (6,132) LP1,TPS                                            780
 132    FORMAT (1X,37X,'WE HAVE CALCULATED A NEGATIVE X0 DURING ITERATION 790
C    INTEGRATE FOR CP EQUATION
 12     CALL TRAPP (X0A,1.,NPART,RIESUM)                                 830
C    CALCULATE NEW CPS ...
        CPSP = CPS                                                       840
        CMCPO = CMCPN                                                    850
        CPS = CI3-A*RIESUM/KC3                                           860
        IF (LTFLG-1) 80,84,80                                            870
 80     IF (CPS-(.25*CI3)) 81,81,130                                     880
 81     LTFLG=1                                                          890
        GO TO 82                                                         900
 84     LTFLG=0                                                          910
        IF (CPS) 89,130,130                                              920
 89     CPS=0.                                                           930
        GO TO 46                                                         940
 130    CMCPN = CI3-CPS                                                  950
C    CALCULATE NEW TP
 13     DCPDX = KC3/DP3*(CI3-CPS)                                        960
        GRAD = DCPDX*DP3                                                 970
        TGRAD = HC*(T-TPS)                                               980
        TPSPP = TPSP                                                     990
        TPSP = TPS                                                      1000
        TMTPO = TMTPN                                                   1010
 51     TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC                            1020
        IF (TPS.LT.0.) TPS=1.                                           1030
        CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                               1040
        DP3 = DP3F(TPS,D03,P)                                           1050
        TMTPN = T-TPS                                                   1060
        GAMMA = BGM/TPS                                                 1070
        BETA = -CPS*H3*DP3/(KP*TPS)                                     1080
        K0 = ALPH2*EXP(-GAMMA)*CI1**EN3                                 1090
C    TEST TEMP,CONCENTRATION FOR 5% LIMIT
        IF (ABS(TMTPO-TMTPN)/TMTPN - .05) 41,41,43                      1100
 41     IF (ABS(CMCPO-CMCPN)/CMCPN - .05) 70,70,43                      1110
C    TEST FOR TEMPERATURE LOOP ... COMPARE LAST 3 TEMPS
 43     IF (AMIN1(TPS,TPSP,TPSPP) - TPSP) 60,71,60                      1120
 60     IF (AMAX1(TPS,TPSP,TPSPP) - TPSP) 46,71,46                      1130
C    TEMPERATURE HAS FLUCTUATED ... TAKE AVERAGE AND RECALCULATE CPS
```

```
 71   TPSPP = TPSP                                                    1140
      TPSP = TPS                                                      1150
      TMTPO = TMTPN                                                   1160
      TPS = (TPSP+TPSPP)/2.                                           1170
      CALL UNBAR (H3,BL,1,TPS,0.,H3,KK)                               1180
      DP3 = DP3F(TPS,D03,P)                                           1190
      DP3P = DP3                                                      1200
      TMTPN = T-TPS                                                   1210
      DCPDX = (HC*(T-TPS)-H4*KC4*CI4)/(H3*DP3)                        1220
      CPSP = CPS                                                      1230
      CMCPO = CMCPN                                                   1240
      CPS = CI3-DP3/KC3*DCPDX                                         1250
      IF (CPS.LT.0.) CPS=0.                                           1260
      CMCPN = CI3-CPS                                                 1270
      LP1 = LP1+1                                                     1280
      IF (LP1-50) 61,61,44                                            1290
C   NO CONVERGENCE YET ... AVERAGE THE CPS'S FOR LAST TWO CALC'S AND REPEAT
 46   CPS = .2*CPS+.8*CPSP                                            1300
      GO TO 53                                                        1310
 22   X00 = WAF1*X0P+WAF2*X0                                          1320
      CPS = CI3/(1.+DP3/(KC3*A-KC3*X00))                              1330
 53   DCPDX = KC3/DP3P*(CI3-CPS)                                      1340
      CMCPN = CI3-CPS                                                 1350
      H3 = H3P                                                        1360
 42   LP1 = LP1+1                                                     1370
      IF (LP1-25) 40,40,44                                            1380
 44   WAF1 = WAF1+.05                                                 1390
      IF (WAF1.GT.0.95) GO TO 99                                      1400
      WAF2 = 1.-WAF1                                                  1410
C   NO CONVERGENCE WITH PRESENT WEIGHTED AVERAGE FACTORS FOR X0
C   REPEAT ITERATION PROCEDURE WITH NEW FACTORS
      GO TO 1                                                         1420
 99   WRITE (6,98)                                                    1430
 98   FORMAT (///20X,'UNABLE TO FIND SUITABLE X0 AFTER  FOUR TRIES OF 25   1440
     X ITERATIONS EACH --- PROGRAM STOP FOLLOWS' )                    1450
      CALL EXIT                                                       1460
C   SATISFACTORY X0 HAS BEEN FOUND
 70   IF (PRINT.EQ.1) WRITE(6,16)LP1,X0                               1470
 16   FORMAT (/// 46X,27HSATISFACTORY X0 FOUND AFTER,I3,7H TRIES  /   1480
     X        57X,5H X0 =,E12.5 )                                     1490
C
C   CALCULATE GRADIENT
C
 131  LP2 = 1                                                         1500
      NX = 24                                                         1510
      NX1 = NX+1                                                      1520
      NXM1 = NX-1                                                     1530
 291  X0A = X0/A                                                      1540
      VNU = -KC3/DP3                                                  1550
      IN11 = 1                                                        1560
      K = 2                                                           1570
      R1 = 0.                                                         1580
      R2 = 0.                                                         1590
      PS1 = 0.                                                        1600
      PS2 = 0.                                                        1610
      DELX0A = (1.-X0A)/FLOAT(NX)                                     1620
C   CALCULATE PROFILE CURVES FOR INTEGRAND FUNCTIONS
      XA = X0A                                                        1630
      DO 770 I=1,NX1                                                  1640
C   CP(X/A) IS A LINEAR PROFILE DUE TO FIRST APPROXIMATION
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```
      IF (LP2.GT.1) GO TO 664                                          1650
      CPX(I) = (XA-X0A)/(1.-X0A)*CPS                                   1660
  664 RHET(I) = K0*CI3**(1-N)*CPX(I)**N*EXP(GAMMA*BETA*(1.-CPX(I)/CI3)/ 1670
     X           (1.+BETA*(1.-CPX(I)/CI3)))                            1680
      DX(I) = XA                                                       1690
      XA = XA+DELX0A                                                   1700
  770 CONTINUE                                                         1710
C     TAKE INTERVAL FUNCT'N MIDPTS AS CONSTANT VALUE FOR CP(X/A) AND RHET
      DO 771 I=1,NX                                                    1720
      CPX(I) = (CPX(I)+CPX(I+1))/2.                                    1730
      RHET(I) = (RHET(I)+RHET(I+1))/2.                                 1740
  771 CONTINUE                                                         1750
      XA = X0A+DELX0A                                                  1760
      CTRM = (A*VNU+1.)/(A*VNU)                                        1770
C     INTEGRAL EQUATION FOLLOWS
C     CPOX(1) IS SPECIAL CASE ... X=X0
      DXL = X0A                                                        1780
      DXU = DXL+DELX0A                                                 1790
      RR1 = 0.                                                         1800
      DO 377 I=1,NX                                                    1810
      RR1 = RR1+RHET(I)*(EVAL2(DXL,DXU)-CTRM*EVAL1(DXL,DXU))           1820
      DXL = DXU                                                        1830
      DXU = DXU+DELX0A                                                 1840
  377 CONTINUE                                                         1850
      CPOX(1) = CI3-A*A/DP3*RR1                                        1860
      IF (CPOX(1).LT.0.) CPOX(1)=0.                                    1870
C     SOLVE GENERAL EQUATION OF TWO INTEGRALS FOR CP(X/A)
  769 DO 772 I=1,INT1                                                  1880
      R1 = R1+RHET(I)*EVAL1(X0A,XA)                                    1890
      X0A = XA                                                         1900
      XA = XA+DELX0A                                                   1910
  772 CONTINUE                                                         1920
      R1 = R1*(1./X0A-CTRM)                                            1930
      XAD = XA                                                         1940
      XA = XA-DELX0A                                                   1950
      DO 773 I=INT1,NXM1                                               1960
      PS1 = PS1+RHET(I+1)*EVAL2(XA,XAD)                                1970
      PS2 = PS2+RHET(I+1)*EVAL1(XA,XAD)                                1980
      XA = XAD                                                         1990
      XAD = XAD+DELX0A                                                 2000
  773 CONTINUE                                                         2010
      R2 = PS1-CTRM*PS2                                                2020
      INT1 = INT1+1                                                    2030
      CPOX(K) = CI3-A*A/DP3*(R1+R2)                                    2040
      IF (CPOX(K).LT.0.) CPOX(K)=0.                                    2050
      X0A = X0/A                                                       2060
      XA = X0A+DELX0A                                                  2070
      K = K+1                                                          2080
      R1 = 0.                                                          2090
      R2 = 0.                                                          2100
      PS1 = 0.                                                         2110
      PS2 = 0.                                                         2120
      IF (K.LE.NX) GO TO 769                                           2130
C     CPOX(NX1) IS SPECIAL CASE ... X=A
      DXL = X0A                                                        2140
      DXU = DXL+DELX0A                                                 2150
      RR2 = 0.                                                         2160
      DO 378 I=1,NX                                                    2170
      RR2 = RR2+RHET(I)*EVAL1(DXL,DXU)                                 2180
      DXL = DXU                                                        2190
```

```
      DXU = DXU+DELXOA                                                  2200
  378 CONTINUE                                                          2210
      CPOX(NX1) = CI3-A*A/DP3*(1.-CTRM)*RR2                             2220
      IF (CPOX(NX1).LT.0.) CPOX(NX1)=0.                                 2230
C   CALCULATE A NEW TPS
      DCPDX = KC3/DP3*(CI3-CPOX(NX1))                                   2240
      H3P = H3                                                          2250
      DP3P = DP3                                                        2260
      TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC                              2270
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                                 2280
      DP3 = DP3F(TPS,D03,P)                                             2290
      TMTPO = TMTPN                                                     2300
      TMTPN = T-TPS                                                     2310
C    TWO PASSES NEEDED BEFORE CHECK ON TEMP,CONC CAN BE MADE
   33 IF (LP2.EQ.1) GO TO 27                                            2320
      CMCPO = CMCPN                                                     2330
      CMCPN = CI3-CPOX(NX1)                                             2340
      IF (ABS(TMTPO-TMTPN)/TMTPN - .05) 26,26,27                        2350
   26 IF (ABS(CMCPO-CMCPN)/CMCPN - .05) 88,88,27                        2360
C
C  CALCULATE NEW CPX(I) PROFILE FOR NEXT PASS
C
   27 DO 55 I=1,NX1                                                     2370
      IF (MOD(LP2,5)) 34,57,34                                          2380
C  CALCULATE WEIGHTED AVERAGE OF OLD AVERAGED AND CALCULATED PROFILES
   34 CPX(I) = .8*CPX(I)+.2*CPOX(I)                                     2390
      GO TO 56                                                          2400
C  AVERAGE PRESENT AND PAST CALCULATED PROFILES EVERY 5TH PASS TO SMOOTH
   57 CPX(I) = (CPOX(I)+PCPOX(I))/2.                                    2410
C  STORE PRESENT CALCULATED PROFILE
   56 PCPOX(I) = CPOX(I)                                                2420
   55 CONTINUE                                                          2430
      CMCPN = CI3-CPX(NX1)                                              2440
      DCPDX = KC3/DP3P*(CI3-CPX(NX1))                                   2450
      TPS = T-(H4*KC4*CI4+H3P*DP3P*DCPDX)/HC                            2460
      IF (TPS.LT.0.) TPS=1.                                             2470
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                                 2480
      DP3 = DP3F(TPS,D03,P)                                             2490
      TMTPO = TMTPN                                                     2500
      TMTPN = T-TPS                                                     2510
      LP2 = LP2+1                                                       2520
      IF (LP2-50) 29,29,30                                              2530
   30 WRITE (6,18) CPOX(NX1)                                            2540
   18 FORMAT (///31X,52HUNABLE TO CONVERGE ON CPS IN  50 TRIES ... CP(X/2550
     XA) =,E12.5)                                                       2560
      WRITE (6,522) GRAD,TGRAD                                          2570
  522 FORMAT (51X,'KC3*(CI3-CPS) =',E12.5 / 54X,'HC*(T-TPS) =',E12.5)   2580
      GO TO 28                                                          2590
   29 GAMMA = BGM/TPS                                                   2600
      BETA = -CPX(NX1)*H3*DP3/(KP*TPS)                                  2610
      K0 = ALPH2*EXP(-GAMMA)*CI1**EN3                                   2620
      GO TO 291                                                         2630
   88 IF (PRINT.EQ.1) WRITE(6,19)(DX(I),CPOX(I),I=1,NX1)                2640
   19 FORMAT (///11X,114HX/A        CP(X/A)        X/A        CP(X/A)   2650
     X X/A        CP(X/A)        X/A        CP(X/A)        X/A        CP(X/A)2660
     X        /(5X,10E12.6))                                            2670
      IF (PRINT.EQ.1) WRITE(6,82)LP2,CPOX(NX1)                          2680
   82 FORMAT (///41X,34HCONCENTRATION GRADIENT FOUND AFTER,I3,6H TRIES / 2690
     X      45X,27HCP(X) AT PARTICLE SURFACE =,E12.5 )                 2700
      GRAD = DCPDX*DP3                                                  2710
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      TGRAD = HC*(T-TPS)                                                    2720
      IF (PRINT.EQ.1) WRITE(6,83)GRAD,TGRAD                                 2730
 83   FORMAT (51X,'KC3*(CI3-CPS) =',E12.5 / 54X,'HC*(T-TPS) =',E12.5)       2740
 28   RETURN                                                                2750
      END                                                                   2760


      SUBROUTINE TRAPP (U,V,NPART,RIESUM)                                    0
C     NUMERICAL INTEGRATION USING TRAPEZOIDAL METHOD
      REAL   K0,KC3                                                         10
      COMMON  /BBBB/DP3,A,KC3,K0,X0A,CPS,CI3,GAMMA,BETA                     20
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.-      30
     X                          B/A)))                                      40
C     FUNCTIONS DEFINING INTEGRANDS
      FOXI1(X,R)=X**2*R                                                     50
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                                           60
      N=NPART-1                                                             70
      PART=NPART                                                            80
      H=(V-U)/PART                                                          90
      UPH = U+H                                                            100
      SUM=0.                                                               110
      CPX1=CPXF(U,X0A,CPS)                                                 120
      CPX2=CPXF(V,X0A,CPS)                                                 130
      RHET1=RHETF(CI3,CPX1,GAMMA,BETA,K0,1)                                140
      RHET2=RHETF(CI3,CPX2,GAMMA,BETA,K0,1)                                150
C     CALCULATE FIRST,LAST TERMS OF RIEMANN SUM FIRST
 4    TRM1=FOXI1(U,RHET1)/2.                                               160
      TRM2=FOXI1(V,RHET2)/2.                                               170
 6    DO 8 I=1,N                                                           180
      CPX=CPXF(UPH,X0A,CPS)                                                190
      RHET = RHETF(CI3,CPX,GAMMA,BETA,K0,1)                                200
      SUM=SUM+FOXI1(UPH,RHET)                                              210
      UPH = UPH+H                                                          220
 8    CONTINUE                                                             230
 9    RIESUM=H*(TRM1+SUM+TRM2)                                             240
 99   RETURN                                                               250
      END                                                                  260


      SUBROUTINE UNBAR (T,IK,XIN,YIN,ZZ,KK)                                 0
      DIMENSION T(1),X(6),Y(6),A(6)                                         10
C     ------------------  MARCH 4, 1961 ---------------              UNBAR004
C     ------------------  MODIFIED 7/62  ------------------          UNBAR005
C     ------------------    TO DO QUADRATIC AND LINEAR INTERPOLATION ALSO UNBAR006
C                                                                     UNBAR007
      II = IK+1                                                             20
      N = 3                                                                 30
      N2=                                                                   40
           IF (T(II)-3.) 700,701,702                                        50
 700       IF (T(II)+0.) 60,701,704                                         60
 704       IF (T(II)-2.) 705,706,701                                        70
 705  N = 1                                                                 80
           GO TO 707                                                        90
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706   N = 2                                                          100
707   N2= 1                                                          110
701   II = II+1                                                      120
702   N1 = N +1                                                      130
            DO 50 L = II,II                                         140
            IF ( T(L) + 0. ) 60,60,51                               150
60     KK = -1                                                      160
       ZZ = 0.                                                      170
         GO TO 9999                                                 180
51    NX = T(L)                                                     190
            IF (T(L+1) + 0. ) 60,52,50                              200
52    NY = 0                                                        210
            GO TO 53                                                220
50    NY = T(L+1)                                                   230
53       CONTINUE                                                   240
      KK  = 0                                                       250
      KY  = 0                                                       260
      XX  = XIN                                                     270
      YY  = YIN                                                     280
      J1  = II+2                                                    290
      J2  = NX+II+1                                                 300
      IF(XX-T(J1))301,306,400                                       310
400         DO 302 J=J1,J2                                          320
            IF (XX-T(J)) 304,304,302                                330
302   CONTINUE                                                      340
309   KK  = 2                                                       350
      XX  = T(J2)                                                   360
308   JX1 = J2-N                                                    370
            GO TO 305                                               380
301   KK  = 1                                                       390
      XX  = T(J1)                                                   400
306   JX1 = J1                                                      410
            GO TO 305                                               420
304         IF (J-J1-1) 301,308,307                                 430
307         IF (J-J2)  305,308,309                                  440
303   JX1 = J-N2                                                    450
305   CONTINUE                                                      460
      XINT  = XX                                                    470
        IF (NY) 1500, 1500, 3000                                    480
1500        DO 1599 L=1,N1                                          490
             X(L) = T(JX1)                                          500
             LY = JX1 + NX                                          510
             Y(L) = T(LY)                                           520
1599    JX1 = JX1+1                                                 530
      I = 1                                                         540
      GO TO 54                                                      550
3000  J1  = J1+NX                                                   560
      J2  = J2+NY                                                   570
      IF(YY-T(J1))311,316,401                                       580
401         DO 312 J=J1,J2                                          590
            IF (YY-T(J)) 314,314,312                                600
312   CONTINUE                                                      610
319   KY  = 4                                                       620
      YY  = T(J2)                                                   630
318   JY1 = J2-N                                                    640
            GO TO 315                                               650
311   KY  = 3                                                       660
      YY  = T(J1)                                                   670
316   JY1 = J1                                                      680
            GO TO 315                                               690
```

```
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 [illegible] Y(J)*  X(J)
56       CO[illegible]
59       [illegible] 3098,9999
9999 KK  [illegible]
         [illegible]
     [illegible]
```

```
      BLOCK DATA                                                        0
      COMMON /MUVST/VISVST(30)                                         10
C     BLOCK DATA FOR VISCOSITY VS TEMPERATURE
      DATA (VISVST(I),I=1,30) / 0.0,1.,13.,0.0,                        20
     X      360.,540.,720.,900.,1080.,1260.,1440.,1620.,1800.,1980.,   30
     X      2160.,2340.,2520.,                                         40
     X      .048 E-4,.070 E-4,.093 E-4,.117 E-4,.141 E-4,.164 E-4,     50
     X      .186 E-4,.207 E-4,.228 E-4,.247 E-4,.266 E-4,.285 E-4,     60
     X      .302 E-4/                                                  70
      END                                                              80
```

```
      BLOCK DATA                                                        0
      COMMON /FTZ/TBLVP(70),TBLH4(42),TBLH3(42),SHTBL1(34),SHTBL2(34),  10
     1        SHTBL3(34),SHTBL4(34),ZTBLD(46),ZTBLAP(46),ZTBLA(46)      20
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 30
     134.60,534.71,538.34,543.91,545.73,560.20,569.98,579.26,579.48,595. 40
     234,610.13,614.08,618.07,627.49,628.82,645.68,650.76,665.57,674.99, 50
     3686.13,692.39,697.47,744.,798.,852.,942.,1032.,1122.,1176.,.0520,. 60
     41479,.2011,.2069,.2398,.2436,.2823,.2920,.3539,.5453,.7367,.9727,. 70
     59823,1.510,2.204,2.462,2.740,3.407,3.562,5.240,5.971,8.065,9.711,1 80
     61.91,13.46,14.70,33.80,73.48,147.0,382.1,823.0,1528.,2131./       90
      DATA  (TBLH4(I),I=1,42 )/0.0,1.,19.0,0.0,0.0,180.,360.,536.4,540., 100
     5720.,900.,1080.,1260.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,27 110
     900.0,2880.,3060.,-1991.34,-1951.02,-1919.50,-1896.04,-1895.70,-188 120
     X2.55,-1878.12,-1879.46,-1884.63,-1892.38,-1901.94,-1912.88,-1924.8 130
     X5,-1937.54,-1950.74,-1964.45,-1978.32,-1992.36,-2006.62/          140
      DATA  (TBLH3(I),I=1,42 )/0.0,1.,19.0,0.0,0.0,180.,360.,536.4,540., 150
     X720.,900.,1080.,1260.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,27 160
     X00.,2880.,3060.,  83.07,1055.57,1103.97,1159.35,1160.40,1213.46,125 170
     X9.64,1298.00,1329.71,1355.28,1375.57,1391.11,1402.52,1410.13,1414. 180
     X57,1416.37,1416.05,1414.15,1410.56/                               190
      DATA  (SHTBL1(I),I=1,34)/0.0,1.,15.0,0.0,540.,720.,900.,1080.,1260 200
     1.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,2700.,2880.,3060.,.380 210
     24,.4601,.5261,.5784,.6212,.6577,.6899,.7185,.7442,.7673,.7879,.800 220
     33,.8226,.8373,.8503/                                              230
      DATA  (SHTBL2(I),I=1,34)/0.0,1.,15.0,0.0,540.,720.,900.,1080.,1260 240
     5.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,2700.,2880.,3060.,.500 250
     65,.5424,.5691,.6344,.6773,.7176,.7553,.7905,.8236,.8541,.8823,.907 260
     75,.9304,.9512,.9697/                                              270
      DATA  (SHTBL3(I),I=1,34)/0.0,1.,15.0,0.0,540.,720.,900.,1080.,1260 280
     9.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,2700.,2880.,3060.,.248 290
     X5,.2495,.2524,.2569,.2624,.2682,.2738,.2790,.2836,.2878,.2914,.294 300
     X6,.2974,.2998,.3019/                                              310
      DATA  (SHTBL4(I),I=1,34)/0.0,1.,15.0,0.0,540.,720.,900.,1080.,1260 320
     X.,1440.,1620.,1800.,1980.,2160.,2340.,2520.,2700.,2880.,3060.,3.41 330
     X94,3.4596,3.4685,3.4765,3.4899,3.5151,3.5454,3.5806,3.6208,3.6654, 340
     X3.7150,3.7696,3.8291,3.8802,3.9288/                               350
      END                                                               360
```

```
      BLOCK DATA                                                        0
```

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```
C   BLOCK DATA FOR SPECIFIC HEAT VS TEMPERATURE
      COMMON /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)                  10
      DATA  (CFTBL1(I),I=1,34) /  0., 1., 15., 0.,                             20
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,         30
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,                 40
C     SPECIFIC HEATS
     X 3.4194, 3.4596, 3.4685, 3.4765, 3.4899, 3.5151, 3.5454, 3.5006,         50
     X 3.6208, 3.6654, 3.7150, 3.7696, 3.8291, 3.8802, 3.9288 /                60
      DATA  (CFTBL2(I),I=1,34) /  0., 1., 15.,  .,                             70
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,         80
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,                 90
C     SPECIFIC HEATS
     X .2465 , .2495 , .2524 , .2569 , .2624 , .2682 , .2738 , .2790 ,         100
     X .2836 , .2878 , .2914 , .2946 , .2974 , .2998 , .3019  /                110
      DATA  (CFTBL3(I),I=1,34) /  0., 1., 15., 0.,                             120
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,         130
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,                 140
C     SPECIFIC HEATS
     X .5005 , .5424 , .5891 , .6344 , .6773 , .7176 , .7553 , .7905 ,         150
     X .8236 , .8541 , .8823 , .9075 , .9304 , .9512 , .9697  /                160
      DATA  (CFTBL4(I),I=1,34) /  0., 1., 15., 0.,                             170
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,         180
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,                 190
C     SPECIFIC HEATS
     X .3604 , .4601 , .5261 , .5784 , .6212 , .6577 , .6899 , .7185 ,         200
     X .7442 , .7673 , .7879 , .8063 , .8226 , .8373 , .8503  /                210
      END                                                                      220
```

```
      BLOCK DATA                                                               0
C     BLOCK DATA FOR HEAT OF REACTION VS TEMPERATURE
      COMMON /CCC/H4TBL(40),H3TBL(40)                                          10
      DATA  (H4TBL(I),I=1,40) /   0., 1., 18., 0.,                             20
C     TEMPERATURES
     X  160. ,  360. ,  536.4 ,  540. ,  720. ,  900. , 1080. ,               30
     X 1260. , 1440. , 1620. , 1800. , 1980. , 2160. , 2340. ,                 40
     X 2520. , 2700. , 2880. , 3060. ,                                         50
C     HEATS OF REACTION
     X-1951.02,-1919.50,-1896.04,-1895.70,-1882.55,-1878.12,-1879.46,          60
     X-1884.63,-1892.38,-1901.94,-1912.88,-1924.85,-1937.54,-1950.74,          70
     X-1964.45,-1978.32,-1992.36,-2006.62  /                                   80
      DATA  (H3TBL(I),I=1,40) /   0., 1., 18., 0.,                             90
C     TEMPERATURES
     X  180. ,  360. ,  536.4 ,  540. ,  720. ,  900. , 1080. ,               100
     X 1260. , 1440. , 1620. , 1800. , 1980. , 2160. , 2340. ,                 110
     X 2520. , 2700. , 2880. , 3060. ,                                         120
C     HEATS OF REACTION
     X1055.57 ,1103.97 ,1159.35 ,1160.40 ,1213.46 ,1259.64 ,1298.00 ,         130
     X1329.71 ,1355.28 ,1375.57 ,1391.11 ,1402.52 ,1410.13 ,1414.57 ,         140
     X1416.37 ,1416.05 ,1414.15 ,1410.56   /                                   150
      END                                                                      160
```

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```
      BLOCK DATA                                                          0
      COMMON /DAVTBL/VPTBL(44)                                           10
C     BLOCK DATA TABLE OF VAPOR PRESSURE VS TEMP  (USED TO FIND TVAP)
      DATA (VPTBL(I),I=1,44) /     0. ,   1. ,  20. ,   0. ,            20
     X      50.  ,  100. , 150. , 200. , 250. , 300. , 350. , 400. ,     30
     X      450. ,  500. , 550. , 600. , 650. , 700. , 750. , 800. ,     40
     X      850. , 900. , 950. , 1000.,                                  50
     X      770. , 820. , 855. , 880. , 905. , 925. , 945. , 965. ,      60
     X      980. , 995. ,1010. ,1025. ,1035. ,1050. ,1060. ,1070. ,      70
     X      1080.,1090. ,1100. ,1110. /                                  80
      END                                                                 90


      BLOCK DATA                                                          0
      COMMON /LIZTBL/DHVST(18),DHLVST(18)                                10
C     BLOCK DATA TABLES FOR DELHV AND DELHL VS TEMP  (USED TO FIND HV)
      DATA  (DHVST(I),I=1,18) / 0., 1., 7., 0.,                          20
     X      180. , 360. , 534.6 , 540. , 720. , 900. , 1080. ,          30
     X      1390.16 , 1332.82 , 1280.02 , 1279.12 , 1237.79 , 1208.80 ,  40
     X      1189.76 /                                                    50
      DATA  (DHLVST(I),I=1,18) / 0., 1., 7., 0.,                         60
     X      180. , 360. , 534.6 , 540. , 720. , 900. , 1080. ,          70
     X      652.14 , 665.96 , 679.61 , 679.89 , 700.89 , 733.19 , 777.22 80
     X       /                                                           90
      END                                                                100
```

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 60'S ... FORMAT EXACTLY AS IN CARD 4
C
C  CARD 6  ... CONTAINS 20'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
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 17A,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              (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                          C
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZO(25),GO(25),ZO(25)          10
      COMMON /BLOK2/A,AP,DELTA,DR,DFA,D0N2H4,D0NH3,R,CGM,RADIUS,NMAX1,   20
     X        NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4  30
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS 40
      COMMON /BVTBLS/AVSZ(234),APVSZ(234),BELVSZ(234)                    50
      COMMON /AAA/VISVST(30),TBLVP(68)                                   60
      COMMON /CCC/H4TBL(40),H3TBL(40)                                    70
      COMMON /LIZTBL/DHVST(18),DHLVST(18)                                80
      COMMON /DAVTBL/VPTBL(44)                                           90
      COMMON /MMM/MI                                                     100
      DIMENSION ZL(25),TL(25),ZLV(25),TLV(25),JZ(25),ZZ(25,75),TT(25,75) 110
      DIMENSION TITLE(14)                                                120
      READ (5,702) NCASE                                                 130
  702 FORMAT (I3)                                                        140
      KOUNT = 1                                                          150
  705 READ (5,608) TITLE                                                 160
  608 FORMAT (14A6)                                                      170
      WRITE (6,609) TITLE                                                180
  609 FORMAT ('1',28X,14A6//)                                            190
C   READ INPUT CONSTANTS
      READ (5,810) NRINGS,NOFZ                                           200
      READ (5,811) (F(I),I=1,NRINGS)                                     210
      READ (5,811) (GO(I),I=1,NRINGS)                                    220
      READ (5,811) (ZO(I),I=1,NRINGS)                                    230
  810 FORMAT (2I3)                                                       240
  811 FORMAT (10E8.4)                                                    250
C   THE SUBSCRIPT 'I' REFERS TO THE ANNULAR REGIONS
C   REGIONS ARE NUMBERED 1,2,...,NRINGS FROM THE CENTER OUTWARD
      I = 0                                                              260
      READ (5,800) ALPHA3,HF,R,MN2H4,MNH3,MN2,MH2,ALPHA1,ALPHA2,AGM,BGM, 270
     X       KP,TF,CF,NMAX1,NMAX2,P,ZEND,D0N2H4,D0NH3,CGM,RADIUS          280
  800 FORMAT (8E10.5)                                                    290
      WRITE (6,36) (J,F(J),GO(J),ZO(J),J=1,NRINGS)                       300
   36 FORMAT (////61X,'PROGRAM INPUT' /46X,'RING',11X,'F',11X,'GO',10X,' 310
     XZO' /(47X,I2,5X,3E12.5))                                           320
      WRITE (6,37) ALPHA3,HF,R,MN2H4,MNH3,MN2,MH2,ALPHA1,ALPHA2,AGM,BGM, 330
     X       KP,TF,CF,NMAX1,NMAX2,P,ZEND,D0N2H4,D0NH3,CGM,RADIUS          340
   37 FORMAT (//5X,'ALPHA3 =',E10.4,3X,'HF =',F10.4,3X,'R =',E10.4,3X,'MN2H 350
     X4 =',E10.4,3X,'MNH3 =',E10.4,3X,'MN2 =',E10.4,3X,'MH2 =',E10.4 //  360
     X      3X,'ALPHA1 =',E10.4,3X,'ALPHA2 =',E10.4,3X,'AGM =',E10.4,3X,  370
     X      'BGM =',E10.4,3X,'KP =',E10.4,3X,'TF =',E10.4,3X,'CF =',E10.4 // 380
     X      5X,'NMAX1 =',E10.4,3X,'NMAX2 =',E10.4,3X,'P =',E10.4,3X,      390
     X      'ZEND =',E10.4,3X,'D04 =',E10.4,3X,'D03 =',E10.4,3X,'CGM =',E10. 400
     X4     /,3X,'RADIUS =',E10.4 /)                                      410
      NZTBL = NOFZ+NRINGS+NOFZ*NRINGS+4                                  420
      NOFZ4 = NOFZ+4                                                     430
      NOFZ5 = NOFZ4+1                                                    440
      NOFZ6 = NOFZ4+NRINGS                                               450
C   READ IN A,AP,DELTA AS 2 TABLES (DIVARIATE)
      READ (5,40) (AVSZ(I),Z=1,4)                                        460
   40 FORMAT (4E8.4)                                                     470
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      READ (5,41) (AVSZ(I),I=5,NOFZ4)                                  480
41    FORMAT (10E8.4)                                                  490
      READ (5,41) (AVSZ(I),I=NOFZ5,NOFZ6)                              500
      I1 = NOFZ6+1                                                     510
      I2 = NOFZ6+NRINGS                                                520
      DO 42 J=1,NOFZ                                                   530
      READ (5,41) (AVSZ(I),I=I1,I2)                                    540
      I1 = I2+1                                                        550
      I2 = I1+NRINGS-1                                                 560
42    CONTINUE                                                         570
      READ (5,40) (APVSZ(I),I=1,4)                                     580
      READ (5,41) (APVSZ(I),I=5,NOFZ4)                                 590
      READ (5,41) (APVSZ(I),I=NOFZ5,NOFZ6)                             600
      I1 = NOFZ6+1                                                     610
      I2 = NOFZ6+NRINGS                                                620
      DO 43 J=1,NOFZ                                                   630
      READ (5,41) (APVSZ(I),I=I1,I2)                                   640
      I1 = I2+1                                                        650
      I2 = I1+NRINGS-1                                                 660
43    CONTINUE                                                         670
      READ (5,40) (DELVSZ(I),I=1,4)                                    680
      READ (5,41) (DELVSZ(I),I=5,NOFZ4)                                690
      READ (5,41) (DELVSZ(I),I=NOFZ5,NOFZ6)                            700
      I1 = NOFZ6+1                                                     710
      I2 = NOFZ6+NRINGS                                                720
      DO 44 J=1,NOFZ                                                   730
      READ (5,41) (DELVSZ(I),I=I1,I2)                                  740
      I1 = I2+1                                                        750
      I2 = I1+NRINGS-1                                                 760
44    CONTINUE                                                         770
      WRITE (6,604)                                                    780
604   FORMAT (///59X,13H A VS Z TABLE)                                 790
      WRITE (6,45) (AVSZ(I),I=1,4)                                     800
      WRITE (6,50)                                                     810
50    FORMAT ( / )                                                     820
      WRITE (6,46) (AVSZ(I),I=5,NOFZ4)                                 830
      WRITE (6,50)                                                     840
      WRITE (6,46) (AVSZ(I),I=NOFZ5,NOFZ6)                             850
      WRITE (6,50)                                                     860
45    FORMAT (39X,4E13.5)                                              870
46    FORMAT (10E13.5)                                                 880
      I1 = NOFZ6+1                                                     890
      I2 = NOFZ6+NRINGS                                                900
      DO 47 J=1,NOFZ                                                   910
      WRITE (6,46) (AVSZ(I),I=I1,I2)                                   920
      I1 = I2+1                                                        930
      I2 = I1+NRINGS-1                                                 940
47    CONTINUE                                                         950
      WRITE (6,606)                                                    960
606   FORMAT (///59X,13HAP VS Z TABLE)                                 970
      WRITE (6,45) (APVSZ(I),I=1,4)                                    980
      WRITE (6,50)                                                     990
      WRITE (6,46) (APVSZ(I),I=5,NOFZ4)                               1000
      WRITE (6,50)                                                    1010
      WRITE (6,46) (APVSZ(I),I=NOFZ5,NOFZ6)                           1020
      WRITE (6,50)                                                    1030
      I1 = NOFZ6+1                                                    1040
      I2 = NOFZ6+NRINGS                                               1050
      DO 48 J=1,NOFZ                                                  1060
      WRITE (6,46) (APVSZ(I),I=I1,I2)                                 1070
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```
      I1 = I2+1                                                          1080
      I2 = I1+NRINGS-1                                                   1090
 48   CONTINUE                                                           1100
      WRITE (6,607)                                                      1110
607   FORMAT (///57X,17H DELTA VS Z TABLE)                               1120
      WRITE (6,45) (DELVSZ(I),I=1,4)                                     1130
      WRITE (6,50)                                                       1140
      WRITE (6,46) (DELVSZ(I),I=5,NOFZ4)                                 1150
      WRITE (6,50)                                                       1160
      WRITE (6,46) (DELVSZ(I),I=NOFZ5,NOFZ6)                             1170
      WRITE (6,50)                                                       1180
      I1 = NOFZ6+1                                                       1190
      I2 = NOFZ6+NRINGS                                                  1200
      DO 49 J=1,NOFZ                                                     1210
      WRITE (6,46) (DELVSZ(I),I=I1,I2)                                   1220
      I1 = I2+1                                                          1230
      I2 = I1+NRINGS-1                                                   1240
 49   CONTINUE                                                           1250
      WRITE (6,27)                                                       1260
 27   FORMAT ('1',22X,'POSITIONS AND TEMPERATURES AT EACH AXIAL STATION  1270
     X ---  LIQUID AND LIQUID-VAPOR REGIONS')                           1280
      DR = RADIUS/FLOAT(NRINGS)                                          1290
C   OBTAIN MIDPOINTS OF ANNULAR RINGS
      RAD(1) = DR/2.                                                     1300
      DO 101 J=2,NRINGS                                                  1310
      RAD(J) = RAD(J-1)+DR                                               1320
101   CONTINUE                                                           1330
      CALL UNBAR (VPTBL,1,P,0.,TVAP,KK)                                  1340
      CALL UNBAR (DHVST,1,TVAP,0.,DELHV,KK)                              1350
      CALL UNBAR (DHLVST,1,TVAP,0.,DELHL,KK)                             1360
      HL = (TVAP-TF)*CF                                                  1370
      HV = HL+DELHV-DELHL                                                1380
875   I = I+1                                                            1390
      LIQVP = 0                                                          1400
      J = 0                                                              1410
      Z = 0.                                                             1420
      DZ = 0.                                                            1430
      DERIV = 0.                                                         1440
      H(I) = HF                                                          1450
      GATZ0(I) = G0(I)+F(I)*Z0(I)                                        1460
879   Z = Z+DZ                                                           1470
      J = J+1                                                            1480
C   STORE CURRENT Z IN OUTPUT BLOCK
      ZZ(I,J) = Z                                                        1490
C   CHECK IF WE HAVE REACHED THE END OF THE INJECTOR FOR THIS RING
      IF (Z-Z0(I)) 34,34,35                                              1500
 34   G = G0(I)+F(I)*Z                                                   1510
      GO TO 78                                                           1520
 35   G = GATZ0(I)                                                       1530
      F(I) = 0.                                                          1540
 78   T = TF+(H(I)-HF)/CF                                                1550
C    STORE CURRENT TEMP IN OUTPUT BLOCK
      TT(I,J) = T                                                        1560
C    CHECK IF WE HAVE REACHED LIQUID-LIQUID VAPOR INTERFACE
      IF (LIQVP.EQ.1) GO TO 102                                          1570
      CALL UNBAR (TBLVP,1,T,0.,VPR,KK)                                   1580
      CALL UNBAR (H4TBL,1,T,0.,H4,KK)                                    1590
      CALL UNBAR (AVSZ,1,Z,RAD(I),A,KK)                                  1600
      CALL UNBAR (APVSZ,1,Z,RAD(I),AP,KK)                                1610
      C4 = VPR*MN2H4/(R*T)                                               1620
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```
      GAMMA = AGM/T                                                          1630
      K = ALPHA1*EXP(-GAMMA)                                                 1640
      DPA = D0N2H4*(T/492.)**1.832*14.7/P*(1.-EXP(-.067*P*492./              1650
     X      (14.7*T)))                                                      1660
      BETA = -C4*H4*DPA/(KP*T)                                               1670
      DERIVO = DERIV                                                         1680
      CALL SLOPE (DERIV)                                                     1690
      IF (MI.GT.20) DERIV=DERIVO                                             1700
      DHDZ = -(H4*DPA*AP*DERIV+F(I)*(H(I)-HF))/G                             1710
      DZ = -H4/(NMAX1*DHDZ)                                                  1720
      H(I) = H(I)+DHDZ*DZ                                                    1730
      IF (H(I)-HL) 879,877,878                                               1740
C   WE HAVE EXCEEDED LIQUID-LIQUID VAPOR INTERFACE FOR THIS RING ---
C   BACKSTEP TO L-LV BOUNDARY
 878  DZ = (HL-H(I))/DHDZ                                                    1750
      H(I) = HL                                                              1760
C   SET FLAG TO INDICATE INTERFACE HAS BEEN REACHED
 877  LIQVP = 1                                                              1770
      GO TO 879                                                              1780
C   WE HAVE REACHED THE LIQUID-LIQUID VAPOR INTERFACE FOR THIS RING
 102  TL(I) = T                                                              1790
      ZL(I) = Z                                                              1800
      CALL LQVP (I,J,DERIV,T,Q,Z,ZZ,TT,DZ)                                   1810
      TLV(I) = T                                                             1820
      ZLV(I) = Z                                                             1830
      JZ(I) = J                                                              1840
C   CHECK IF ALL RINGS HAVE BEEN PROCESSED
      IF (I-NRINGS) 875,870,870                                              1850
 870  DO 25 I=1,NRINGS                                                       1860
      JN = JZ(I)                                                             1870
      WRITE (6,28) I                                                         1880
      WRITE (6,26) (ZZ(I,J),TT(I,J),J=1,JN)                                  1890
 25   CONTINUE                                                               1900
 26   FORMAT (9X,'Z',12X,'T',4(12X,'Z',12X,'T') / (1X,10E13.5) )             1910
 28   FORMAT (//65X,'RING',I3)                                               1920
      WRITE (6,613)                                                          1930
 613  FORMAT (1H1,27X,75H**********                    LIQUID REGION        1940
     X   ********** )                                                        1950
      LAST = NRINGS-1                                                        1960
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                                                        1970
      IF (ABS(ZL(I)-ZL(I+1)).LT..01*ZL(I)) ZL(I+1)=ZL(I)                     1980
      IF (ABS(ZLV(I)-ZLV(I+1)).LT..01*ZLV(I)) ZLV(I+1)=ZLV(I)                1990
 700  CONTINUE                                                               2000
      WRITE (6,88) (I,ZL(I),RAD(I),TL(I),I=1,NRINGS)                         2010
 88   FORMAT (//23X,'POSITION AND TEMPERATURE AT LIQUID - LIQUID VAPOR I     2020
     XNTERFACE FOR EACH ANNULAR REGION' /                                    2030
     X      36X,57H RING       AXIAL POSITION   RADIAL POSITION   TEMPERA  2040
     XTURE  /                                                                2050
     X      (38X,I2,6X,E12.5,6X,E12.5,4X,E12.5) )                           2060
      WRITE (6,90)                                                           2070
 90   FORMAT (////27X,75H**********                    LIQUID-VAPOR REGION   2080
     X      ********** )                                                    2090
      WRITE (6,89) (I,ZLV(I),RAD(I),TLV(I),I=1,NRINGS)                       2100
 89   FORMAT (//24X,'POSITION AND TEMPERATURE AT LIQUID VAPOR - VAPOR IN     2110
     XTERFACE FOR EACH ANNULAR REGION' /                                     2120
     X      36X,57H RING       AXIAL POSITION   RADIAL POSITION   TEMPERA  2130
     XTURE  /                                                                2140
     X      (38X,I2,6X,E12.5,6X,E12.5,4X,E12.5) )                           2150
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C   PROCEED ON TO VAPOR REGION
      CALL VAPOR (ALPHA3,ZLV,TLV)                                          216C
      KOUNT = KOUNT+1                                                      217C
      IF (KOUNT.LE.NCASE) GO TO 705                                        218C
      WRITE (6,107)                                                        219C
  107 FORMAT (////48X,35H******  OPERATIONS COMPLETE  ****** )             220C
      STOP                                                                 221C
      END                                                                  222C
```

```
      SUBROUTINE LGVP (I,J,DERIV,T,G,Z,ZZ,TT,DZ)                            C
C   THIS ROUTINE HANDLES REACTOR CALCULATIONS FOR LIQUID VAPOR REGIONS
C   OF EACH ANNULAR RING
      REAL  NMAX2                                                           1C
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZ0(25),G0(25),Z0(25)             2C
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,D0N2H4,D0NH3,R,CGM,RADIUS,NMAX1,      3C
     X        NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4     4C
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS    5C
      COMMON /BVTBLS/AVSZ(234),APVSZ(234),DELVSZ(234)                       6C
      COMMON /CCC/H4TBL(40),H3TBL(40)                                       7C
      DIMENSION ZZ(25,75),TT(25,75)                                         8C
C   ASSUME TEMPERATURE CONSTANT IN LIQUID VAPOR REGION
      CALL UNBAR (H4TBL,1,T,0.,H4,KK)                                       9C
  182 CALL UNBAR (APVSZ,1,Z,RAD(I),AP,KK)                                   10C
      DPA = D0N2H4*(T/492.)**1.832*14.7/P*(1.-EXP(-.067*P*492./             11C
     X      (14.7*T)))                                                     12C
      DHDZ = -(H4*DPA*AP*DERIV+F(I)*(H(I)-HF))/G                            13C
      DZ = -H4/(NMAX2*DHDZ)                                                 14C
      Z = Z+DZ                                                              15C
      J = J+1                                                               16C
C   STORE CURRENT Z IN OUTPUT BLOCK
      ZZ(I,J) = Z                                                           17C
      TT(I,J) = T                                                           18C
C   CHECK IF WE HAVE REACHED THE INJECTOR TIP FOR THIS RING
      IF (Z-Z0(I)) 34,34,35                                                 19C
   34 G = G0(I)+F(I)*Z                                                      20C
      GO TO 78                                                              21C
   35 G = GATZ0(I)                                                          22C
      F(I) = 0.                                                             23C
   78 H(I) = H(I)+DHDZ*DZ                                                   24C
      IF (H(I)-HV) 182,195,184                                              25C
C   WE HAVE EXCEEDED LIQUID VAPOR-VAPOR INTERFACE FOR THIS RING ---
C   BACKSTEP TO LV-V BOUNDARY
  184 DZ = (HV-H(I))/DHDZ                                                   26C
      Z = Z+DZ                                                              27C
      ZZ(I,J) = Z                                                           28C
      H(I) = HV                                                             29C
  195 RETURN                                                                30C
      END                                                                   31C
```

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      SUBROUTINE VAPOR (ALPHA3,ZLV,TLV)                                     C
C   THIS ROUTINE HANDLES REACTOR CALCULATIONS FOR VAPOR REGION OF EACH
C   ANNULAR RING
      REAL  LAMDA,NH1,NRR1,NR2,NRR2,NR3,NRR3,NR4,NRR4,KC4,MH2,MN2,MNH3,     1C
     X      MN2H4,MBAR                                                     2C
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      INTEGER VAPOR,VP                                                          30
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZ0(25),G0(25),Z0(25)                 40
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,D0N2H4,D0NH3,R,CGM,RADIUS,NMAX1,          50
     X       NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4         60
      COMMON /BLOK3/KV,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS       70
      COMMON /BVTBLS/AVSZ(234),APVSZ(234),DELVSZ(234)                           80
      COMMON /AAA/VISVST(30),TBLVP(68)                                          90
      COMMON /CCC/H4TBL(40),H3TBL(40)                                          100
      COMMON /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)                  110
      DIMENSION  HH4(25),XV(25),TLV(25),CI1(25),CI2(25),CI3(25),CI4(25),       120
     X           RH0(25),RHOM(25),T(25),ZLV(25),ZV0(25),IFN(25),MIX(10),       130
     X           G(25),ZZ(25),F1(25),F2(25),F3(25),F4(25),F3D(25)              140
      DIMENSION  TT(25),C1(25),C2(25),C3(25),C5(25),GR(25),TGR(25),            150
     X           CK4(25),DPDZ(25),Z00(25),NZ0(25)                              160
      VAPOR = 0                                                                170
      IFFLG = 0                                                                180
      VP = VAPOR+1                                                             190
      M = 2                                                                    200
      N = 1                                                                    210
      NM1 = NRINGS-1                                                           220
      WRITE (6,598)                                                            230
598   FORMAT ('1',29X,'**************************      VAPOR REGION      **     240
     X**************************')                                             250
C     CALCULATE CONCENTRATIONS AT INTERFACES FOR EACH RING
      DO 37 I=1,NRINGS                                                         260
      CALL UNBAR (H4TBL,1,TLV(I),0.,HH4(I),KK)                                 270
      XV(I) = (HF-H(I))/HH4(I)                                                 280
      X1 = (1.-XV(I))/(1.+XV(I))                                               290
      X2 = XV(I)/(1.+XV(I))                                                    300
      PRT = P/(R*TLV(I))                                                       310
      CI1(I) = .5*PRT*MH2*X2                                                   320
      CI2(I) = .5*PRT*MN2*X2                                                   330
      CI3(I) = PRT*MNH3*X2                                                     340
      CI4(I) = PRT*MN2H4*X1                                                    350
      RH0(I) = CI1(I)+CI2(I)+CI3(I)+CI4(I)                                     360
      RHOM(I) = ALPHA3*CI4(I)*EXP(-CGM/TLV(I))                                 370
      T(I) = TLV(I)                                                            380
C     SET INITIAL VAPOR REGION VALUES FOR G
      IF (ZLV(I)-Z0(I)) 590,590,591                                            390
590   G(1) = G0(I)+F(I)*ZLV(I)                                                 400
      GO TO 37                                                                 410
591   G(1) = GATZ0(I)                                                          420
      F(I) = 0.                                                                430
37    CONTINUE                                                                 440
      WRITE (6,38) CI4(1),CI3(1),CI2(1),CI1(1)                                 450
38    FORMAT (//43X,'CONCENTRATIONS AT LIQUID VAPOR - VAPOR INTERFACE'/        460
     X       47X,'N2H4          NH3          N2          H2'/41X,4E12.5 )     470
      SUM = CI1(1)/MH2+CI2(1)/MN2+CI3(1)/MNH3+CI4(1)/MN2H4                     480
      FRAC1 = CI1(1)/(MH2*SUM)                                                 490
      FRAC2 = CI2(1)/(MN2*SUM)                                                 500
      FRAC3 = CI3(1)/(MNH3*SUM)                                                510
      FRAC4 = CI4(1)/(MN2H4*SUM)                                               520
      FRAC3D = (FRAC1/FRAC2-1.)/(3.-FRAC1/FRAC2)                               530
      WRITE (6,39) FRAC1,FRAC2,FRAC3,FRAC4,FRAC3D                              540
39    FORMAT (///40X,'MFRAC1', 6X,'MFRAC2' 6X,'MFRAC3' 6X,'MFRAC4' 6X,         550
     X       'FRAC3D' / 35X,5E12.5 )                                           560
      DPDZ = 0.                                                                570
C     SUBROUTINE ORDER STORES INTERFACE AXIAL STATIONS IN ASCENDING ORDER
      CALL ORDER (ZLV,ZV0)                                                     580
      Z = ZV0(1)                                                               590
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C   GET ZO'S STORED IN ASCENDING ORDER
      CALL ORDER (ZO,ZOO)                                                  600
C   SET N (ZO INDICATOR) TO IGNORE INJECTOR TIPS IF LESS THAN SMALLEST ZVAP
      IF (ZOO(NRINGS).LT.ZVO(1)) N=NRINGS+1                                610
C   FIND AND LABEL ALL DISTINCT INTERFACES
      J = 1                                                                620
      IFACE = 1                                                            630
      IFN(1) = 1                                                           640
      DO 74 I=2,NRINGS                                                     650
      IF (ZVO(J)-ZVO(I)) 72,73,72                                          660
   73 J = 1                                                                670
      GO TO 74                                                             680
   72 J = 1                                                                690
C   IFACE = TOTAL NUMBER OF DISTINCT INTERFACES
      IFACE = IFACE+1                                                      700
      IFN(IFACE) = J                                                       710
   74 CONTINUE                                                             720
C   FIND AND LABEL ALL DISTINCT ZO'S
      J = 1                                                                730
      NOZO = 1                                                             740
      NZO(1) = 1                                                           750
      DO 227 I=2,NRINGS                                                    760
      IF (ZOO(J)-ZOO(I)) 228,229,228                                       770
  229 J = 1                                                                780
      GO TO 227                                                            790
  228 J = 1                                                                800
C   NOZO = TOTAL NUMBER OF DISTINCT ZO'S
      NOZO = NOZO+1                                                        810
      NZO(NOZO) = J                                                        820
  227 CONTINUE                                                             830
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                                                840
   22 VAPOR = 1                                                            850
      VP = VP+1                                                            860
      CALL DELTAZ (CI1,CI2,CI3,CI4,T,G,RHO,RHOM,CK4,GR,TGR,Z,DZ)           870
      GO TO 8                                                              880
C   USE CONSTANT DZ VALUE FOR INITIAL PORTIONS OF VAPOR REGION
   23 DZZ = (ZVO(NRINGS)-ZVO(1))/25.                                       890
      DZ = DZZ                                                             900
    8 ZP = Z                                                               910
      IF (VAPOR.EQ.1) GO TO 15                                             920
      IF (IFFLG-1) 40,42,40                                                930
   40 IF (DZ.LT.DZZ) DZ=DZZ                                                940
      GO TO 15                                                             950
   42 DZ = DELZ                                                            960
      IFFLG = 0                                                            970
   15 Z = Z+DZ                                                             980
C   TEST IF WE HAVE REACHED THE END OF THE REACTOR
      IF (Z-ZEND) 43,43,44                                                 990
   44 Z = ZEND                                                            1000
      DZ = ZEND-ZP                                                        1010
C   TEST IF ALL INTERFACES HAVE BEEN ENCOUNTERED
   43 IF (VAPOR-1) 28,33,28                                               1020
C   STILL WITHIN REGION OF VARIOUS ANNULAR INTERFACES --- NOW MUST TEST
C   FOR CURRENT Z EXCEEDING NEXT INTERFACE POSITION
   28 MM = IFN(M)                                                         1030
      IF (Z-ZVO(MM)) 30,30,31                                             1040
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)                                                  1050
      DZ = ZVO(MM)-ZP                                                   1060
      Z = ZVO(MM)                                                       1070
      IFFLG = 1                                                         1080
      M = M+1                                                           1090
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                                             1100
 32   VAPOR = 1                                                         1110
C     SET UP MIXING TERM INDICATOR FOR EACH RING AT THIS AXIAL STATION
 30   DO 10 J=1,NRINGS                                                  1120
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                                                      1130
C     TEST IF WE ARE IN FIRST OR LAST RING
        IF (J-1) 1,11,1                                                 1140
 1      IF (J-NRINGS) 2,12,2                                            1150
C     IF Z<ZVAP FOR THIS RING THEN WE ARE STILL IN LIQUID AREA
 2      IF (Z-ZLV(J)) 10,10,16                                          1160
 16     IF (Z-ZLV(J-1)) 3,3,4                                           1170
 4      MIX(J) = 2                                                      1180
 3      IF (Z-ZLV(J+1)) 10,10,5                                         1190
 5      IF (MIX(J)-2) 6,7,6                                             1200
 6      MIX(J) = 3                                                      1210
        GO TO 10                                                        1220
 7      MIX(J) = 4                                                      1230
        GO TO 10                                                        1240
C     FIRST AND LAST RINGS ARE SPECIAL CASES
 11     IF (Z-ZLV(2)) 10,10,13                                          1250
 13     MIX(J) = 3                                                      1260
        GO TO 10                                                        1270
 12     IF (Z-ZLV(NRINGS-1)) 10,10,14                                   1280
 14     MIX(J) = 2                                                      1290
 10     CONTINUE                                                        1300
 33     IF (N.GT.NOZO) GO TO 225                                        1310
        NN = NZO(N)                                                     1320
C     IF SMALLEST CURRENT ZO IS ZERO MOVE ON TO PROGRAM CALC'S
        IF (ZOO(NN)) 225,225,230                                        1330
C     TEST IF CURRENT Z EXCEEDS SMALLEST REMAINING ZO
C     YES --- BACKSTEP TO INJECTOR TIP
 230    IF (Z-ZOO(NN)) 225,225,226                                      1340
 226    DZ = Z-ZOO(NN)                                                  1350
        Z = ZOO(NN)                                                     1360
        N = N+1                                                         1370
C     SET UP CALCULATIONS FOR TEMP AND CONCENTRATION
 225    DO 20 J=1,NRINGS                                                1380
C     TEST IF WE ARE PRECISELY AT LAST INTERFACE
        IF (Z-ZVO(NRINGS)) 41,41,77                                     1390
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                                            1400
C     WE ARE IN THE ALL-VAPOR REGION OF THE REACTOR --- MIX PARAMETER NOW
C     FIXED FOR ALL RINGS
 29     MIX(1) = 3                                                      1410
        MIX(NRINGS) = 2                                                 1420
        DO 9 I=2,NM1                                                    1430
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      MIX(I) = 4                                                        1440
 9    CONTINUE                                                          1450
C    INCREMENT VP TO AVOID REDUNDANT SETTINGS OF 'MIX'
      VP = VP+1                                                         1460
      GO TO 27                                                          1470
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                                            1480
C    SET UP PRELIMINARY CALCULATIONS FOR DWDZ TERMS
 27   CALL UNBAR (AVSZ,1,ZP,RAD(J),A,KK)                                1490
      CALL UNBAR (APVSZ,1,ZP,RAD(J),AP,KK)                              1500
      CALL UNBAR (DELVSZ,1,ZP,RAD(J),DELTA,KK)                          1510
      CALL UNBAR (H4TBL,1,T(J),0.,H4,KK)                                1520
      CALL UNBAR (CFTBL4,1,T(J),0.,CF4,KK)                              1530
      CALL UNBAR (CFTBL3,1,T(J),0.,CF3,KK)                              1540
      CALL UNBAR (CFTBL2,1,T(J),0.,CF2,KK)                              1550
      CALL UNBAR (CFTBL1,1,T(J),0.,CF1,KK)                              1560
C    TEST IF Z HAS EXCEEDED INJECTOR TIP FOR THIS RING
      IF (Z-Z0(J)) 34,34,35                                             1570
 34   G(J) = G0(J)+F(J)*ZP                                              1580
      GO TO 63                                                          1590
 35   G(J) = GATZ0(J)                                                   1600
      F(J) = 0.                                                         1610
 63   CFBAR = (CF1*CI1(J)+CF2*CI2(J)+CF3*CI3(J)+CF4*CI4(J))/(CI1(J)+    1620
     X         CI2(J)+CI3(J)+CI4(J))                                    1630
      RHOM(J) = ALPHA3*CI4(J)*EXP(-C6M/T(J))                            1640
      EPSLN = -A*G(J)/(5.*RHO(J)*DELTA)                                 1650
      LAMDA = -A*CFBAR*G(J)/(5.*DELTA)                                  1660
      MX = MIX(J)                                                       1670
      GO TO (56,57,58,59), MX                                           1680
C    STATEMENT 56 --- NO MIXING TERMS USED
 56   NR1 = 0.                                                          1690
      NR2 = 0.                                                          1700
      NR3 = 0.                                                          1710
      NR4 = 0.                                                          1720
      QR1 = 0.                                                          1730
      QRN = 0.                                                          1740
      NRR1 = 0.                                                         1750
      NRR2 = 0.                                                         1760
      NRR3 = 0.                                                         1770
      NRR4 = 0.                                                         1780
      QRR1 = 0.                                                         1790
      GO TO 60                                                          1800
C    STATEMENT 57 --- INWARD MIXING ONLY
 57   NR1 = EPSLN*(CI1(J)-CI1P)/DR                                      1810
      NR2 = EPSLN*(CI2(J)-CI2P)/DR                                      1820
      NR3 = EPSLN*(CI3(J)-CI3P)/DR                                      1830
      NR4 = EPSLN*(CI4(J)-CI4P)/DR                                      1840
      QR1 = LAMDA*(T(J)-TP)/DR                                          1850
      QRN = (NR1*CF1+NR2*CF2+NR3*CF3+NR4*CF4)*(T(J)-TP)/DR              1860
      NRR1 = 0.                                                         1870
      NRR2 = 0.                                                         1880
      NRR3 = 0.                                                         1890
      NRR4 = 0.                                                         1900
      QRR1 = 0.                                                         1910
      GO TO 60                                                          1920
C    STATEMENT 58 --- OUTWARD MIXING ONLY
 58   NR1 = 0.                                                          1930
      NR2 = 0.                                                          1940
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      NR3 = 0.                                                                  1950
      NR4 = 0.                                                                  1960
      QR1 = 0.                                                                  1970
      QRN = 0.                                                                  1980
220   NRR1 = EPSLN*(CI1(J+1)-CI1(J))/DR                                         1990
      NRR2 = EPSLN*(CI2(J+1)-CI2(J))/DR                                         2000
      NRR3 = EPSLN*(CI3(J+1)-CI3(J))/DR                                         2010
      NRR4 = EPSLN*(CI4(J+1)-CI4(J))/DR                                         2020
      QRR1 = LAMDA*(T(J+1)-T(J))/DR                                             2030
      GO TO 60                                                                  2040
C     STATEMENT 59 --- BOTH INWARD AND OUTWARD MIXING
 59   NR1 = EPSLN*(CI1(J)-CI1P)/DR                                              2050
      NR2 = EPSLN*(CI2(J)-CI2P)/DR                                              2060
      NR3 = EPSLN*(CI3(J)-CI3P)/DR                                              2070
      NR4 = EPSLN*(CI4(J)-CI4P)/DR                                              2080
      QR1 = LAMDA*(T(J)-TP)/DR                                                  2090
      QRN = (NR1*CF1+NR2*CF2+NR3*CF3+NR4*CF4)*(T(J)-TP)/DR                      2100
223   NRR1 = EPSLN*(CI1(J+1)-CI1(J))/DR                                         2110
      NRR2 = EPSLN*(CI2(J+1)-CI2(J))/DR                                         2120
      NRR3 = EPSLN*(CI3(J+1)-CI3(J))/DR                                         2130
      NRR4 = EPSLN*(CI4(J+1)-CI4(J))/DR                                         2140
      QRR1 = LAMDA*(T(J+1)-T(J))/DR                                             2150
C     CHECK IF WE ARE IN ALL-VAPOR REGION
 60   IF (Z-ZVO(NRINGS)) 61,61,62                                               2160
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)           2170
      GO TO 64                                                                  2180
 62   GRAD = GR(J)                                                              2190
      TGRAD = TGR(J)                                                            2200
      KC4 = CK4(J)                                                              2210
 64   W1 = CI1(J)/RHO(J)                                                        2220
      W2 = CI2(J)/RHO(J)                                                        2230
      W3 = CI3(J)/RHO(J)                                                        2240
      W4 = CI4(J)/RHO(J)                                                        2250
      DW1DZ = (.5*MH2/MN2H4*(RHOM(J)*DELTA+AP*KC4*CI4(J))+1.5*AP*GRAD*          2260
     X          MH2/MNH3+(NR1-NRR1)*DELTA/DR-NRR1*DELTA/RAD(J)-F(J)*W1)/       2270
     X          G(J)                                                           2280
      DW2DZ = (.5*MN2/MN2H4*(RHOM(J)*DELTA+AP*KC4*CI4(J))+.5*AP*GRAD*           2290
     X          MN2/MNH3+(NR2-NRR2)*DELTA/DR-NRR2*DELTA/RAD(J)-F(J)*W2)/       2300
     X          G(J)                                                           2310
      DW3DZ = (MNH3/MN2H4*(RHOM(J)*DELTA+AP*KC4*CI4(J))-AP*GRAD)+(NR3-          2320
     X           NRR3)*DELTA/DR-NRR3*DELTA/RAD(J)-F(J)*W3)/G(J)                 2330
      DW4DZ = (F(J)-RHOM(J)*DELTA-AP*KC4*CI4(J)+(NR4-NRR4)*DELTA/DR-            2340
     X           NRR4*DELTA/RAD(J)-F(J)*W4)/G(J)                                2350
C     READY PROGRAM FOR TEMP,CONCENTRATION CALCULATIONS
      MBAR = (CI1(J)+CI2(J)+CI3(J)+CI4(J))/(CI1(J)/MH2+CI2(J)/MN2+              2360
     X        CI3(J)/MNH3+CI4(J)/MN2H4)                                         2370
      WMSM = W1/MH2+W2/MN2+W3/MNH3+W4/MN2H4                                     2380
      DMDZ = -MBAR/WMSM*(DW1DZ/MH2+DW2DZ/MN2+DW3DZ/MNH3+DW4DZ/MN2H4)           2390
      DHDZ = -(F(J)*(H(J)-HF)+AP*TGRAD+DELTA*(H4*RHOM(J)-(QR1-QRR1)/DR)+        2400
     X        QRR1*DELTA/RAD(J)+QRN*DELTA)/G(J)                                 2410
      DTDZ = DHDZ/CPBAR                                                         2420
      DRODZ = RHO(J)*(DMDZ/MBAR-DTDZ/T(J)+DPBDZ/(144.*P))                       2430
      DC1DZ = RHO(J)*DW1DZ+W1*DRODZ                                             2440
      DC2DZ = RHO(J)*DW2DZ+W2*DRODZ                                             2450
      DC3DZ = RHO(J)*DW3DZ+W3*DRODZ                                             2460
      DC4DZ = RHO(J)*DW4DZ+W4*DRODZ                                             2470
C     STORE TEMP,CONCENTRATIONS FOR INWARD RADIAL MIX CALCS IN NEXT RING
      CI1P = CI1(J)                                                             2480
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      C12P = CI2(J)                                                    2490
      CI3P = CI3(J)                                                    2500
      CI4P = CI4(J)                                                    2510
      TP = T(J)                                                        2520
      CI1(J) = CI1(J)+DC1DZ*DZ                                         2530
      CI2(J) = CI2(J)+DC2DZ*DZ                                         2540
      CI3(J) = CI3(J)+DC3DZ*DZ                                         2550
      CI4(J) = CI4(J)+DC4DZ*DZ                                         2560
      IF (CI1(J).LT.0.) CI1(J)=0.                                      2570
      IF (CI2(J).LT.0.) CI2(J)=0.                                      2580
      IF (CI3(J).LT.0.) CI3(J)=0.                                      2590
      IF (CI4(J).LT.0.) CI4(J)=0.                                      2600
      T(J) = T(J)+DTDZ*DZ                                              2610
      IF (T(J).LT.0.) GO TO 98                                         2620
      H(J) = H(J)+DHDZ*DZ                                              2630
C     STORE Z,TEMP,AND CONCENTRATIONS IN OUTPUT BLOCK
      ZZ(J) = Z                                                        2640
      TT(J) = T(J)                                                     2650
      C1(J) = CI1(J)                                                   2660
      C2(J) = CI2(J)                                                   2670
      C3(J) = CI3(J)                                                   2680
      C5(J) = CI4(J)                                                   2690
      SUM = CI1(J)/MH2+CI2(J)/MN2+CI3(J)/MNH3+CI4(J)/MN2H4             2700
      IF (CI4(J).LT.0.) SUM=SUM-CI4(J)/MN2H4                           2710
      IF (CI3(J).LT.0.) SUM=SUM-CI3(J)/MNH3                            2720
      FRAC1 = CI1(J)/(MH2*SUM)                                         2730
      FRAC2 = CI2(J)/(MN2*SUM)                                         2740
      FRAC3 = CI3(J)/(MNH3*SUM)                                        2750
      FRAC4 = CI4(J)/(MN2H4*SUM)                                       2760
      FRAC3D = (FRAC1/FRAC2-1.)/(3.-FRAC1/FRAC2)                       2770
      F1(J) = FRAC1                                                    2780
      F2(J) = FRAC2                                                    2790
      F3(J) = FRAC3                                                    2800
      F4(J) = FRAC4                                                    2810
      F3D(J) = FRAC3D                                                  2820
      GO TO 20                                                         2830
C     NO FURTHER CALCULATIONS FOLLOW FOR THIS RING --- ZERO OUT OUTPUT BLOCK
C     AND MOVE ON TO NEXT RING
   96 ZZ(J) = 0.                                                       2840
      TT(J) = 0.                                                       2850
      C1(J) = 0.                                                       2860
      C2(J) = 0.                                                       2870
      C3(J) = 0.                                                       2880
      C5(J) = 0.                                                       2890
      F1(J) = 0.                                                       2900
      F2(J) = 0.                                                       2910
      F3(J) = 0.                                                       2920
      F4(J) = 0.                                                       2930
      F3D(J) = 0.                                                      2940
   20 CONTINUE                                                         2950
      P = P+DPBDZ*DZ/144.                                              2960
      IF (P.LT.0.) GO TO 94                                            2970
C     CALCULATE DPDZ FOR PRESSURE CHANGES IN EACH RING
      SUMP = 0.                                                        2980
      DO 75 J=1,NRINGS                                                 2990
      CALL UNBAR (VISVST,1,T(J),0.,VIS,KK)                             3000
      CALL UNBAR (AVSZ,1,Z,RAD(J),A,KK)                                3010
      CALL UNBAR (DELVSZ,1,Z,RAD(J),DELTA,KK)                          3020
      RHO(J) = CI1(J)+CI2(J)+CI3(J)+CI4(J)                             3030
      RHOM(J) = ALPHA3*CI4(J)*EXP(-CGM/T(J))                           3040
```

```
      DPDZ(J) = -(1.-DELTA)/DELTA**3*(1.75+75.*VIS*(1.-DELTA)/(A*G(J)))*     3050
     X            G(J)**2/(64.4*A*RHO(J))                                   3060
      SUMP = SUMP+DPDZ(J)*RAD(J)                                            3070
 75   CONTINUE                                                              3080
      DPDDZ = 2.*DR*SUMP/RADIUS**2                                          3090
      WRITE (6,599)                                                         3100
 599  FORMAT (  /// 28X,'RING',11X,'Z',10X,'TEMP',8X,'N2H4',9X,'NH3',      3110
     X       9X,'N2',10X,'H2'    )                                          3120
      WRITE (6,600) (J,ZZ(J),TT(J),C5(J),C3(J),C2(J),C1(J),J=1,NRINGS)      3130
 600  FORMAT (29X,I2,5X,6E12.5)                                             3140
      WRITE (6,97) P                                                        3150
 97   FORMAT (//54X,'PRESSURE =',E12.5)                                     3160
      WRITE (6,36) (F1(J),F2(J),F3(J),F4(J),F3D(J),J=1,NRINGS)              3170
 36   FORMAT (//86X,'EQUIVALENT' / 40X,'MFRAC1',6X,'MFRAC2',6X,'MFRAC3',    3180
     X       6X,'MFRAC4',6X,'FRAC3D' / (35X,5E12.5))                        3190
      WRITE (6,606)                                                         3200
 606  FORMAT (///25X,'**********************************************       3210
     X**************************')                                         3220
      DO 108 J=1,NRINGS                                                     3230
      IF (TT(J).LT.TLV(J)) GO TO 106                                        3240
 108  CONTINUE                                                              3250
C    CHECK IF WE HAVE REACHED THE END OF THE REACTOR
      IF (Z-ZEND) 17,99,99                                                  3260
C    CHECK IF WE HAVE REACHED ALL-VAPOR REGION
 17   IF (Z-ZVO(NRINGS)) 8,21,21                                            3270
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)            3280
      VAPOR = 1.                                                            3290
      VP = VP+1                                                             3300
      IF (VP.GT.3) VP=3                                                     3310
      GO TO 8                                                               3320
 94   WRITE (6,95)                                                          3330
 95   FORMAT (//30X,'THE PROGRAM HAS CALCULATED A NEGATIVE PRESSURE ---     3340
     XRETURN AND TERMINATE' )                                               3350
      GO TO 99                                                              3360
 98   WRITE (6,103) J                                                       3370
 103  FORMAT (//23X,'THE PROGRAM HAS CALCULATED A NEGATIVE TEMPERATURE I    3380
     XN RING',I3,' --- RETURN AND TERMINATE' )                              3390
      GO TO 8                                                               3400
 106  WRITE (6,107) J                                                       3410
 107  FORMAT (// 7X,'THERE IS A PUDDLE OF COLD HYDRAZINE AT THE LIQUID-V    3420
     XAPOR/VAPOR INTERFACE IN RING',I3,' --- TRY USING A LARGER VALUE FO    3430
     XR GO')                                                                3440
 99   RETURN                                                                3450
      END                                                                   3460
```

```
      SUBROUTINE ORDER (ZV,ZVO)                                              0
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,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS     10
      DIMENSION  ZV(100),ZVO(100)                                            20
      LAST = NRINGS-1                                                        30
      DO 10 I=1,NRINGS                                                       40
      ZVO(I) = ZV(I)                                                         50
 10   CONTINUE                                                               60
      DO 20 J=1,LAST                                                         70
      DO 15 I=1,LAST                                                         80
```

```
      IF (ZVO(I)-ZVO(I+1)) 15,15,4                                        90
 4    TEMP = ZVO(I)                                                       100
      ZVO(I) = ZVO(I+1)                                                   110
      ZVO(I+1) = TEMP                                                     120
15    CONTINUE                                                            130
20    CONTINUE                                                            140
      RETURN                                                              150
      END                                                                 160

      SUBROUTINE DELTAZ (CI1,CI2,CI3,CI4,T,G,RHO,RHOM,CK4,GR,TGR,Z,DZ)     0
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             10
      COMMON /BLOK1/F(25),H(25),RAD(25),GATZ0(25),G0(25),Z0(25)           20
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,D0N2H4,D0NH3,R,CGM,RADIUS,NMAX1,    30
     X        NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4  40
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS  50
      COMMON /BVTBLS/AVSZ(234),APVSZ(234),DELVSZ(234)                     60
      COMMON /CCC/H4TBL(40),H3TBL(40)                                     70
      COMMON /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)             80
      DIMENSION  T(25),CI1(25),CI2(25),CI3(25),CI4(25),G(25),RHO(25),     90
     X           PHOM(25),DWDZ(25),DWDZ0(25),DTDZ(25),DTDZ0(25),GR(25),   100
     X           ,GR(25),CK4(25)                                          110
      DO 20 J=1,NRINGS                                                    120
      CALL UNBAR (AVSZ,1,Z,RAD(J),A,KK)                                   130
      CALL UNBAR (APVSZ,1,Z,RAD(J),AP,KK)                                 140
      CALL UNBAR (DELVSZ,1,Z,RAD(J),DELTA,KK)                             150
      CALL UNBAR (H4TBL,1,T(J),0.,H4,KK)                                  160
      CALL UNBAR (CFTBL4,1,T(J),0.,CF4,KK)                                170
      CALL UNBAR (CFTBL3,1,T(J),0.,CF3,KK)                                180
      CALL UNBAR (CFTBL2,1,T(J),0.,CF2,KK)                                190
      CALL UNBAR (CFTBL1,1,T(J),0.,CF1,KK)                                200
C     CHECK CURRENT Z WITH INJECTOR TIP FOR EACH RING
      IF (Z-Z0(J)) 11,12,12                                               210
 11   G(J) = G0(J)+F(J)*Z                                                 220
      GO TO 13                                                            230
 12   G(J) = GATZ0(J)                                                     240
      F(J) = 0.                                                           250
 13   CFBAR = (CF1*CI1(J)+CF2*CI2(J)+CF3*CI3(J)+CF4*CI4(J))/(CI1(J)+      260
     X          CI2(J)+CI3(J)+CI4(J))                                    270
      EPSLN = -A*G(J)/(5.*RHO(J)*DELTA)                                   280
      LAMDA = -A*CFBAR*G(J)/(5.*DELTA)                                    290
C     FIRST AND LAST RINGS ARE SPECIAL CASES
      IF (J-1) 1,2,1                                                      300
 1    IF (J-NRINGS) 3,4,3                                                 310
C     STANDARD MODE --- BOTH INWARD AND OUTWARD MIXING
 3    NR1 = EPSLN*(CI1(J)-CI1(J-1))/DR                                    320
      NR2 = EPSLN*(CI2(J)-CI2(J-1))/DR                                    330
      NR3 = EPSLN*(CI3(J)-CI3(J-1))/DR                                    340
      NR4 = EPSLN*(CI4(J)-CI4(J-1))/DR                                    350
      GR1 = LAMDA*(T(J)-T(J-1))/DR                                        360
      GRN = (NR1*CF1+NR2*CF2+NR3*CF3+NR4*CF4)*(T(J)-T(J-1))/DR            370
      NRR1 = EPSLN*(CI1(J+1)-CI1(J))/DR                                   380
      GRR1 = LAMDA*(T(J+1)-T(J))/DR                                       390
      GO TO 10                                                            400
C     FIRST RING --- OUTWARD MIXING ONLY
 2    NR1 = 0.                                                            410
```

```
      NR2 = 0.                                                          420
      NR3 = 0.                                                          430
      NR4 = 0.                                                          440
      QR1 = 0.                                                          450
      QRN = 0.                                                          460
      NRR1 = EPSLN*(CI1(J+1)-CI1(J))/DR                                 470
      QRR1 = LAMDA*(T(J+1)-T(J))/DR                                     480
      GO TO 10                                                          490
C   LAST RING --- INWARD MIXING ONLY
 4    NR1 = EPSLN*(CI1(J)-CI1(J-1))/DR                                  500
      NR2 = EPSLN*(CI2(J)-CI2(J-1))/DR                                  510
      NR3 = EPSLN*(CI3(J)-CI3(J-1))/DR                                  520
      NR4 = EPSLN*(CI4(J)-CI4(J-1))/DR                                  530
      QR1 = LAMDA*(T(J)-T(J-1))/DR                                      540
      QRN = (NR1*CF1+NR2*CF2+NR3*CF3+NR4*CF4)*(T(J)-T(J-1))/DR          550
      NRR1 = 0.                                                         560
      QRR1 = 0.                                                         570
 10   CALL SGRAD (CI1(J),CI2(J),CI3(J),CI4(J),G(J),T(J),GR(J),TGR(J),J) 580
      GRAD = GR(J)                                                      590
      TGRAD = TGR(J)                                                    600
      CK4(J) = KC4                                                      610
      W1 = CI1(J)/RHO(J)                                                620
      DWDZ(J) = (.5*MH2/MN2H4*(RHOM(J)*DELTA*AP*KC4*CI4(J))+1.5*AP*GRAD*  630
     X           MH2/MNH3+(NR1-NRR1)*DELTA/DR-NRR1*DELTA/RAD(J)-F(J)*W1)  640
     X           /G(J)                                                  650
      DHDZ = -(F(J)*(H(J)-HF)+AP*TGRAD+DELTA*(H4*RHOM(J)-(QR1-QRR1)/DR)+  660
     X       QRR1*DELTA/RAD(J)+QRN*DELTA)/G(J)                          670
      DTDZ(J) = ABS(DHDZ)/CFBAR                                         680
 20   CONTINUE                                                          690
C   FIND LARGEST OF DWDZ'S
      CALL ORDER (DWDZ,DWDZ0)                                           700
C   FIND LARGEST OF DTDZ'S
      CALL ORDER (DTDZ,DTDZ0)                                           710
C   CALCULATE NEW DZ
      DZ1 = .01/DWDZ0(NRINGS)                                           720
      DZ2 = 30./DTDZ0(NRINGS)                                           730
C   TAKE DELTAZ AS THE SMALLER OF DZ1 AND DZ2
      DZ = AMIN1(DZ1,DZ2)                                               740
      RETURN                                                            750
      END                                                               760
```

```
      SUBROUTINE SLOPE (RATE)                                            0
      REAL  K                                                           10
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,D0N2H4,D0NH3,R,C0M,RADIUS,NMAX1,   20
     X         NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4  30
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS  40
      COMMON /MMM/MI                                                     50
      DIMENSION K(1),     GMMA(1),BETA(1),DPA(1),CG(1),S(210),FST(210),  60
     1SLC(210),D(210),CPA(210),CPB(210),E(210),A(1),TERM1(210),          70
     2TERM2(210),C(210),XXX(210),XOA(210)                                80
      CG(1)=C4                                                           90
      GMMA(1)=GAMMA                                                     100
      PRES=P                                                            110
      EM12=1                                                            120
      DIFF=D0N2H4                                                       130
      IFLAG=0                                                           140
      JFLAG = 0                                                         150
```

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```
      ALLOW = .05                                                        160
      FRAC=.99                                                           170
   12 B=0.0                                                              180
  702 I=1                                                                190
      NOT=0                                                              200
      ADIV=100.                                                          210
      BDIV=100.                                                          220
      TOL=.01                                                            230
      STORE=1.0                                                          240
      KJ=0                                                               250
      HOLD=0.                                                            260
      NI=0                                                               270
   13 MI=0                                                               280
      IL=0                                                               290
      IK=0                                                               300
      MM=0                                                               310
      IM=0                                                               320
      F=0.5                                                              330
   20 MM=MM+1                                                            340
      ADR=B/ADIV                                                         350
      BDR=(A(I)-B)/BDIV                                                  360
      JINT=BDIV                                                          370
      INIT=ADIV                                                          380
      IF(MM.EQ.1) GO TO 15                                               390
      GO TO 16                                                           400
   15 MMAX=JINT+1                                                        410
      MAX=MMAX-1                                                         420
      MINT=0                                                             430
      GO TO 17                                                           440
   16 MMAX=INIT+JINT+1                                                   450
      MINT=INIT+1                                                        460
      MAX=MMAX-1                                                         470
   17 X=0.0                                                              480
      DO 40 IJ=1,MMAX                                                    490
      IF(IJ.GT.MINT) GO TO 49                                            500
      X=FLOAT(IJ-1)*ADR                                                  510
      GO TO 23                                                           520
   49 KMJ=IJ-MINT                                                        530
      X=B+FLOAT(KMJ)*BDR                                                 540
   23 CP=CG(I)*X/(A(I)-B)-(B/(A(I)-B))*CG(I)                             550
      IF(CP.LT.0.0) CP=0.0                                               560
C     THIS IS THE GENERAL EQUATION FOR A LINE WITH NEGATIVE Y-INTERCEPT
   24 FACT1=K(I)*(CG(I))**(1.-EN12)*(CP)**EN12                           570
      EFACT=GMMA(I)*BETA(I)*(1.-CP/CG(I))/(1.+BETA(I)*(1.-CP/CG(I)))     580
      IF(EFACT.GT.88.)EFACT=88.                                          590
      FACT2=EXP(EFACT)                                                   600
      IF(X) 37,40,37                                                     610
   37 RCP=FACT1*FACT2                                                    620
   35 S(IJ)=(1./X-1./A(I))*X**2*RCP                                      630
   40 CONTINUE                                                           640
   50 SUM=0.0                                                            650
      SUMA=0.0                                                           660
      DO 60 IL=2,MAX                                                     670
      IF(IL.GT.MINT) GO TO 61                                            680
      SUM=SUM+S(IL)                                                      690
      GO TO 60                                                           700
   61 SUMA=SUMA+S(IL)                                                    710
   60 CONTINUE                                                           720
      S(1)=0.                                                            730
      SGMA=(S(1)+2.*SUM)*(ADR/(2.*DPA(I)))+(S(MMAX)+2.*SUMA)*(BDR/(2.    740
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     10*DPA(I))}                                                        750
      D2=SGMA-FRAC*CG(I)                                                760
      TOT=D2+TOL*CG(I)                                                  770
      IF(MM-1) 110,110,112                                              780
112   IF(D2)1,1,2                                                       790
1     IF(TOT)2,230,230                                                  800
2     GO TO 115                                                         810
110   IF(IFLAG.EQ.1)GO TO 115                                           820
      IF(D2)150,115,115                                                 830
115   IF(MM-1) 20,120,140                                               840
120   XOLD=B                                                            850
      D1=D2                                                             860
C     CHANGE THE EQUATION OF T E LINE
      B=.999999  *A(I)                                                  870
      GO TO 20                                                          880
C     USE PRECEDING RESULTS TO ESTIMATE B FOR NEW LINE
140   TEMP=B                                                            890
      MI=MI+1                                                           900
      B=B+(D2/(D2-D1))*(XOLD-B)                                         910
1741  XOLD=TEMP                                                         920
      D1=D2                                                             930
143   IF(MI-20) 145,145,147                                             940
145   GO TO 20                                                          950
147   IF (JFLAG.EQ.1) GO TO 230                                         960
      B = .9*A(I)                                                       970
      JFLAG = 1                                                         980
      GO TO 702                                                         990
C     INITIAL CHOICE THRU ORIGIN IS SATISFACTORY
150   KO=1                                                             1000
      IFLAG=1                                                          1010
      X=0.                                                             1020
C     CALCULATE THE VALUE OF THE TWO INTEGRALS FOR ALL DR (101 POINTS)
      DO 170 II=1,MMAX                                                 1030
      X=FLOAT(II-1)*BDR                                                1040
      CP=CG(I)*X/(A(I)-B)-(B/(A(I)-B))*CG(I)                           1050
      TERM1(II)=K(I)*(CG(I))**(1.-EN12)*(CP)**EN12                     1060
      TERM2(II)=EXP(GMMA(I)*BETA(I)*(1.-CP/CG(I))/(1.+BETA(I)*(1.-CP/CG(  1070
     1I))))                                                            1080
      XXX(II)=X                                                        1090
      XOA(II)=XXX(II)/A(I)                                             1100
      RCP = TERM1(II)*TERM2(II)                                        1110
      FST(II)=X*X*RCP                                                  1120
      IF(X) 165,170,165                                                1130
165   SEC(II)=(1./X-1./A(I))*X*X*RCP                                   1140
170   CONTINUE                                                         1150
C     THE TRAPEZOIDAL RULE IS USED TO EVALUATE BOTH INTEGRALS
172   C(1)=0.                                                          1160
173   DO 175 JJ=2,MMAX                                                 1170
      IF(JJ.GT.MINT) GO TO 176                                         1180
      C(JJ)=C(JJ-1)+(FST(JJ)+FST(JJ-1))*(ADR/(2.*DPA(I)))              1190
      GO TO 175                                                        1200
176   C(JJ)=C(JJ-1)+(FST(JJ)+FST(JJ-1))*(BDR/(2.0*DPA(I)))            1210
175   CONTINUE                                                         1220
      SEC(1)=0.                                                        1230
      D(1) = 0.                                                        1240
      DO 180 KK=2,MMAX                                                 1250
      IF(KK.GT.MINT) GO TO 179                                         1260
      D(KK)=D(KK-1)+(SEC(KK-1)+SEC(KK))*(ADR/(2.*DPA(I)))              1270
      GO TO 180                                                        1280
179   D(KK)=D(KK-1)+(SEC(KK-1)+SEC(KK))*(BDR/(2.0*DPA(I)))             1290
```

```
  180  CONTINUE                                                          130(
C      THE VALUE OF CP AT X=0 IS  CG -D(101)
       E(1)=D(MMAX)                                                      131(
   186 CPA(1)=0.0                                                        132(
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)                                                    133(
       IF(KJ.EQ.1) GO TO 185                                             134(
       IF(IM.EQ.0) GO TO 185                                             135(
       IF(N1.EQ.1) GO TO 368                                             136(
  185  SAM=0.0                                                           137(
       DO 190 LL=2,MMAX                                                  138(
       IF(LL.GT.MINT) GO TO 188                                          139(
       E(LL)=E(LL-1)-(SEC(LL)+SEC(LL-1))*(DR/(2.*DPA(I)))                140(
       SAM=FLOAT(LL-1)*ADR                                               141(
       GO TO 189                                                         142(
  188  E(LL)=E(LL-1)-(SEC(LL)+SEC(LL-1))*(BDR/(2.0*DPA(I)))             143(
       SAM=SAM+BDR                                                       144(
   189 CPA(LL)=CG(I)-((1./SAM)-(1./A(I)))*C(LL)-E(LL)                    145(
       IF(LL.LT.MINT) CPA(LL)=0.0                                        146(
       IF(CPA(LL).LT.0.0) CPA(LL)=0.0                                    147(
  190  CONTINUE                                                          148(
       IF(KJ.EQ.1) GO TO 200                                             149(
       X=0.                                                              150(
       IF(IM.EQ.0) GO TO 250                                             151(
       IK=1                                                              152(
       GO TO 280                                                         153(
C      THE NEXT ITERATION USES THE VALUES OF CP JUST CALCULATED
  192  DO 200 LI=1,MMAX                                                  154(
       IF(LI.GT.MINT) GO TO 195                                          155(
       X=FLOAT(LI-1)*ADR                                                 156(
       GO TO 199                                                         157(
   195 KLK=LI-MINT                                                       158(
       X=B+FLOAT(KLK)*BDR                                                159(
  199  CONTINUE                                                          160(
       TERM1(LI)=K(I)*(CG(I))**(1.-EN12)*(CPA(LI))**EN12                 161(
       TERM2(LI)= EXP(GMMA(I)*BETA(I)*(1.-CPA(LI)/CG(I))/(1.+BETA(I)*(1.-  162(
     1CPA(LI)/CG(I))))                                                   163(
       XXX(LI)=X                                                         164(
       XOA(LI)=XXX(LI)/A(I)                                              165(
       RCP=TERM1(LI)*TERM2(LI)                                           166(
       FST(LI)=X*X*RCP                                                   167(
       IF(X) 200,200,193                                                 168(
   193 SEC(LI)=(1./X-1./A(I))*X*X*RCP                                    169(
   200 CONTINUE                                                          170(
       GO TO 172                                                         171(
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)                        172(
       IF(B.GT..998*A(I)) GO TO 322                                      173(
C      THE RANGE OF X FROM ZERO TO A IS USED
  237  X=0.                                                              174(
       NI=1                                                              175(
       DO 240 NN=1,MMAX                                                  176(
       IF(NN.GT.MINT) GO TO 246                                          177(
       X=FLOAT(NN-1)*ADR                                                 178(
       GO TO 354                                                         179(
   246 KJK=NN-MINT                                                       180(
       X=B+FLOAT(KJK)*BDR                                                181(
  354  IF(IM.GE.1) GO TO 353                                             182(
   238 CPB(NN) = CG(I)*X/(A(I)-B) - (B/(A(I)-B))*CG(I)                   183(
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      IF(CPB(NN).LT.0.0) CPB(NN)=0.0                                    1840
  353 TERM1(NN)=K(I)*(CG(I))**(1.-EN12)*(CPB(NN))**EN12                 1850
      TERM2(NN)= EXP(GMMA(I)*BETA(I)*(1.-CPB(NN)/CG(I))/(1.+BETA(I)*(1.- 1860
     1CPB(NN)/CG(I))))                                                  1870
      XXX(NN)=X                                                         1880
      XOA(NN)=XXX(NN)/A(I)                                              1890
      RCP = TERM1(NN)*TERM2(NN)                                         1900
      FST(NN)=X*X*RCP                                                   1910
      IF(X) 240,240,247                                                 1920
  247 SEC(NN) = (1./X-1./A(I))*X*X*RCP                                  1930
  240 CONTINUE                                                          1940
      GO TO 172                                                         1950
  368 DO 370 NL=1,MMAX                                                  1960
      CPB(NL)=CPA(NL)                                                   1970
  370 CONTINUE                                                          1980
      GO TO 185                                                         1990
  250 DO 260 IL=1,MMAX                                                  2000
  252 CPA(IL)=.5*CPA(IL)+.5*CPB(IL)                                     2010
  260 CONTINUE                                                          2020
      IK=0                                                              2030
C     THE VALUES OF X AT A AND NEAREST A ARE USED IN FINDING THE DERIVATIVE
  280 DERIF=(CG(I)-CPA(MAX))/BDR                                        2040
      IM=IM+1                                                           2050
      IF(IM.GT.99.AND.IFLAG.EQ.1)GO TO 701                              2060
      IF(IM.GT.99)GO TO 328                                             2070
  310 IF(KJ.EQ.1) IK=1                                                  2080
      IF(ABS(DERIF-HOLD)-ALLOW*DERIF)3,3,321                            2090
    3 IF(IK.EQ.1)GO TO 322                                              2100
  321 HOLD=DERIF                                                        2110
      IF(KJ.EQ.1) GO TO 192                                             2120
      IF(IK.EQ.1) GO TO 250                                             2130
      GO TO 192                                                         2140
  322 RATE=DERIF                                                        2150
  777 IF (B.GT..998*A(I)) GO TO 327                                     2160
  327 RETURN                                                            2170
  328 PERC=(ABS(DERIF-HOLD)/DERIF)*100.                                 2180
      ALL=100.*ALLOW                                                    2190
      GO TO 322                                                         2200
C     SIMPLIFIED VERSION DOES NOT ''CONVERGE'' IN 99 ITERATIONS
C     SET B=.000001*A     ,    AND START OVER
  701 B=.000001*A(I)                                                    2210
      WRITE (6,700)                                                     2220
  700 FORMAT (/ 84H INITIAL CHOICE THRU ORIGIN SEEMINGLY OK, BUT RESULTS 2230
     X ROTTEN AFTER 99 ITERATIONS .../48H SET X0=.000001*A AND USE MORE  2240
     XREFINED TECHNIQUE /)                                              2250
      ADR=B/ADIV                                                        2260
      BDR=(A(I)-B)/BDIV                                                 2270
      MMAX=INIT+JINT+1                                                  2280
      MINT=INIT+1                                                       2290
      MAX=MMAX-1                                                        2300
      IM=0                                                              2310
      KJ=0                                                              2320
      GO TO 237                                                         2330
      END                                                               2340


      SUBROUTINE SGRAD (CI1,CI2,CI3,CI4,G,T,GRAD,TGRAD,JRING)           0
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,X0A,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  X0BLOK(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                                                    510
      BETA = -CPS*H3*DP3/(KP*TPS)                                        520
      K0 = ALPH2*EXP(-GAMMA)/CI1**1.6                                    530
C   LINEAR EXTRAPOLATION USED TO GUESS AT X0
      X0P = X0                                                           540
      X0 = A-CPS/DCPDX                                                   550
      X0BLOK(L) = X0                                                     560
      X0A = X0/A                                                         570
      IF (X0) 11,12,12                                                   580
 11   X0 = 0.                                                            590
      X0A = 0.                                                           600
      CPS = CI3/(DP3/(A*KC3)+1.)                                         610
      DCPDX = CI3/A                                                      620
      TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC                               630
      IF (TPS.LT.0.) TPS=1.                                              640
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                                  650
      DP3 = DP3F(TPS,D03,P)                                              660
      DP3P = DP3                                                         670
      H3P = H3                                                           680
      TMTPN = T-TPS                                                      690
      GAMMA = BGM/TPS                                                    700
      BETA = -CPS*H3*DP3/(KP*TPS)                                        710
      K0 = ALPH2*EXP(-GAMMA)/CI1**1.6                                    720
      WRITE (6,132) LP1,TPS                                              730
 132  FORMAT (///37X,'WE HAVE CALCULATED A NEGATIVE X0 DURING ITERATION  740
     X0',I3,/39X,'SET X0 = 0. , CALCULATE TPS =',E11.6,' , AND CONTINUL  750
     X ')                                                               760
      GO TO 131                                                          770
C   INTEGRATE FOR CP EQUATION
 12   CALL TRAPP (X0A,1.,NPART,RIESUM,CI3)                               780
C   CALCULATE NEW CPS ...
      CPSP = CPS                                                         790
      CMCP0 = CMCPN                                                      800
      CPS = CI3-A*RIESUM/KC3                                             810
      IF (LTFLG-1) 80,84,80                                              820
 80   IF (CPS-(.25*CI3)) 81,81,87                                        830
 81   LTFLG = 1                                                          840
      GO TO 22                                                           850
 84   LTFLG = 0                                                          860
      IF (CPS) 89,87,87                                                  870
 89   CPS = 0.                                                           880
      GO TO 46                                                           890
 87   CMCPN = CI3-CPS                                                    900
C   CALCULATE NEW TP
 13   DCPDX = KC3/DP3*(CI3-CPS)                                          910
      GRAD = DCPDX*DP3                                                   920
      TGRAD = HC*(T-TPS)                                                 930
      TPSPP = TPSP                                                       940
      TPSP = TPS                                                         950
      TMTP0 = TMTPN                                                      960
 51   TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC                               970
      IF (TPS.LT.0.) TPS=1.                                              980
 2    CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                                  990
      DP3 = DP3F(TPS,D03,P)                                             1000
      TMTPN = T-TPS                                                     1010
      GAMMA = BGM/TPS                                                   1020
      BETA = -CPS*H3*DP3/(KP*TPS)                                       1030
      K0 = ALPH2*EXP(-GAMMA)/CI1**1.6                                   1040
C   TEST TEMP,CONCENTRATION FOR 5% LIMIT
      IF (ABS(TMTP0-TMTPN)/TMTPN - .05) 41,41,43                        1050
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 41   IF (ABS(CMCPO-CMCPN)/CMCPN - .05) 131,131,43                          106
C   TEST FOR TEMPERATURE LOOP ... COMPARE LAST 3 TEMPS
 43   IF (AMIN1(TPS,TPSP,TPSPP) - TPSP) 60,71,60                            107
 60   IF (AMAX1(TPS,TPSP,TPSPP) - TPSP) 46,71,46                            108
C   TEMPERATURE HAS FLUCTUATED ... TAKE AVERAGE AND RECALCULATE CPS
 71   TPSPP = TPSP                                                          109
      TPSP = TPS                                                            110
      TMTPO = TMTPN                                                         111
      TPS = (TPSP+TPSPP)/2.                                                 112
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                                     113
      DP3 = DP3F(TPS,D03,P)                                                 114
      DP3P = DP3                                                            115
      TMTPN = T-TPS                                                         116
      DCPDX = (HC*(T-TPS)-H4*KC4*CI4)/(H3*DP3)                              117
      CPSP = CPS                                                            118
      CMCPO = CMCPN                                                         119
      CPS = CI3-DP3/KC3*DCPDX                                               120
      IF (CPS.LT.0.) CPS=0.                                                 121
      CMCPN = CI3-CPS                                                       122
      LP1 = LP1+1                                                           123
      L = L+1                                                               124
      IF (LP1-25) 61,61,44                                                  125
C   NO CONVERGENCE YET ... AVERAGE THE CPS'S FOR LAST TWO CALC'S AND REPEAT
 2    CPS = .2*CPS+.8*CPSP                                                  126
      GO TO 53                                                              127
C   CALCULATE WEIGHTED AVERAGE OF PRESENT AND PREVIOUS X0
 22   X00 = WAF1*X0P+WAF2*X0                                                128
      CPS = CI3/(1.+DP3/(KC3*A-KC3*X00))                                    129
 53   DCPDX = KC3/DP3P*(CI3-CPS)                                            130
      CMCPN = CI3-CPS                                                       131
      H3 = H3P                                                              132
 42   LP1 = LP1+1                                                           133
      L = L+1                                                               134
      IF (LP1-25) 40,40,44                                                  135
 44   WAF1 = WAF1+.05                                                       136
      IF (WAF1.GT..95) GO TO 99                                             137
      WAF2 = 1.-WAF1                                                        138
C   NO CONVERGENCE WITH PRESENT WEIGHTED AVERAGE FACTORS FOR X0 ---
C   REPEAT ITERATION PROCEDURE WITH NEW
      GO TO 1                                                               139
 99   LM1 = L-1                                                             140
      WRITE (6,98)                                                          141
 98   FORMAT (///20X,'UNABLE TO FIND SUITAB          ER FOUR TRIES OF 25    142
     XITERATIONS EACH --- PROGRAM STOP FOLLO                                143
      WRITE (6,96) (X0BLOK(I),I=1,LM1)                                      144
 96   FORMAT (//52X,'X0 VALUES CALCULATED IN SGRAD' / (10E13.5))            145
      CALL DUMP                                                             146
C
C   SATISFACTORY X0 HAS BEEN FOUND
C   CALCULATE GRADIENT
C
 131  LP2 = 1                                                               147
      NX = P4                                                               148
      NX1 = NX+1                                                            149
      NXM1 = NX-1                                                           150
 291  XOA = X0/A                                                            151
      VNU = -KC3/DP3                                                        152
      INT1 = 1                                                              153
      L = 2                                                                 154
      R1 = 0.                                                               155
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      R2 = 0.                                                          1560
      PS1 = 0.                                                         1570
      PS2 = 0.                                                         1580
      DELXOA = (1.-XOA)/FLOAT(NX)                                      1590
C     CALCULATE PROFILE CURVES FOR INTEGRAND FUNCTIONS
      XA = XOA                                                         1600
      DO 770 I=1,NX1                                                   1610
C     CP(X/A) IS A LINEAR PROFILE DURING FIRST APPROXIMATION
      IF (LP2.GT.1) GO TO 664                                          1620
      CPX(I) = (XA-XOA)/(1.-XOA)*CPS                                   1630
664   RHET(I) = K0*CI3**(1-N)*CPX(I)**N*EXP(GAMMA*BETA*(1.-CPX(I)/CI3))/ 1640
     X          (1.+BETA*(1.-CPX(I)/CI3)))                            1650
      DX(I) = XA                                                       1660
      XA = XA+DELXOA                                                   1670
770   CONTINUE                                                         1680
C     TAKE INTERVAL FUNCT'N MIDPTS AS CONSTANT VALUE FOR CP(X/A) AND RHET
      DO 771 I=1,NX                                                    1690
      CPX(I) = (CPX(I)+CPX(I+1))/2.                                    1700
      RHET(I) = (RHET(I)+RHET(I+1))/2.                                 1710
771   CONTINUE                                                         1720
      XA = XOA+DELXOA                                                  1730
      CTRM = (A*VNU+1.)/(A*VNU)                                        1740
C     INTEGRAL EQUATION FOLLOWS
C     CPOX(1) IS SPECIAL CASE ... X=X0
      DXL = XOA                                                        1750
      DXU = DXL+DELXOA                                                 1760
      RR1 = 0.                                                         1770
      DO 377 I=1,NX                                                    1780
      RR1 = RR1+RHET(I)*(EVAL2(DXL,DXU)-CTRM*EVAL1(DXL,DXU))           1790
      DXL = DXU                                                        1800
      DXU = DXU+DELXOA                                                 1810
377   CONTINUE                                                         1820
      CPOX(1) = CI3-A*A/DP3*RR1                                        1830
      IF (CPOX(1).LT.0.) CPOX(1)=0.                                    1840
C     SOLVE GENERAL EQUATION OF TWO INTEGRALS FOR CP(X/A)
769   DO 772 I=1,INT1                                                  1850
      R1 = R1+RHET(I)*EVAL1(XOA,XA)                                    1860
      XOA = XA                                                         1870
      XA = XA+DELXOA                                                   1880
772   CONTINUE                                                         1890
      R1 = R1*(1./XOA-CTRM)                                            1900
      XAD = XA                                                         1910
      XA = XA-DELXOA                                                   1920
      DO 773 I=INT1,NXM1                                               1930
      PS1 = PS1+RHET(I+1)*EVAL2(XA,XAD)                                1940
      PS2 = PS2+RHET(I+1)*EVAL1(XA,XAD)                                1950
      XA = XAD                                                         1960
      XAD = XAD+DELXOA                                                 1970
773   CONTINUE                                                         1980
      R2 = PS1-CTRM*PS2                                                1990
      INT1 = INT1+1                                                    2000
      CPOX(L) = CI3-A*A/DP3*(R1+R2)                                    2010
      IF (CPOX(L).LT.0.) CPOX(L)=0.                                    2020
      XOA = X0/A                                                       2030
      XA = XOA+DELXOA                                                  2040
      L = L+1                                                          2050
      R1 = 0.                                                          2060
      R2 = 0.                                                          2070
      PS1 = 0.                                                         2080
      PS2 = 0.                                                         2090
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      IF (L.LE.NX) GO TO 769                                              2100
C   CPOX(NX1) IS SPECIAL CASE ... X=A
      DXL = X0A                                                           2110
      DXU = DXL+DELX0A                                                    2120
      RR2 = 0.                                                            2130
      DO 378 I=1,NX                                                       2140
      RR2 = RR2+RHET(I)*EVAL1(DXL,DXU)                                    2150
      DXL = DXU                                                           2160
      DXU = DXU+DELX0A                                                    2170
  378 CONTINUE                                                            2180
      CPOX(NX1) = CI3-A*A/DP3*(1.-CTRM)*RR2                               2190
      IF (CPOX(NX1).LT.0.) CPOX(NX1)=0.                                   2200
C   CALCULATE A NEW TPS
      DCPDX = KC3/DP3*(CI3-CPOX(NX1))                                     2210
      H3P = H3                                                            2220
      DP3P = DP3                                                          2230
      TPS = T-(H4*KC4*CI4+H3*DP3*DCPDX)/HC                                2240
      IF (TPS.LT.0.) TPS=1.                                               2250
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                                   2260
      DP3 = DP3F(TPS,D03,P)                                               2270
      TMTPO = TMTPN                                                       2280
      TMTPN = T-TPS                                                       2290
C   TWO PASSES NEEDED BEFORE CHECK ON TEMP,CONC CAN BE MADE
   33 IF (LP2.EQ.1) GO TO 27                                              2300
      CMCPO = CMCPN                                                       2310
      CMCPN = CI3-CPOX(NX1)                                               2320
      IF (ABS(TMTPO-TMTPN)/TMTPN - .05) 26,26,27                          2330
   26 IF (ABS(CMCPO-CMCPN)/CMCPN - .05) 49,49,27                          2340
C   CALCULATE NEW CPX(I) PROFILE FOR NEXT PASS
   27 DO 55 I=1,NX1                                                       2350
      IF (MOD(LP2,5)) 34,57,34                                            2360
C  CALCULATE WEIGHTED AVERAGE OF OLD AVERAGED AND CALCULATED PROFILES
   34 CPX(I) = .8*CPX(I)+.2*CPOX(I)                                       2370
      GO TO 56                                                            2380
C  AVERAGE PRESENT AND PAST CALCULATED PROFILES EVERY 5TH PASS TO SMOOTH
   57 CPX(I) = (CPOX(I)+PCPOX(I))/2.                                      2390
C  STORE PRESENT CALCULATED PROFILE
   56 PCPOX(I) = CPOX(I)                                                  2400
   55 CONTINUE                                                            2410
      CMCPN = CI3-CPX(NX1)                                                2420
      DCPDX = KC3/DP3P*(CI3-CPX(NX1))                                     2430
      TPS = T-(H4*KC4*CI4+H3P*DP3P*DCPDX)/HC                              2440
      IF (TPS.LT.0.) TPS=1.                                               2450
      CALL UNBAR (H3TBL,1,TPS,0.,H3,KK)                                   2460
      DP3 = DP3F(TPS,D03,P)                                               2470
      TMTPO = TMTPN                                                       2480
      TMTPN = T-TPS                                                       2490
      LP2 = LP2+1                                                         2500
      IF (LP2-50) 29,29,30                                                2510
   30 WRITE (6,18) CPOX(NX1)                                              2520
   18 FORMAT (///31X,52HUNABLE TO CONVERGE ON CPS IN  50 TRIES ... CP(X/  2530
     XA) =,E12.5)                                                         2540
      WRITE (6,522) GRAD,TGRAD                                            2550
  522 FORMAT (51X,'KC3*(CI3-CPS) =',E12.5 / 54X,'HC*(T-TPS) =',E12.5)     2560
      GO TO 28                                                            2570
   29 GAMMA = BGM/TPS                                                     2580
      BETA = -CPX(NX1)*H3*DP3/(KP*TPS)                                    2590
      K0 = ALPH2*EXP(-GAMMA)/CI1**1.6                                     2600
      GO TO 291                                                           2610
   49 GRAD = DCPDX*DP3                                                    2620
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      TGRAD = HC*(T-TPS)                                                2630
 28   RETURN                                                            2640
      END                                                               2650

      SUBROUTINE TRAPP (U,W,NPART,RIESUM,CI3)                            0
C     NUMERICAL INTEGRATION USING TRAPEZOIDAL METHOD
      REAL   K0,KC3                                                     10
      COMMON /AAAA/DP3,X0,X0A,CPS                                       20
      COMMON /BLOK2/A,AP,DELTA,DR,DPA,D0N2H4,D0NH3,R,CGM,RADIUS,NMAX1,  30
     X        NMAX2,ALPHA1,ALPHA2,BETA,AGM,BGM,P,ZEND,MH2,MN2,MNH3,MN2H4 40
      COMMON /BLOK3/K,K0,KP,KC3,KC4,HF,HL,HV,TF,CF,CFBAR,GAMMA,C4,NRINGS 50
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.-  60
     X                    B/A)))                                        70
C     FUNCTIONS DEFINING INTEGRANDS
      FOXI1(X,R)=X**2*R                                                 80
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                                       90
      N=NPART-1                                                        100
      PART=NPART                                                       110
      D=(W-U)/PART                                                     120
      UPH=U+D                                                          130
      SUM=0.                                                           140
      CPX1=CPXF(U,X0A,CPS)                                             150
      CPX2=CPXF(W,X0A,CPS)                                             160
      RHET1=RHETF(CI3,CPX1,GAMMA,BETA,K0,1)                            170
      RHET2=RHETF(CI3,CPX2,GAMMA,BETA,K0,1)                            180
C     CALCULATE FIRST,LAST TERMS OF RIEMANN SUM FIRST
 4    TRM1=FOXI1(U,RHET1)/2.                                           190
      TRM2=FOXI1(W,RHET2)/2.                                           200
 6    DO 8 I=1,N                                                       210
      CPX=CPXF(UPH,X0A,CPS)                                            220
      RHET = RHETF(CI3,CPX,GAMMA,BETA,K0,1)                            230
      SUM=SUM+FOXI1(UPH,RHET)                                          240
      UPH=UPH+D                                                        250
 8    CONTINUE                                                         260
 9    RIESUM=D*(TRM1+SUM+TRM2)                                         270
 99   RETURN                                                           280
      END                                                              290

       SUBROUTINE  UNBAR(T,IK,XIN,YIN,ZZ,KK)                             0
      DIMENSION T(1),X(6),Y(6),A(6)                                     10
C                                                                  UNBAR003
C  ------------------  MARCH 4, 1961 ------------                  UNBAR004
C  ------------------  MODIFIED 7/62  -----------------            UNBAR005
C  ------------------  TO DO QUADRATIC AND LINEAR INTERPOLATION ALSO UNBAR006
C                                                                  UNBAR007
      II = IK+1                                                         20
      N = 3                                                             30
      N2= 2                                                             40
           IF (T(II)-3.) 700,701,702                                    50
 700       IF (T(II)+0.) 60,701,704                                     60
 704       IF (T(II)-2.) 705,706,701                                    70
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 705  N = 1                                                              80
           GO TO 707                                                     90
 706  N = 2                                                             100
 707  N2= 1                                                             110
 701  II = II+1                                                         120
 702  N1 = N +1                                                         130
           DO 50 L = II,II                                              140
           IF ( T(L) + 0. ) 60,60,51                                    150
 60     KK = -1                                                        160
        ZZ = 0.                                                         170
           GO TO 9999                                                   180
 51    NX = T(L)                                                       190
           IF (T(L+1) + 0. ) 60,52,50                                   200
 52    NY = 0                                                          210
           GO TO 53                                                     220
 50    NY = T(L+1)                                                     230
 53        CONTINUE                                                    240
       KK  = 0                                                         250
       KY  = 0                                                         260
       XX  = X1N                                                       270
       YY  = Y1N                                                       280
       J1  = II+2                                                      290
       J2  = NX+II+1                                                   300
       IF(XX-T(J1))301,306,400                                         310
 400       DO 302 J=J1,J2                                            320
           IF (XX-T(J)) 304,304,302                                     330
 302   CONTINUE                                                        340
 309   KK  = 2                                                         350
       XX  = T(J2)                                                     360
 308   JX1 = J2-N                                                      370
           GO TO 305                                                    380
 301   KK  = 1                                                         390
       XX  = T(J1)                                                     400
 306   JX1 = J1                                                        410
           GO TO 305                                                    420
 304       IF (J-J1-1) 301,306,307                                     430
 307       IF (J-J2)   303,308,309                                     440
 303   JX1 = J-N2                                                      450
 305   CONTINUE                                                        460
       XINT  = XX                                                      470
       IF (NY) 1500, 1500, 3000                                        480
 1500      DO 1599 L=1,N1                                            490
           X(L) = T(JX1)                                               500
            LY = JX1 + NX                                              510
           Y(L) = T(LY)                                                520
 1599    JX1 = JX1+1                                                   530
       I = 1                                                           540
       GO TO 54                                                        550
 3000  J1  = J1+NX                                                     560
       J2  = J2+NY                                                     570
       IF(YY-T(J1))311,316,401                                         580
 401       DO 312 J=J1,J2                                            590
           IF (YY-T(J)) 314,314,312                                    600
 312   CONTINUE                                                        610
 319   KY  = 6                                                         620
       YY  = T(J2)                                                     630
 318   JY1 = J2-N                                                      640
           GO TO 315                                                    650
 311   KY  = 3                                                         660
       YY  = T(J1)                                                     670
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```
316  JY1 = J1                                                          680
          GO TO 315                                                    690
314       IF (J-J1-1) 311,316,317                                      700
317       IF (J-J2)   313,318,319                                      710
313  JY1 = J-N2                                                        720
315  CONTINUE                                                          730
     JX2  = JX1                                                        740
     LY   = JY1 + NY*(JX2-II-1)                                        750
     LY1 = LY                                                          760
          DO 3099 L=1,N1                                               770
     X(L) = T(JX2)                                                     780
     Y(L) = T(LY1)                                                     790
     LY1  = LY1+NY                                                     800
3099 JX2  = JX2+1                                                      810
     I    = 0                                                          820
          GO TO 54                                                     830
3098 Y(1)  = ZZ                                                        840
          DO 4400 I=1,N                                                850
     LY1 = LY+I                                                        860
     Y(I+1) = 0.                                                       870
          DO 4050 MM=1,N1                                              880
     Y(I+1) = Y(I+1) + T(LY1)*X(MM)                                    890
4050 LY1 = LY1+NY                                                      900
4400  CONTINUE                                                         910
          DO 4199 L=1,N1                                               920
     X(L) = T(JY1)                                                     930
4199 JY1  = JY1+1                                                      940
     XINT = YY                                                         950
     I=  1                                                             960
54   D   = 1.                                                          970
     X(N+2) = X(1)                                                     980
     X(N+3) = X(2)                                                     990
          DO 55 J=1,N1                                                1000
     A(J+1) = X(J+1) - X(J)                                           1010
     TPAL1  = XINT - X(J)                                             1020
      IF ( TPAL1 ) 57,58,57                                           1030
 58    ZZ = Y (J)                                                     1040
      X(1) = 0.                                                       1050
      X(2) = 0.                                                       1060
      X(3) = 0.                                                       1070
      X(4) = 0.                                                       1080
      X(J) = 1.0                                                      1090
      GO TO 59                                                        1100
 57  D = D * TPAL1                                                    1110
          GO TO (711,712,713) ,N                                      1120
711  X(J)  = TPAL1/A(J+1)                                            1130
          GO TO 55                                                    1140
712  X(J)  = -TPAL1                                                  1150
          GO TO 55                                                    1160
713  X(J)  = (X(J+2)-X(J))*TPAL1                                     1170
55       CONTINUE                                                    1180
     A(1) = A(N+2)                                                    1190
     ZZ = 0.                                                          1200
         DO 56 J=1,N1                                                1210
       X(J) = D/(A(J)*A(J+1)*  X(J))                                 1220
     ZZ = ZZ + Y(J)*  X(J)                                           1230
56       CONTINUE                                                    1240
 59        IF (I) 3098,3098,9999                                      1250
9999 KK  = KK+KY                                                     1260
         RETURN                                                      1270
```

```
      END                                                                1280
```

```
      BLOCK DATA                                                            0
C     BLOCK DATA FOR VISCOSITY VS TEMPERATURE
      COMMON /AAA/VISVST(30),TBLVP(68)                                     10
      DATA  (VISVST(I),I=1,30) /  0., 1., 13., 0.,                         20
C     TEMPERATURES
     X  360.  ,  540.  ,  720.  ,  900.  , 1080.  , 1260.  , 1440.  ,      30
     X 1620.  , 1800.  , 1980.  , 2160.  , 2340.  , 2520.  ,               40
C     VISCOSITIES
     X.048 E-4,.070 E-4,.093 E-4,.117 E-4,.141 E-4,.164 E-4,.186 E-4,      50
     X.207 E-4,.228 E-4,.247 E-4,.266 E-4,.285 E-4,.302 E-4 /              60
C     BLOCK DATA FOR VAPOR PRESSURE AS FUNCTION OF TEMPERATURE
      DATA  (TBLVP(I),I=1,68) /  0. ,  1. ,  32. ,  0. ,                   70
C     TEMPERATURES
     X  492. ,  519. ,  528.4,  529.1,  534.6,  534.7,  538.8,  543.9,     80
     X  545.7,  560.2,  570.0,  579.3,  579.5,  595.3,  610.1,  614.1,     90
     X  618.1,  627.5,  628.8,  645.7,  650.8,  665.6,  675.0,  692.4,    100
     X  697.5,  744.0,  798.0,  852.0,  942.0, 1032.0, 1122.0, 1176.0,    110
C     VAPOR PRESSURES
     X .052  , .148  , .201  , .207  , .240  , .282  , .292  , .354  ,     120
     X .545  , .737  , .973  , .982  , 1.51  , 2.20  , 2.46  , 2.74  ,     130
     X 3.41  , 3.56  , 5.24  , 5.97  , 8.07  , 9.71  , 11.91 , 13.46 ,     140
     X 14.70 , 33.80 , 73.48 , 147.  , 382.  , 823.  , 1528. , 2131.  /    150
      END                                                                  160
```

```
      BLOCK DATA                                                            0
C     BLOCK DATA FOR SPECIFIC HEAT VS TEMPERATURE
      COMMON /DDD/CFTBL4(34),CFTBL3(34),CFTBL2(34),CFTBL1(34)              10
      DATA  (CFTBL1(I),I=1,34) /  0., 1., 15., 0.,                         20
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,     30
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,            40
C     SPECIFIC HEATS
     X 3.4194, 3.4596, 3.4685, 3.4765, 3.4899, 3.5151, 3.5454, 3.5006,     50
     X 3.6208, 3.6654, 3.7150, 3.7696, 3.8291, 3.8802, 3.9288 /            60
      DATA  (CFTBL2(I),I=1,34) /  0., 1., 15., 0.,                         70
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,     80
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,            90
C     SPECIFIC HEATS
     X .2485 , .2495 , .2524 , .2569 , .2624 , .2682 , .2738 , .2790 ,    100
     X .2836 , .2878 , .2914 , .2946 , .2974 , .2998 , .3019  /           110
      DATA  (CFTBL3(I),I=1,34) /  0., 1., 15., 0.,                         120
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,    130
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,            140
C     SPECIFIC HEATS
     X .5005 , .5424 , .5891 , .6344 , .6773 , .7176 , .7553 , .7905 ,    150
     X .8236 , .8541 , .8823 , .9075 , .9304 , .9512 , .9697  /           160
      DATA  (CFTBL4(I),I=1,34) /  0., 1., 15., 0.,                         170
C     TEMPERATURES
     X  540. ,  720. ,  900. , 1080. , 1260. , 1440. , 1620. , 1800. ,    180
     X 1980. , 2160. , 2340. , 2520. , 2700. , 2880. , 3060. ,            190
```

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      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 , 1280.82 , 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
```