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MATHEMATICAL MODELS FOR THE TRANSIENT BEHAVIOR OF A PACKED BED REACTOR

BY

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A THESIS

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled MATHEMATICAL MODELS FOR THE TRANSIENT BEHAVIOR OF A PACKED BED REACTOR, submitted by John E. Feick, B.Sc., in partial fulfilment of the requirements for the degree of Doctor of Philosophy.

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ABSTRACT

Three mathematical models of varying degree of complexity have been used to describe the transient behavior of a packed bed tubular reactor. The method followed in the solution of these models is essentially the same. The partial differential equations describing heat and mass transfer in the reactor and within the catalyst particles are finite differenced in the spatial variables and the resulting sets of nonlinear ordinary differential equations are solved by an alternating direction explicit procedure. Using this method it has been shown that the time integration of the transient equations is reduced to the sequential solution of a series of nonlinear algebraic equations; each equation containing only one unknown variable. For this purpose the simple Newton-Raphson iterative procedure was found to be adequate.

The overall stability of the numerical method was not proven theoretically because of the nonlinear nature of the problem. The approach taken was to satisfy the criteria for stability in the corresponding linear problem and to compute the nonlinear term at the most advanced time step of the transient integration. This latter procedure necessitates the use of an iterative procedure to solve each algebraic equation but in

many cases it was a necessary condition for stability. The primary advantages of this method are its computational efficiency and general application to the equations describing heat and mass transfer both within a single catalyst particle and within the reactor, regardless of the form of rate expression. Also, due to the nature of the finite difference scheme and the alternating direction explicit procedure, the corresponding linear problem does not require any restriction on the size of the space or time increments. The effect of nonlinear terms may limit the size of the time increment, however this problem was not encountered.

The most complex model developed, accounts for radial and axial diffusion within the reactor and the possible resistance to heat and mass transfer between the external fluid and the catalyst as well as within the catalyst pellets themselves. In the examples discussed in this work, a comparison of this complex model with simpler models of a chemical reactor, indicate the importance of including these phenomena.

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I INTRODUCTION AND LITERATURE SURVEY

The last decade has seen remarkable advances in the mathematical representation of chemical processes and chemical process equipment. This perhaps has been spurred by the simultaneous development and availability of large scale digital computers and the development of efficient numerical methods in the field of matrix iterative analysis. The simulation of packed bed tubular reactors and individual catalyst particles, in particular, has received widespread attention.

The behavior of packed bed reactors has generally been characterized by a pair of second order partial differential equations describing heat and mass transfer in the external field of the reactor. Here, the external field is taken to mean the fluid, gas or liquid, which is flowing around the catalyst particles. Without the appropriate physical constants; these equations are of the general form:

$$\frac{\partial^2 C}{\partial X^2} + \left[\frac{\partial^2 C}{\partial R^2} + \frac{1}{R}\frac{\partial C}{\partial R}\right] - \frac{\partial C}{\partial X} = \frac{\partial C}{\partial t} + r' \qquad \text{(I-1)}$$

$$\frac{\partial^2 T}{\partial X^2} + \left[\frac{\partial^2 T}{\partial R^2} + \frac{1}{R}\frac{\partial T}{\partial R}\right] - \frac{\partial T}{\partial X} = \frac{\partial T}{\partial t} + r'' \qquad \text{(I-2)}$$

Here r' represents the disappearance of reactant due to chemical reaction or diffusion towards a catalyst where reaction occurs, and r" represents the disappearance or appearance of heat due to chemical reaction or diffusion from a reacting catalyst. Being second order, these equations require two boundary conditions. A study of the physical situation indicates that one of these is at the reactor entrance and the other is at the exit, making this a boundary value problem. If the resistance to heat and mass transfer between the external field and the catalyst and also within the catalyst particles themselves, is taken into account, then additional equations describing this phenomena are required.

The general approach to date has been to make several simplifying assumptions; finite difference the resulting equations; and then solve this finite differenced form by an appropriate numerical method. These types of computations have required the use of a digital computor. The boundary value nature of the problem and the non-linear coupling of the independent variables through the reaction rate term have provided the main obstacles to a solution of the entire problem. These features have required that the problem be modified so that the resulting form will be amenable to a numerical solution

by existing techniques. The progress in this field may be illustrated by a review of several recent publications.

C. Barkelew, (1), in 1959 assumed that the radial and axial diffusion of heat and mass in the external field was negligible compared with transport by flow. It was also assumed that there was no resistance to heat and mass transfer between the external field and the catalyst, and within the catalyst itself. The modified forms of equations (I-1) and (I-2) were then reduced to steady state form and numerically integrated. This investigation yielded several qualitative observations regarding the stability of tubular reactors.

A series of papers, (2), (3), (4), by Shean-lin Liu and Neal R. Amundson in 1962-63 deal with a more quantitative stability analysis. Their first paper, (2) deals with the adiabatic operation of a packed bed tubular reactor. It assumes no radial or axial diffusion of heat and mass within the reactor and neglects internal mass and temperature gradients within the catalyst particles. The resulting equations are solved by the method of characteristics, (5). Their second paper, (3), adds the effect of non-adiabatic behavior to their previous analysis. The third publication, (4), includes the effect of axial mixing on the transport of heat and mass within the reactor. The resulting transient equations

are finite differenced using an implicit procedure over the time interval. The finite differenced form is then solved at each time step using a method peculiar to tri-diagonal matrices due to Thomas, (6). Each stage of the time integration requires trial and error calculations. This same model of a packed bed reactor, with the omission of heat and mass transfer between the external field and the catalyst, was presented by E.S. Lee, (7), in 1966. He used a quasi-linearization technique, (8), to solve the nonlinear finite difference equations.

Carberry and Wendel, (9), in 1963 formulated and solved a steady-state model which assumed that heat and mass were diffused in the axial direction only. The resistance to heat and mass transfer between the external field and the catalyst was taken into account. The catalyst particles were assumed to be isothermal, thus enabling an effectiveness factor for the catalyst in each finite differenced reactor element to be calculated in terms of a Thiele modulus, (10). This Thiele modulus is a function of the rate constant, the particle diameter, and the diffusion coefficient within the catalyst. The finite differenced sets of equations were solved by a straight iterative procedure using the Thomas method for tri-diagonal

matrices. This represents the first attempt to account for the intraparticle diffusion of reactant within the general framework of a complete reactor model.

In 1968, Shean-lin Liu, (11), formulated a steady state model which accounted for heat and mass transfer by diffusion in the radial direction but not in the axial direction. A resistance to heat and mass transfer between the external field and the catalyst particles was not taken into account. The effectiveness factor for the catalyst particles was calculated as a function of the diffusion parameters, the rate constant, and the particle diameter, (12). The finite differenced set of equations was solved by an implicit iterative scheme based on Saul'yev's method, (13).

The most sophisticated model to date has been presented by McGuire and Lapidus, (14), in 1965. A complete transient model was formulated which included axial and radial diffusion in the external field, a resistance to heat and mass transfer between the external fluid and the catalyst particles, and intraparticle diffusion of heat and mass. The external field was formulated as an initial value problem by dividing the reactor bed into radial and axial increments and considering these finite cells as a series of well-stirred reactors as presented in an earlier paper by Deans and Lapidus, (15). The differential equations describing

heat and mass transfer within the catalyst particles are finite differenced and solved at each time step using the Thomas method. The initial value nature of the external field allows the sequential solution of the equations for each reactor cell at each time step.

Several papers since 1960, (16), (17), (18), (19), have dealt extensively with the effect of intra-particle concentration and temperature gradients upon the effectiveness factor for catalyst pellets. Here, the effectiveness factor is defined as the ratio of the overall rate of reaction occurring within the catalyst pellet, to that rate of reaction which would occur if the interior of the catalyst were exposed to the surface conditions. Many of the numerical methods presented are particular to the choice of a rate expression for chemical reaction.

The main contribution of the work presented here is a more correct representation of the external field as a boundary value problem, considering both heat and mass diffusion in the radial and axial directions. The resistance to heat and mass transfer both within the catalyst particles and between the particles and the fluid is also considered. The numerical techniques used in the solution of the nonlinear finite differenced equations are both efficient and entirely independent of the chemical rate expression. The alternating direction

explicit procedure used in the transient integration is considered to have superior stability characteristics in the numerical solution.

II MATHEMATICAL MODELS OF PACKED BED REACTORS

The transport of heat and mass within a packed bed reactor can be adequately described by a set of simultaneous nonlinear partial differential equations. These equations are the result of differential heat and material balances about the component parts of the reactor; namely the external field, the catalyst particles, and the boundaries. The physical situation being considered is a radially symmetric tubular reactor packed with spherical catalyst particles. It will be assumed that there is no volume change with chemical reaction. This will encompass equimolar reactions and cases with small reactant concentrations. Without this assumption, momentum balances would have to be written both for the external field and the catalyst particles. It will also be assumed that the diffusion parameters, the heat capacity and density of the fluid, and the heat of reaction are constant. The numerical method used to solve the differential equations can accommodate those cases where any of these parameters can be specified as a function of position in the reactor or within the catalyst particle. However because of the nonlinearities introduced it cannot handle those cases where they are a function of the dependent variables such as temperature and concentration. The bulk velocity profile and the bed porosity are also assumed to be

constant. It is realized that studies on turbulent flow in packed bed reactors have indicated that the velocity is somewhat higher along the reactor wall than in the centre because of a looser packing. If this velocity profile is known as a function of reactor radius, then the above restriction may be relaxed. Chemical reaction will be considered to occur only within the porous structure of the catalyst. Furthermore, the chemical reaction will be assumed to be of the form: A → products. This restriction is for convenience only and is not necessary for the general case. If there is a multiple reaction occurring then a mass balance must be written for each reacting species, and the heat balance must account for the total heat of reaction.

The following phenomena may have significant effects upon the transient and steady-state behavior of the reactor.

i) Radial and axial diffusion of heat and mass
ii) A resistance to heat and mass transfer between the external field and the catalyst particles.
iii) A resistance to heat and mass transfer within the porous structure of the catalyst particles.
iv) A resistance to heat transfer across the reactor wall.

v) The heat capacities of the external field and the catalyst particles.

A. HOMOGENEOUS MODEL:

The first and simplest model to be considered is one which assumes that there is no resistance to heat and mass transfer between the external field and the catalyst and there are no significant temperature and concentration gradients within the catalyst. Using these assumptions, the following pair of partial differential equations can be used to describe the reactor.

$$\varepsilon_R D_a \frac{\partial^2 C}{\partial X^2} + \varepsilon_R D_r \left[\frac{\partial^2 C}{\partial R^2} + \frac{1}{R}\frac{\partial C}{\partial R}\right] - \varepsilon_R u \frac{\partial C}{\partial X} = (1-\varepsilon_R) f(C,T) + (\varepsilon_R + (1-\varepsilon_R)\varepsilon_P) \frac{\partial C}{\partial t} \qquad \text{(II-1a)}$$

$$\varepsilon_R K_a \frac{\partial^2 T}{\partial X^2} + \varepsilon_R K_r \left[\frac{\partial^2 T}{\partial R^2} + \frac{1}{R}\frac{\partial T}{\partial R}\right] - \varepsilon_R \rho_f Z_f u \frac{\partial T}{\partial X} = (1-\varepsilon_R)\ \Delta H\ f(C,T) + (\varepsilon_R \rho_f Z_f + (1-\varepsilon_R)\ \rho_P Z_P) \frac{\partial T}{\partial t} \qquad \text{(II-2a)}$$

The boundary conditions may be formulated as follows:

$$\frac{\partial^2 C}{\partial X^2} = \frac{\partial^2 T}{\partial X^2} = 0;\ X = 0,\ X = L \qquad \text{(II-3)}$$

$$\frac{\partial C}{\partial R} = \frac{\partial T}{\partial R} = 0;\quad R = 0 \qquad \text{(II-4)}$$

Heat loss at reactor wall = $h_w A_o (T-T_w)$ (II-5)

The system will be completely defined with the specification of any initial conditions.

This model has been termed a homogeneous model since it assumes that there is no variation in temperature or concentration between the centre of a given catalyst particle and the external fluid adjacent to the catalyst. This representation of the reactor accounts for radial and axial diffusion of heat and mass due to turbulent mixing within the reactor. This model would be useful under conditions where there is negligible resistance to heat and mass transfer across the particle surface. These conditions may be present when there is a high fluid velocity through the reactor. Temperature and concentration gradients within the catalyst itself will be insignificant in cases where there is a low heat of reaction and a high thermal conductivity and diffusion coefficient within the catalyst or in cases where the catalyst particles are very small.

B. SURFACE RESISTANCE MODEL:

This model is an extension of the homogeneous model to include the effects of a resistance to heat and mass transfer across the film at the catalyst surface. However it also assumes that the gradients within the catalyst particles are negligible. Equations (II-1a)

and (II-2a) must now be modified to describe the behavior of the external field. Here the depletion and accumulation terms will be the transfer of heat and mass between the external field and the catalyst.

$$\varepsilon_R D_a \frac{\partial^2 C}{\partial X^2} + \varepsilon_R D_r \left[\frac{\partial^2 C}{\partial R^2} + \frac{1}{R} \frac{\partial C}{\partial R}\right] - \varepsilon_R u \frac{\partial C}{\partial X} =$$

$$S_v k_g (C - C_s) + \varepsilon_R \frac{\partial C}{\partial t} \qquad \text{(II-1b)}$$

$$\varepsilon_R K_a \frac{\partial^2 T}{\partial X^2} + \varepsilon_R K_r \left[\frac{\partial^2 T}{\partial R^2} + \frac{1}{R} \frac{\partial T}{\partial R}\right] - \varepsilon_R \rho_f Z_f u \frac{\partial T}{\partial X} =$$

$$S_v k_g (T - T_s) + \varepsilon_R \rho_f Z_f \frac{\partial T}{\partial t} \qquad \text{(II-2b)}$$

These equations will apply only to the temperature and concentration of the external field. The boundary conditions (II-3), (II-4), and (II-5) remain unchanged.

The following two additional equations will describe the behavior of the temperature and concentration at the surface and within the catalyst particles.

$$S_v k_g (C - C_s) = V_v f(C_s, T_s) + \varepsilon_p V_v \frac{\partial C_s}{\partial t} \qquad \text{(II-6b)}$$

$$S_v h_g (T - T_s) = V_v \Delta H f(C_s, T_s) + \rho_p Z_p V_v \frac{\partial T_s}{\partial t} \qquad \text{(II-7b)}$$

Again, the specification of some initial conditions is necessary to completely define the system.

This model then, will go beyond the application of the homogeneous model to include the cases where there is a significant concentration or temperature difference between the external field and the catalyst particles.

C. INTERNAL RESISTANCE MODEL:

This model is intended to account for all of the previously listed phenomena affecting the performance of a non-adiabatic packed bed reactor. Internal concentration and temperature gradients within the catalyst particles will now determine the rate of reaction. In many cases this model will give results significantly different from the previous models, where it was assumed that the entire catalyst particle exists under the same conditions as are present on its surface.

The pair of partial differential equations describing the behavior of the external field for this model will be the same as those for the surface resistance model, (II-1b) and (II-2b). Again the boundary conditions (II-3), (II-4), and (II-5) remain unchanged. Equations (II-6b) and (II-7b) must be slightly modified to describe heat and mass transfer across the film at the particle surface and chemical reaction at the surface of the catalyst particle.

They become:

$$S_v k_g (C-C_s) + D_p S_v \left.\frac{\partial C_p}{\partial r}\right|_{r=r_o} = f(C_s,T_s)\Big|_{r=r_o} + \varepsilon_p \left.\frac{\partial C_s}{\partial t}\right|_{r=r_o} \quad \text{(II-6c)}$$

$$S_v h_g (T-T_s) + K_p S_v \left.\frac{\partial T_p}{\partial r}\right|_{r=r_o} = \Delta H\, f(C_s,T_s)\Big|_{r=r_o} + \rho_p Z_p \left.\frac{\partial T_p}{\partial t}\right|_{r=r_o} \quad \text{(II-7c)}$$

These equations apply only at the outside surface boundary of the catalyst.

If the catalyst packing is considered to be composed of uniform porous spherical particles, the following pair of equations describe the transport of heat and mass with chemical reaction within the particles themselves.

$$D_p \left[\frac{\partial^2 C_p}{\partial r^2} + \frac{2}{r}\frac{\partial C_p}{\partial r}\right] = f(C_p,T_p) + \varepsilon_p \frac{\partial C_p}{\partial t} \quad \text{(II-8)}$$

$$K_p \left[\frac{\partial^2 T_p}{\partial r^2} + \frac{2}{r}\frac{\partial T_p}{\partial r}\right] = \Delta H\, f(C_p,T_p) + \rho_p Z_p \frac{\partial T_p}{\partial t} \quad \text{(II-9)}$$

A mass transfer parameter q_M may be defined as

$$q_M = \frac{r_o \eta f (C_s, T_s)}{3 k_g C_s} = \frac{C-C_s}{C_s} \qquad \text{(II-12)}$$

Similarly, a heat transfer parameter q_H may be defined as:

$$q_H = \frac{r_o \eta \Delta H f (C_s, T_s)}{3 h_g T_s} = \frac{T-T_s}{T_s} \qquad \text{(II-13)}$$

Thus if the parameters q_M and q_H are examined over the expected range of operating variables and are found to be less than 0.001, then the error in assuming $C=C_S$ and $T=T_S$ will be less than 0.1%. Thus in the absence of internal catalyst gradients, the homogeneous model would represent the system as well as the surface resistance model.

ii) If heat and mass transfer within the catalyst itself is examined, Prater, (20), has shown that the following relation holds at any point within the catalyst at steady-state regardless of particle geometry or chemical rate expression.

$$T_p - T_s = \frac{-\Delta H \, D_p}{K_p} (C_s - C_p) \qquad \text{(II-14)}$$

where H, D_p, and K_p are independent of concentration or temperature. The maximum temperature difference within the catalyst is thus given by

$$(T_p - T_s)_{max} = \frac{-\Delta H \; D_p \; C_s}{K_p} \qquad \text{(II-15)}$$

Defining a heat of reaction parameter, β, as

$$\beta = \frac{(T_p - T_s)_{max}}{T_s} = \frac{-\Delta H \; D_p \; C_s}{K_p \; T_s} \qquad \text{(II-16)}$$

indicates that if $|\beta|$ is less than 0.001, the assumption of an isothermal catalyst would be warranted.

A diffusion parameter, Φ, may be defined as

$$\Phi = r_o \sqrt{\frac{f(C_s, T_s)}{D_p \; C_s}} \qquad \text{(II-17)}$$

It has been shown by Weisz, (16), that for an isothermal case; if $\Phi \leq 0.3$ for a second order reaction, or $\Phi \leq 1.0$ for a first order reaction, or $\Phi \leq 6.0$ for a zero order reaction, then diffusion effects may be considered negligible.

Thus an examination of these parameters over the expected range of operating conditions should indicate whether or not the internal resistance model would be that much more an improved representation of the reactor so as to warrant its use.

III NUMERICAL METHODS

An analytic solution to the partial differential equations set forth in section II does not appear possible. The numerical approach taken was to finite difference the entire set of equations for each model and solve the resulting systems of nonlinear differential equations. These equations are of the general form:

$$\underline{A}\,\underline{x} = \frac{\partial \underline{x}}{\partial t} + \underline{f}(x) + \underline{k} \qquad \text{(III-1)}$$

where $\underline{A}$ is an mxm constant matrix

$\underline{x}$ is the column vector of unknown variables

$\underline{f}(x)$ is the column vector of nonlinear functions of the unknown variables

$\underline{k}$ is a constant column vector.

It will be instructive to first examine a system of linear algebraic equations of the form:

$$\underline{A}\ \underline{x} = \underline{k} \qquad \text{(III-2)}$$

Such a system of equations might result from the finite differencing of the steady-state diffusion equation, $\nabla^2 x = 0$, with a Neumann or Dirichelet boundary condition at either end.

The matrix $\underline{A}$, may be partitioned into three separate matrices, $\underline{A} = \underline{D} - \underline{E} - \underline{F}$ where:

$\underline{D}$ is a diagonal matrix consisting of the diagonal entries of $\underline{A}$

$\underline{E}$ is a strictly lower triangular matrix whose entries are the negatives of the entries of $\underline{A}$ below the main diagonal.

$\underline{F}$ is a strictly upper triangular matrix whose entries are the negatives of the entries of $\underline{A}$ above the main diagonal.

Equation (III-2) may now be written as;

$(\underline{D} - \underline{E} - \underline{F})\ \underline{x} = \underline{k}$; or upon multiplying by a scalar, ω, and rearranging a few terms:

$$(\underline{D} - \omega\underline{E})\ \underline{x} = \left[(1-\omega)\ \underline{D} + \omega\underline{F}\right]\ \underline{x} + \omega\underline{k} \qquad \text{(III-3)}$$

This gives rise to the iterative scheme:

$$\underline{x}^{(n+1)} = (\underline{D} - \omega\underline{E})^{-1}\ \left[(1-\omega)\ \underline{D} + \omega\underline{F}\right]\ \underline{x}^{(n)} + \omega\underline{k} \qquad \text{(III-4)}$$

The matrix $(\underline{D} - \omega\underline{E})$ is lower triangular and $\underline{x}^{(n)}$ is known. Thus the system of equations can easily be solved by back-substitution for $\underline{x}^{(n+1)}$ beginning with $x_1^{(n+1)}$. If $\omega > 1$ this iterative scheme is referred to as point successive overrelaxation, (PSOR), (21). If the matrix $\underline{A}$ is diagonally dominant, real, and symmetric this method of solution is stable for all $0 < \omega < 2$. An iteration scheme is stable if regardless of the initial guess vector, $\underline{x}^{(0)}$, the successive

solution vectors, $\underline{x}^{(n)}$, approach the true solution, $\underline{x}^*$, of the algebraic equations, (III-2), as the number of iterations, n, approaches infinity. Wachspress, (22), has shown that the above scheme, (III-4), can be stable even if $\underline{A}$ is not symmetric, provided that certain other requirements are met, among them being that the algebraic equations are consistently ordered.

The above scheme, (III-4), may be altered slightly so that at odd iterations the system of equations, $(\underline{D} - \omega\underline{E})\ \underline{x}^{(n+1)} = \left[(1 - \omega)\ \underline{D} + \omega\underline{F}\right]\ \underline{x}^{(n)} + \omega\underline{k}$ is solved sequentially beginning with $x_1^{(n+1)}$ and at even iterations the system of equations, $(D - \omega\underline{E})\ \underline{x}^{(n+1)} = \left[(1 - \omega)\ \underline{D} + \omega\underline{E}\right]\ \underline{x}^{(n)} + \omega\underline{k}$, (III-5), is solved sequentially beginning with $x_m^{(n+1)}$. This scheme is referred to as point symmetric successive overrelaxation and is also stable for all $0 < \omega < 2$, (21).

For diagonally dominant, real and symmetric matrices, it is of practical interest to determine the relaxation factor, ω, which will yield the desired result with the fewest number of iterations. It can be shown, (21), that this optimum ω is given by,

$$\omega_b = \frac{2}{1 + \sqrt{1-\rho(B)^2}}$$, where $\rho(B)$ is the spectral radius of the matrix $\underline{B} = \underline{D}^{-1}\ (\underline{E} + \underline{F})$. Upon examining

$$\left[\underline{M} - \frac{\underline{I}}{\Delta t}\right] \underline{x}^{(t+1)} = \left[-\underline{N} - \frac{\underline{I}}{\Delta t}\right] \underline{x}^{(t)} \quad \text{(III-8)}$$

or

$$\left[\underline{N} - \frac{\underline{I}}{\Delta t}\right] \underline{x}^{(t+1)} = \left[-\underline{M} - \frac{\underline{I}}{\Delta t}\right] x^{(t)} \quad \text{(III-9)}$$

If these two matrix equations are solved alternately at every other time step, then this method of iteration is known as the alternating direction explicit procedure, (ADEP), (23). This method is stable for all Δt if both $\underline{M}$ and $\underline{N}$ are diagonally dominant.

The ADEP can be shown to be analagous to point symmetric successive overrelaxation, (PSSOR), for solving elliptic equations where the solution of each time step corresponds to the solution of each iteration. The following illustration will show the relationship between ω and Δt for a rather special case.

Suppose $\underline{A}$ is diagonally dominant, real, and symmetric. The solution of the i^{th} equation for x_i on a forward sweep, (equation (III-4)), at the $(n+1)^{th}$ iteration is as follows, assuming $\underline{A}$ to be tri-diagonal:

$$a_{i,i-1}\, x_{i-1}^{(n+1)} + \frac{a_{i,i}}{\omega}\, x_i^{(n+1)} = -\frac{a_{i,i}}{1-\omega}\, x_i^{(n)} - a_{i,i+1}\, x_{i+1}^{(n)} + k_i$$

Now, on the further assumption that, $a_{i,i-1} = a_{i,i+1} = \frac{-a_{i,i}}{2} = a$, there results:

$$a\, x_{i-1}^{(n+1)} - \frac{2a}{\omega}\, x_i^{(n+1)} = \frac{2a}{1-\omega}\, x_i^{(n)} - a\, x_{i+1}^{(n)} + k_i$$

$$\text{or} \quad x_i^{(n+1)} = \frac{\omega}{2}\, x_{i-1}^{(n+1)} + \frac{\omega}{2}\, x_{i+1}^{(n)} - \frac{\omega k_i}{2a} - \frac{\omega}{1-\omega}\, x_i^{(n)} \qquad \text{(III-10)}$$

This can be compared to the forward sweep, (equation (III-8)), of the ADEP at the t+1 time level.

$$a\, x_{i-1}^{(t+1)} - \left[a + \frac{1}{\Delta t}\right] x_i^{(t+1)} = \left[a - \frac{1}{\Delta t}\right] x_i^{(t)} - a\, x_{i+1}^{(t)} + k_i$$

$$\text{or} \quad x_i^{(t+1)} = \frac{a\Delta t}{a\Delta t+1}\, x_{i-1}^{(t+1)} + \frac{a\Delta t}{a\Delta t+1}\, x_{i+1}^{(t)} - \left[\frac{a\Delta t-1}{a\Delta t+1}\right] x_i^{(t)} - \frac{t\, k_i}{a\Delta t+1} \qquad \text{(III-11)}$$

Comparing the terms of equations (III-10) and (III-11), the following relation is seen to hold:

$$\frac{a\Delta t}{a\Delta t+1} = \frac{\omega}{2} \quad \text{or} \quad t = \frac{2\omega}{a(2-\omega)} \qquad \text{(III-12)}$$

It can also be seen that the range of stability ($0 < \omega < 2$) for PSSOR corresponds to the range of

stability ($0 < \Delta t < \infty$) for the ADEP. If the assumption that $a_{i,i-1} = a_{i,i+1} = \frac{-a_{i,i}}{2}$ is neglected then a much more complicated expression for Δt in terms of will result. However it will be of the same general form as (III-12). For this case, a given time step Δt would correspond to an iterative scheme for the elliptic case which used a different relaxation factor, ω, for each algebraic equation of (III-4).

It is now of interest to proceed towards a solution of the nonlinear elliptic and parabolic equations of the general form:

$$\underline{A}\ \underline{x} = \underline{f}(x) + \underline{k} \text{ (elliptic)} \qquad \text{(III-13)}$$

and

$$\underline{A}\ \underline{x} = \frac{\partial \underline{x}}{\partial t} + \underline{f}(x) + \underline{k} \text{ (parabolic)} \qquad \text{(III-14)}$$

If the time derivative in equation (III-14) is approximated by a first order finite difference expression, then both matrix equations can be expressed in the form as shown below:

$$\underline{M}\ \underline{x}^{(n+1)} + \underline{N}\ \underline{x}^{(n)} = \underline{f}(x) + \underline{k} \qquad \text{(III-15)}$$

Here, $\underline{M} = \frac{\underline{D}}{\omega} - \underline{E}$ and $\underline{N} = \frac{(\omega-1)}{\omega}\ \underline{D} - \underline{F}$ for the elliptic case, and $\underline{M} = \underline{D}' - \frac{\underline{I}}{\Delta t} - \underline{E}$ and $\underline{N} = \underline{D}'' + \frac{\underline{I}}{\Delta t} - \underline{F}$ for the parabolic case. Here the transient term $\frac{\underline{I}}{\Delta t}$ is

included in the matrices $\underline{M}$ and $\underline{N}$ for simplicity, so that the following discussion will apply equally to the solution of nonlinear elliptic or parabolic equations.

Three schemes are suggested for solving these types of equations.

1) The first scheme is one where the nonlinear function, f(x), is calculated at the known iteration or time step.

$$\underline{M}\,\underline{x}^{(n+1)} + \underline{N}\,\underline{x}^{(n)} = \underline{f}(x)^{(n)} + \underline{k} \qquad \text{(III-16)}$$

This type of solution is no more difficult than solving the matrix equation, (III-4), since $\underline{f}(x)^{(n)}$ is always known from the previous iteration. However, in many cases the time step, Δt, or the acceleration parameter, ω, must be kept very small to ensure stability. This can be a prohibitive restriction since, as Δt or ω decreases, the number of iterations required to reach a solution increases.

ii) The second scheme is one where the nonlinear function, f(x), is calculated at the latest iteration or time step.

$$\underline{M}\,\underline{x}^{(n+1)} + \underline{N}\,\underline{x}^{(n)} = \underline{f}(x)^{(n+1)} + \underline{k} \qquad \text{(III-17)}$$

This method will involve solving a set of nonlinear algebraic equations at every iteration. It must be

remembered that the matrix $\underline{M}$ is lower triangular. Thus, starting with x_1, in the first equation, each succeeding equation need only be solved for one unknown. To illustrate this more clearly, suppose that $\underline{A}$ is tri-diagonal and that the i^{th} equation is being solved for x_i at the $(n+1)^{th}$ iteration. The equation would be as follows:

$$m_{i,i-1}\, x_{i-1}^{(n+1)} + m_{i,i}\, x_i^{(n+1)} + n_{i,i}\, x_i^{(n)} + n_{i,i+1}\, x_{i+1}^{(n)} = f(x_i)^{(n+1)} + k_i.$$

$x_{i-1}^{(n+1)}$ is known from the solution of the preceding equation, (i-1), and $x_i^{(n)}$ and $x_{i+1}^{(n)}$ are known from the preceding iteration, (n). Thus the only known variable is $x_i^{(n+1)}$. This equation can then be solved by any suitable iterative technique. The simple Newton-Raphson procedure, (6), was found to be satisfactory, using $x_i^{(n)}$ as the initial guess in solving the equation for $x_i^{(n+1)}$. This method of solving the nonlinear matrix equation is more difficult than the procedure which computes the nonlinear term at the known iteration since an iterative procedure is required to solve each algebraic equation. However, no stability problems were encountered in the problems to which this method was applied.

iii) The third scheme is a combination of the above two schemes, using the average value of the nonlinear

function, f(x), over the $(n)^{th}$ and $(n+1)^{th}$ iteration.

$$\underline{M}\,\underline{x}^{(n+1)} + \underline{N}\,\underline{x}^{(n)} = \frac{\underline{f}(x)^{(n+1)}}{2} + \frac{\underline{f}(x)^{(n)}}{2} + \underline{k} \quad \text{(III-18)}$$

The set of equations yielded from this approximation can be solved in the same manner as method (ii). Its only advantage is in the solution of the parabolic equation. Here each iteration is the calculation of a transient time step and the average value of $\underline{f}(x)$ over each time step will provide a greater degree of accuracy. However, often the increased accuracy of this method must be sacrificed in order to utilize the greater stability of the second method (ii).

IV MODEL OF CATALYST PARTICLE

The formulation and solution of a mathematical model for a single catalyst particle, besides being valuable in itself, will serve to illustrate the use of the numerical methods developed in section III.

It has been pointed out that if there is a significant heat of reaction associated with a chemical reaction then both temperature and concentration gradients will be established within the porous solid catalyst. These will depend on the rate at which heat and mass diffuse throughout the particle. If the reaction kinetics are a function of both temperature and concentration, then the rate of chemical reaction will vary throughout the catalyst pellet. It is obvious that catalyst effectiveness must be considered in the simulation of fixed bed catalytic reactors.

This discussion will be confined to the case where mass transfer occurs only by diffusion within the particle. Heat and mass transfer, together with chemical reaction within a catalyst pellet at steady-state may then be described by a pair of nonlinear ordinary differential equations. These simultaneous equations are coupled by the nonlinear reaction rate expression. The two equations may be represented as follows:

$$D_P \nabla^2 C_P = f(C_P, T_P) \qquad \text{(IV-1)}$$

$$K_P \nabla^2 T_P = \Delta H\, f(C_B, T_P) \qquad \text{(IV-2)}$$

with the boundary conditions:

$$C_P = C_{Po}, \quad T_P = T_{Po}; \quad r = r_o \qquad \text{(IV-3)}$$

$$\frac{\partial C_P}{\partial r} = 0 \quad , \quad \frac{\partial T_P}{\partial r} = 0 \; ; \quad r = r_o \qquad \text{(IV-4)}$$

The method of solution of these equations involves finite differencing the spatial derivatives and solving the resulting system of nonlinear algebraic equations. The finite difference approximation may be obtained by considering a mass and heat balance around a finite elemental volume of catalyst. A uniform spherical catalyst pellet will be assumed although the following development is applicable to an infinite cylinder model or a one dimensional infinite slab. Equal radial increments will not be assumed since in many cases it is desirable to have more grid points closer to the catalyst surface, where the bulk of the reaction often occurs.

Referring to Figure (1), consider a volume element bounded by the surfaces $r_{i+\frac{1}{2}}$ and $r_{i-\frac{1}{2}}$ as shown in dashed lines. A mass balance on the reactant about this volume yields:

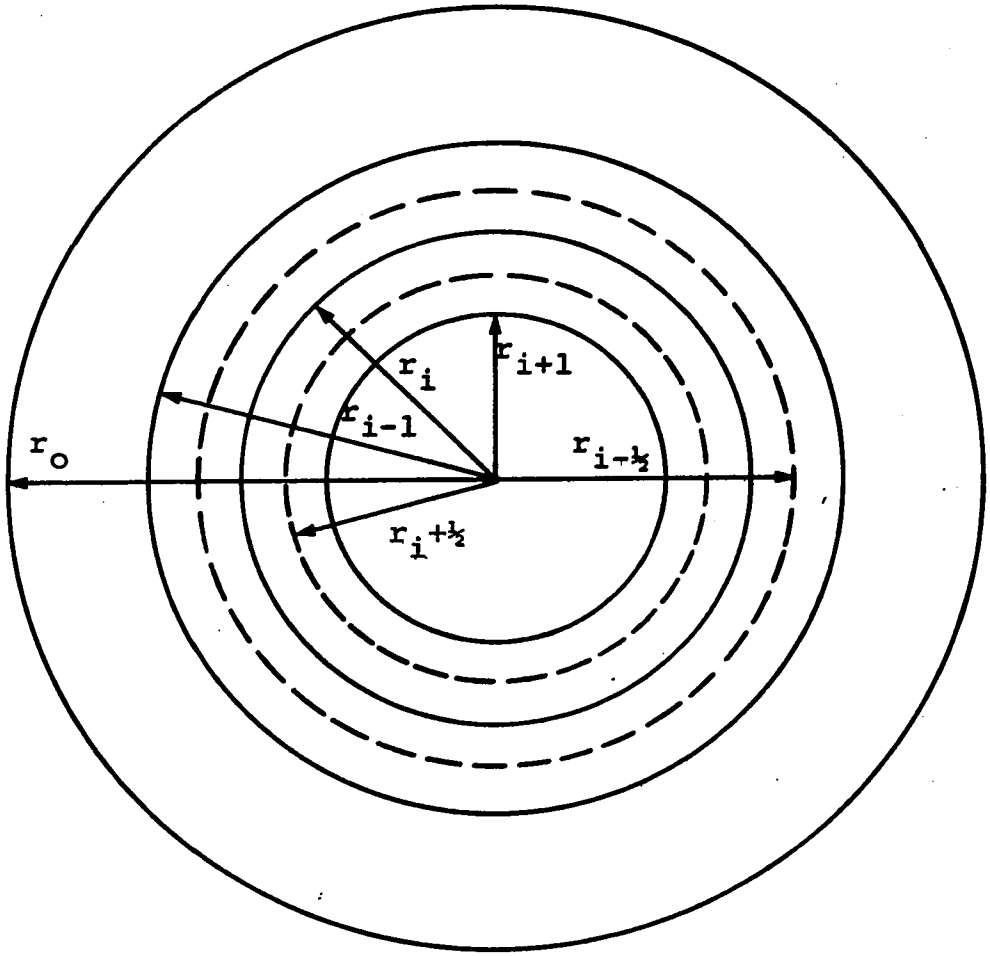

FIGURE 1 ELEMENTAL SPHERICAL SHELL VOLUME WITHIN CATALYST PARTICLE

i) Mass transfer in by diffusion

$$= - D_P \, 4\pi \left[\frac{r_i + r_{i-1}}{2}\right]^2 \left[\frac{C_{Pi} - C_{Pi-1}}{r_{i-1} - r_i}\right]$$

ii) Mass transfer out by diffusion

$$= - D_P \, 4\pi \left[\frac{r_i + r_{i+1}}{2}\right]^2 \left[\frac{C_{Pi+1} - C_{Pi}}{r_i - r_{i+1}}\right]$$

iii) Depletion of reactant due to chemical reaction

$$= \frac{4}{3} \pi \left[\left[\frac{r_i + r_{i-1}}{2}\right]^3 - \left[\frac{r_i + r_{i+1}}{2}\right]^3\right] f(C_{Pi}, T_{Pi})$$

Substituting these terms into a balance equation and rearranging the coefficients gives:

$$D_P \left[\frac{(r_i + r_{i-1})^2}{r_{i-1} - r_i}\right] C_{Pi-1} - D_P \left[\frac{(r_i + r_{i-1})^2}{r_{i-1} - r_i} + \frac{(r_i + r_{i+1})^2}{r_i - r_{i+1}}\right] C_{Pi}$$

$$+ D_P \left[\frac{(r_i + r_{i+1})^2}{r_i - r_{i+1}}\right] C_{Pi+1} = \frac{1}{6} \left[(r_i + r_{i-1})^3 - (r_i + r_{i-1})^3\right] f(C_{Pi}, T_{Pi}) \qquad \text{(IV-5)}$$

A similar heat balance yields:

$$K_P \left[\frac{(r_i + r_{i-1})^2}{r_{i-1} - r_i}\right] T_{Pi-1} - K_P \left[\frac{(r_i + r_{i-1})^2}{r_{i-1} - r_i} + \frac{(r_i + r_{i+1})^2}{r_i - r_{i+1}}\right] T_{Pi} + K_P \left[\frac{(r_i + r_{i+1})^2}{r_i - r_{i+1}}\right] T_{Pi+1}$$

$$= \frac{\Delta H}{6} \left[(r_i + r_{i-1})^3 - (r_i + r_{i+1})^3\right] f(C_{Pi}, T_{Pi}) \quad \text{(IV-6)}$$

If the catalyst has been divided into ℓ increments then the balance equations for the increment at the centre of the catalyst are:

$$D_P\, r_{\ell-1}\, C_{P\ell-1} - D_P\, r_{\ell-1}\, C_{P\ell} = \frac{r_{\ell-1}^3}{6} f\,(C_{P\ell}, T_{P\ell})$$

$$K_P\, r_{\ell-1}\, T_{P\ell-1} - K_P\, r_{\ell-1}\, C_{P\ell} = \frac{r_{\ell-1}^3}{6} \Delta H\, f\,(C_{P\ell}, T_{P\ell})$$

The other boundary condition is one of constant temperature and concentration, C_{Po} and T_{Po}, at the surface of the catalyst. The equations at the outside volume increment become:

$$-D_P \left[\frac{(r_1 + r_o)^2}{r_o - r_1} + \frac{(r_1 + r_2)^2}{r_1 - r_2}\right] C_{P1} + D_P \left[\frac{(r_1 + r_2)^2}{r_1 - r_2}\right] C_{P2}$$

$$= \frac{1}{6}\left[(r_1 + r_o)^3 - (r_1 + r_2)^3\right] f(C_{P1}, T_1) -$$

$$D_P \left[\frac{(r_1 + r_o)^2}{r_o - r_1}\right] C_{Po}$$

and

$$- K_P \left[\frac{(r_1 + r_o)^2}{r_o - r_1} + \frac{(r_1 + r_2)^2}{r_1 - r_2}\right] T_{P1} + K_P \left[\frac{(r_1 + r_2)^2}{r_1 - r_2}\right] T_{P2}$$

$$= \frac{\Delta H}{6}\left[(r_1 + r_o)^3 - (r_1 + r_2)^3\right] f\ (C_{P1}, T_{P1}) - K_P$$

$$\left[\frac{(r_1 + r_o)^2}{r_o - r_1}\right] T_{Po}$$

These equations together are seen to be of the form:

$$a_{1,1}\, C_{P1} + a_{1,2}\, C_{P2} = b_1\, f(C_{P,}, T_{P1}) + S_1$$

$$a_{2,1}\, C_{P1} + a_{2,2}\, C_{P2} + a_{2,3}\, C_{P3} = b_2\, f(C_{P2}, T_{P2})$$

$$a_{3,2}\, C_{P2} + a_{3,3} + a_{3,4}\, C_{P4} = b_3\, f(C_{P3}, T_{P3})$$

$$\vdots \qquad\qquad \vdots$$

$$a_{\ell,\ell-1}\, C_{P\ell-1} + a_{\ell,\ell}\, C_{P\ell} = b_\ell\, f(C_{P\ell}, T_{P\ell})$$

The heat balance equations can be characterized by this same form.

In matrix notation, these equations become:

$$\underline{A}_P \; \underline{C}_P = \underline{B}_P \; \underline{f} \; (C_P, T_P) + \underline{s}_P \qquad \text{(IV-7)}$$

$$\underline{U}_P \; \underline{T}_P = \underline{P}_P \; \underline{f} \; (C_P, T_P) + \underline{v}_P \qquad \text{(IV-8)}$$

It is seen that both the matrices $\underline{A}_P$ and $\underline{U}_P$ are diagonally dominant, real and symmetric. If these matrix equations, (IV-7) and (IV-8) were linear they could be solved either by PSOR or the ADEP, and the stability of the numerical solution would be guaranteed.

These two matrix equations may be solved by PSOR as applied to nonlinear equations in section III. However, here, both sets of equations must be solved simultaneously. Partitioning $\underline{A}_P$ into $\underline{M}_P + \underline{N}_P$ and $\underline{U}_P$ into $\underline{Q}_P + \underline{R}_P$ as shown for PSOR, and choosing an initial guess of $\underline{C}_P^{(o)} = C_{Po}$ and $\underline{T}_P^{(o)} = T_{Po}$, the iterative scheme which computes the nonlinear term at the previous iteration proceeds as follows:

$$\underline{M}_P \; \underline{C}_P^{(1)} = - \underline{N}_P \; \underline{C}_P^{(o)} + \underline{B}_P \; \underline{f} \; (C_P, T_P)^{(o)} + \underline{s}_P \qquad \text{(IV-9)}$$

$$\underline{Q}_P \; \underline{T}_P^{(1)} = - \underline{R}_P \; \underline{T}_P^{(o)} + \underline{P}_P \; \underline{f} \; (C_P, T_P)^{(o)} + \underline{v}_P \qquad \text{(IV-10)}$$

The entire right hand side of both matrix equations is known, and since $\underline{M}_P$ and $\underline{Q}_P$ are lower triangular matrices, these two matrix equations can be solved very simply. On the second iteration the values of $\underline{C}_P^{(1)}$ and $\underline{T}_P^{(1)}$ are

introduced into the right hand side and $\underline{C}_P^{(2)}$ and $\underline{T}_P^{(2)}$ are again easily calculated. This iterative procedure is continued until none of the elements of $\underline{C}_P^{(n+1)}$ and $\underline{T}_P^{(n+1)}$ differ in the third significant figure from their previous values of $\underline{C}_P^{(n)}$ and $\underline{T}_P^{(n)}$. Computationally, this procedure is quite simple; however in many of the examples, the numerical solution became unstable. In all of these trial runs, an acceleration parameter of $\omega = 1.75$ was used. In some of those cases for which the numerical solution became unstable, it was possible to correct this condition by using a smaller value of ω. This resulted in a larger number of iterations required to reach a final solution. Sometimes, this number of iterations became prohibitively large from the viewpoint of practical utility.

The second scheme tried, was the procedure which computes the nonlinear term at the most advanced iteration. Here the overall iteration scheme proceeds as follows:

$$\underline{M}_P \, \underline{C}_P^{(1)} = - \underline{N}_P \, \underline{C}_P^{(o)} + \underline{B}_P \, \underline{f} \, (C_P, T_P)^{(1)} + \underline{s}_P \qquad \text{(IV-11)}$$

$$\underline{Q}_P \, \underline{T}_P^{(1)} = - \underline{R}_P \, \underline{T}_P^{(o)} + \underline{P}_P \, \underline{f} \, (C_P, \underline{T}_P)^{(1)} + \underline{v}_P \qquad \text{(IV-12)}$$

Again, the fact that $\underline{M}_P$ and $\underline{Q}_P$ are lower triangular matrices still provides a computational advantage. Upon examining the first algebraic equation of

introduced into the right hand side and $\underline{C}_p^{(2)}$ and $\underline{T}_p^{(2)}$ are again easily calculated. This iterative procedure is continued until none of the elements of $\underline{C}_p^{(n+1)}$ and $\underline{T}_p^{(n+1)}$ differ in the third significant figure from their previous values of $\underline{C}_p^{(n)}$ and $\underline{T}_p^{(n)}$. Computationally, this procedure is quite simple; however in many of the examples, the numerical solution became unstable. In all of these trial runs, an acceleration parameter of $\omega = 1.75$ was used. In some of those cases for which the numerical solution became unstable, it was possible to correct this condition by using a smaller value of ω. This resulted in a larger number of iterations required to reach a final solution. Sometimes, this number of iterations became prohibitively large from the viewpoint of practical utility.

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$$\underline{Q}_p \, \underline{T}_p^{(1)} = - \underline{R}_p \, \underline{T}_p^{(o)} + \underline{P}_p \, \underline{f} \, (C_p, \underline{T}_p)^{(1)} + \underline{v}_p \qquad \text{(IV-12)}$$

Again, the fact that $\underline{M}_p$ and $\underline{Q}_p$ are lower triangular matrices still provides a computational advantage. Upon examining the first algebraic equation of

each of the matrix equations, (IV-11) and (IV-12), it is seen that the only unknown variables are $C_{P1}^{(1)}$ and $T_{P1}^{(1)}$. Furthermore, these two equations provide a linear relationship between $C_{P1}^{(1)}$ and $T_{P}^{(1)}$. If the expression for the rate term provided by equation (IV-12), is substituted into equation, (IV-11), this linear relationship is characterized by the general form:

$$\underline{M}_P \, \underline{C}_P^{(1)} = - \underline{N}_P \, \underline{C}_P^{(o)} + \underline{s}_P + \underline{P}_P^{-1} \, \underline{B}_P \left[\underline{Q}_P \, \underline{T}_P^{(1)} + \underline{R}_P \, \underline{T}_P^{(o)} - \underline{V}_P \right] \qquad \text{(IV-13)}$$

Therefore in the first algebraic equation of (IV-11) this linear relationship between $C_{P1}^{(1)}$ and $T_{P1}^{(1)}$ may be substituted for $T_{P}^{(1)}$ in the rate term $f\,(C_{P1},T_{P1})^{(1)}$. Now, all that remains is one nonlinear algebraic equation in one unknown variable $C_{P1}^{(1)}$. This equation was solved using the Newton-Raphson procedure and only required a few iterations. Once $C_{P1}^{(1)}$ has been calculated, $T_{P1}^{(1)}$ may be calculated by simple substitution into the linear relation between $C_{P1}^{(1)}$ and $T_{P1}^{(1)}$. Proceeding to the second algebraic equations, it is seen that $C_{P2}^{(1)}$ and $T_{P2}^{(1)}$ are the only unknown variables. Again they may be calculated using the same procedure as outlined above. This is continued until the entire vectors $\underline{C}_P^{(1)}$ and $\underline{T}_P^{(1)}$ have been computed. Then these

values are substituted for $\underline{C}_p^{(o)}$ and $\underline{T}_p^{(o)}$ in equations (IV-11) and (IV-12) and the entire overall procedure is repeated to solve for $\underline{C}_p^{(2)}$ and $\underline{T}_p^{(2)}$. This iterative procedure is continued until a final solution is reached.

DISCUSSION OF RESULTS:

A variety of cases involving widely differing parameters and rate expressions were run using the computational scheme where the nonlinear term is calculated at the most advanced iteration. In these cases an acceleration parameter of $\omega = 1.75$ was used. The determination of an optimum acceleration parameter for the nonlinear problem will be discussed later. The above examples were run on an IBM 360/67 computer using thirty catalyst grid points. The computation time for each case was approximately 20 seconds. Once the steady-state concentration and temperature profiles were found, a third order correct integrating procedure was used to compute the average rate of reaction throughout the catalyst. Comparing this with the rate of reaction at the surface conditions, C_{Po} and T_{Po}, enabled the calculation of an effectiveness factor.

These computations were carried out for the three one-dimensional geometries of a sphere, an infinite cylinder, and an infinite slab. The parameters used to characterize the physical, thermodynamic and kinetic

constants of each case are as follows:

i) First Order Reaction: $r' = k_o e^{-\frac{A'}{T_C}}$

$$\alpha = \frac{A'}{T_o} \; ; \; \beta = - \frac{C_o \; H \; D_P}{K_P \; T_o} \; ; \; \Psi = r_o \sqrt{\frac{k_o \; e^{-\frac{A'}{T_o}}}{D_P}}$$

ii) Second Order Reaction: $r' = k_o e^{-\frac{A'}{T}} C^2$

$$\alpha = - \frac{-\Delta H \; A' \; C_o \; D_P}{K_P \; T_o^2} \; ; \; \Psi = r_o \sqrt{\frac{k_o e^{-\frac{A'}{T_o}} C_o}{D_P}}$$

iii) Langmuir-Hinshelwood Rate equation:

$$r' = \frac{k_o \; e^{-\frac{A'}{T}} \; K_1 \; C}{1 + K_1 C + K_2 C_o - K_2 C}$$

$$\alpha = \frac{A'}{T_o} \; ; \beta = - \frac{\Delta H \; C_o \; D_P}{K_P \; T_o} \; ; \; \Psi = r_o \sqrt{\frac{k_o \; e^{-\frac{A'}{T_o}}}{D_P \; C_o}}$$

A selected set of results for all three reaction expressions are presented in Tables (1), (2), and (3). Their comparison with previously published results reveals no inconsistencies.

Some comment is in order regarding the catalyst grid spacing. It is obvious that the higher the number

TABLE 1

FIRST ORDER REACTION - (SPHERE)

γ	Ψ	β	ITERATIONS	η	$\eta_{(16)}$
10	10	0.6	48	.776	.79
10	10	.0	37	.270	.27
10	10	-.6	37	.138	.13
20	1.0	0.6	45	28.8	26.0
20	1.0	.0	34	.940	.94
20	1.0	-.6	34	.650	.63
30	0.5	0.6	51	254.	250.
30	0.5	.0	28	.984	.98
30	0.5	-.6	24	.804	.80

$\eta_{(16)}$ refers to the results published in reference (16)

TABLE 2

SECOND ORDER REACTION - (INFINITE SLAB)

Ψ	α	ITERATIONS	η	$\eta_{(18)}$
0.5	5.0	34	1.44	1.5
0.5	.0	30	.863	.86
0.5	-5.0	29	.690	.70
1.0	5.0	40	1.82	1.7
1.0	.0	29	.648	.65
1.0	-5.0	35	.442	.45
5.0	5.0	41	.370	.39
5.0	.0	40	.160	.16
5.0	-5.0	37	.101	.10

$\eta_{(18)}$ refers to the results published in reference (18)

TABLE 3

LANGMUIR-HINSHELWOOD REACTION - (INFINITE SLAB)

Ψ	γ	β	K_1C_o	K_2C_o	ITERATIONS	η'	$\eta_{(19)}$
0.5	40	.1	1.0	10.0	27	.960	.95
0.5	40	.0	1.0	10.0	26	.854	.82
1.0	40	.1	1.0	5.0	34	1.25	1.3
1.0	40	.0	1.0	5.0	30	.747	.73
2.0	40	.1	1.0	1.0	47	1.72	2.0
2.0	40	.0	1.0	1.0	39	.651	.62
0.5	40	.1	10.0	10.0	34	1.32	1.3
0.5	40	.0	10.0	10.0	29	.937	.80
1.0	40	.1	10.0	5.0	56	2.95	3.5
1.0	40	.0	10.0	5.0	37	.859	.81
2.0	40	.1	10.0	1.0	60	1.58	2.2
2.0	40	.0	10.0	1.0	144	.673	.63

$\eta_{(19)}$ refers to the results published in reference (19)

of grid points, the more equations there will be at each iteration to solve. Another consideration is the fact that in many highly reactive cases, most of the reaction occurs in the outer one third or even in some cases in the outer one twentieth of the catalyst particle. Thus, a grid spacing was chosen which gave a very narrow spacing near the outer wall of the catalyst where the concentration and temperature gradients could be very steep, and a rather wide spacing near the centre of the catalyst where these profiles are quite flat. For a normalized radius this spacing was as follows: (0, 1/2, 3/4, 7/8, 15/16, ... , $\frac{8207}{8208}$, $\frac{16415}{16416}$, 1). Then each of these spaces was divided in half to give a total of thirty increments.

It was noticed that the choice of the physical representation of the catalyst particle had a very pronounced effect upon its effectiveness factor. A comparison of the three geometric models is given in Table (4) for a first order reaction. It is seen that regardless of the heat effects; whether they be exothermic, endothermic, or isothermal; the effectiveness factor of the slab was less than that for a cylinder, and the effectiveness factor of the cylinder was less than that for a sphere, where all three representations have the same radius. This is due to the fact that a greater proportion of the catalyst volume is closer

TABLE 4

COMPARISON OF DIFFERENT GEOMETRIC MODELS OF CATALYST FOR FIRST ORDER REACTION

γ	Ψ	β	η (SPHERE)	η (CYLINDER)	η (SLAB)
10	10.	0.6	.776	.531	.272
10	1.0	.0	.940	.893	.762
10	0.5	-.6	.905	.843	.691
20	10.	0.6	3.23	2.17	1.093
20	1.0	.0	.940	.894	.764
20	0.5	-.6	.848	.762	.583
30	10.	0.6	13.3	8.89	4.45
30	1.0	.0	.940	.894	.765
30	0.5	-.6	.804	.706	.517

to the surface for a spherical particle than for either a cylindrical or slab type of particle, and it is in this outer volume where most of the reaction occurs. It is suggested that considerable attention should be paid to the choice of which geometric model best approximates the shape of a particular catalyst under investigation.

It was also shown in a few cases that for some combinations of diffusion parameters and heats of reaction, more than one steady state condition could exist within the catalyst. This means that the rate of heat removal equalled the rate of heat generation for more than one steady state condition. For these parameters, two stable steady-state conditions were found; one corresponding to a low reactive state and the other to a high reactive state. Here the term, stable, is used in the sense that when the particle is operating at one of these steady states and a small perturbation is applied to the boundary conditions, the disturbed steady-state profiles will return to their original steady-state upon the removal of the perturbation.

Theoretically, a third steady-state condition is possible, intermediate between the other two. However this steady state is unstable to any perturbation, however small, and could not be found using

numerical methods since even round-off errors which are unavoidable in a discrete model, would cause the results to go towards either of the stable steady-state conditions. Of the stable operating conditions; that one which was closest to the choice of initial conditions, $\underline{C}_p^{(o)}$ and $\underline{T}_p^{(o)}$, was the one which resulted from the computations. The other steady-state could be produced by changing the initial conditions. Figures (2) and (3) show the two stable concentration and temprature profiles which could exist within a catalyst particle under identical boundary conditions. These figures are for a first order reaction and parameters of: $\gamma = 20$, $\Psi = 0.5$, and $\beta = +0.6$. It is seen that in the low reaction condition there is a small gradual depletion of reactant towards the centre of the catalyst, accompanied by a gradual increase in temperature. In the highly reactive case the temperature climbs very rapidly from the surface of the catalyst. The high rate of reaction associated with this high temperature causes a sharp depletion of the reactant until half-way through the catalyst there is a negligible amount of reactant left.

This phenomena of multiple steady states has been indicated by other investigators (14) and its effect has been shown to play a major role in the overall stability of some packed bed reactors.

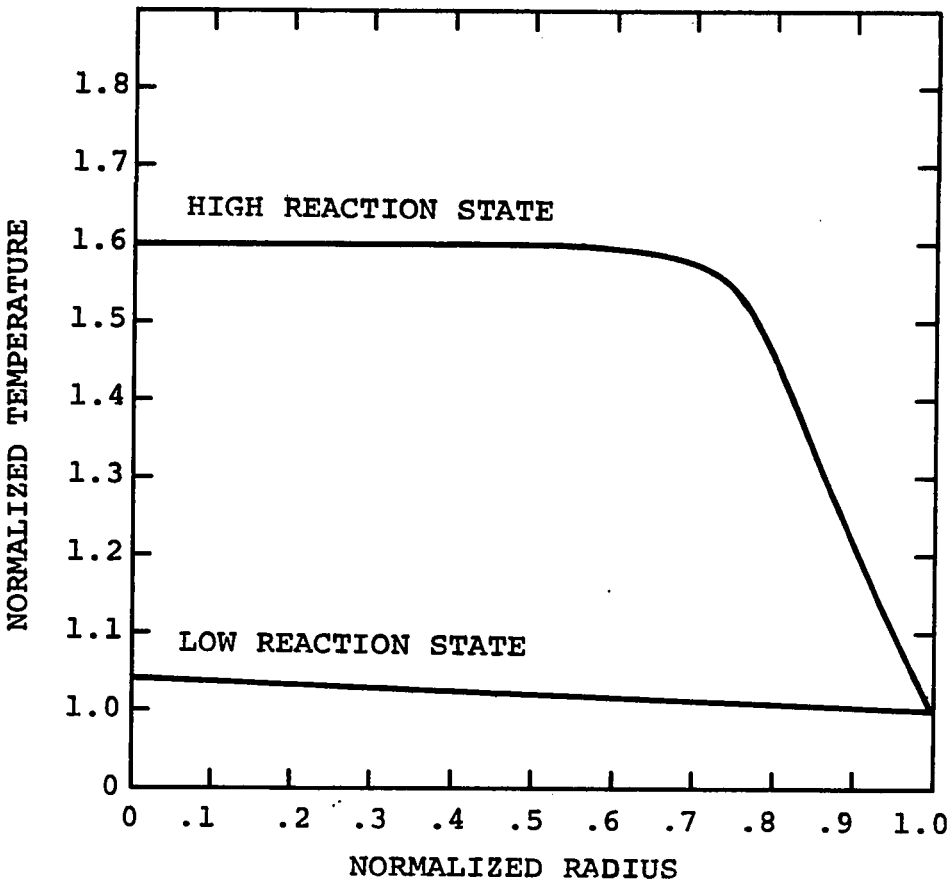


FIGURE 2 MULTIPLE STEADY-STATE TEMPERATURE PROFILES WITHIN SPHERICAL CATALYST

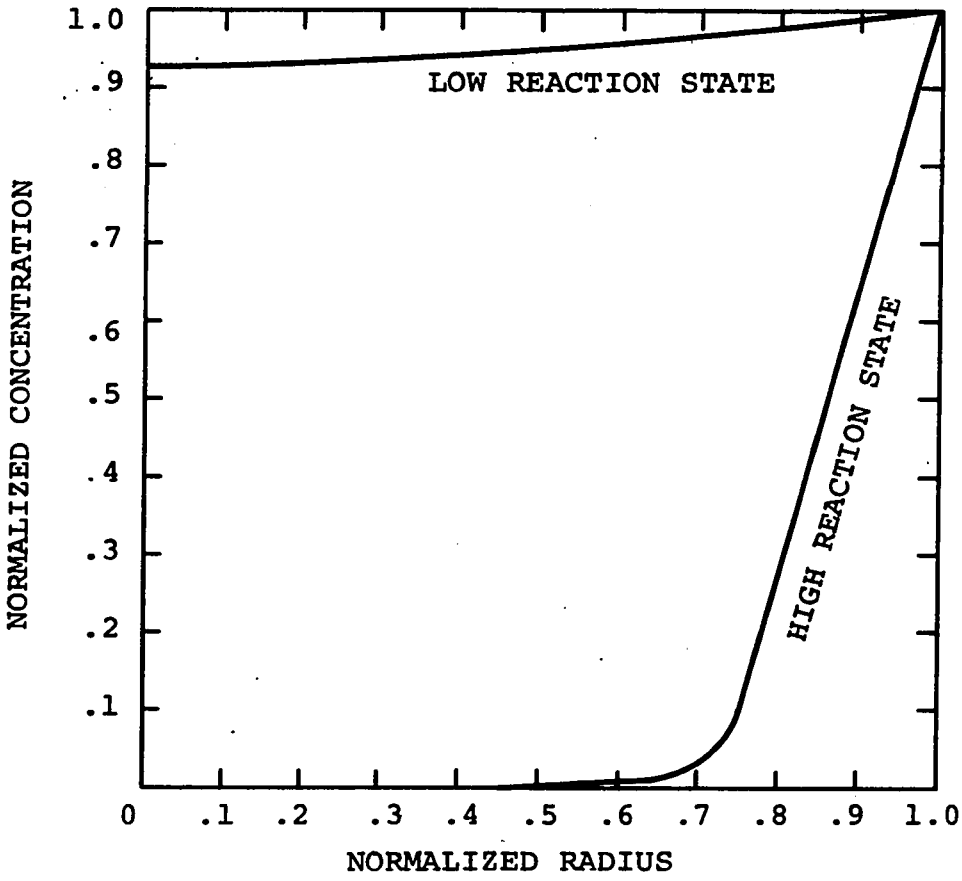


FIGURE 3 MULTIPLE STEADY-STATE CONCENTRATION PROFILES WITHIN SPHERICAL CATALYST

It is of interest to investigate the possibility of determining an optimum acceleration parameter, ω, for computations of this nonlinear type. For the linear case this optimum ω can be determined theoretically as shown in section III from

$$\omega_b = \frac{2}{1 + \sqrt{1 - \rho(B)^2}}$$

where $\rho(B)$ is the spectral radius of the matrix $\underline{B} = \underline{D}^{-1} (\underline{E} + \underline{F})$. For one particular set of parameters and a first order reaction, several runs were made using different values of ω on either side of the theoretically optimum ω for the corresponding linear case. The number of iterations required to reach a solution was then compared with number of iterations when using the linear optimum ω. These results are presented in Table (5). It is seen that the optimum ω for the linear problem is very close to the optimum ω for the nonlinear examples. Thus if many runs are to be carried out it would be advantageous to use the optimum acceleration parameter, ω_b, as provided by the linear problem.

TABLE 5

ACCELERATION PARAMETER (ω)	NUMBER OF ITERATIONS		
	SPHERE	CYLINDER	SLAB
1.50	71	74	74
1.60	52	52	52
1.65	40	41	40
ω*	43	43	43
1.70	42	43	56
1.75	77	51	49
1.80	99	96	110

ω* = 1.678 sphere

1.681 cylinder

1.687 slab

V HOMOGENEOUS MODEL OF REACTOR

As previously described in section II, the homogeneous model is intended to describe a packed bed reactor where there is a negligible resistance to heat and mass transfer across the surface of the catalyst particles and where there are no concentration or temperature gradients within the catalyst itself. The partial differential equations describing heat and mass transfer in the external field are:

$$\varepsilon_R D_a \frac{\partial^2 C}{\partial X^2} + \varepsilon_R D_r \left[\frac{\partial^2 C}{\partial R^2} + \frac{1}{R} \frac{\partial C}{\partial R}\right] - \varepsilon_R u \frac{\partial C}{\partial X}$$

$$= (1 - \varepsilon_R) f(C,T) + (\varepsilon_R + (1 - \varepsilon_R) \varepsilon_P) \frac{\partial C}{\partial t} \quad \text{(II-1a)}$$

$$\varepsilon_R K_a \frac{\partial^2 T}{\partial X^2} + \varepsilon_R K_r \left[\frac{\partial^2 T}{\partial R^2} + \frac{1}{R} \frac{\partial T}{\partial R}\right] - \varepsilon_R u \rho_f z_f \frac{\partial T}{\partial X}.$$

$$= (1 - \varepsilon_R) \Delta H f(C,T) + (\varepsilon_R \rho_f z_f + (1 - \varepsilon_R) \rho_P z_P) \frac{\partial T}{\partial t} \quad \text{(II-2a)}$$

The finite difference analogue of these equations may be obtained by considering a material and heat balance about a finite volume element of the reactor. Since the reactor is assumed to be radially symmetric, the grid system may be represented on a longitudinal plane section through the centre-line of the reactor, bounded by the reactor wall, the reactor centre-line, the entrance, and

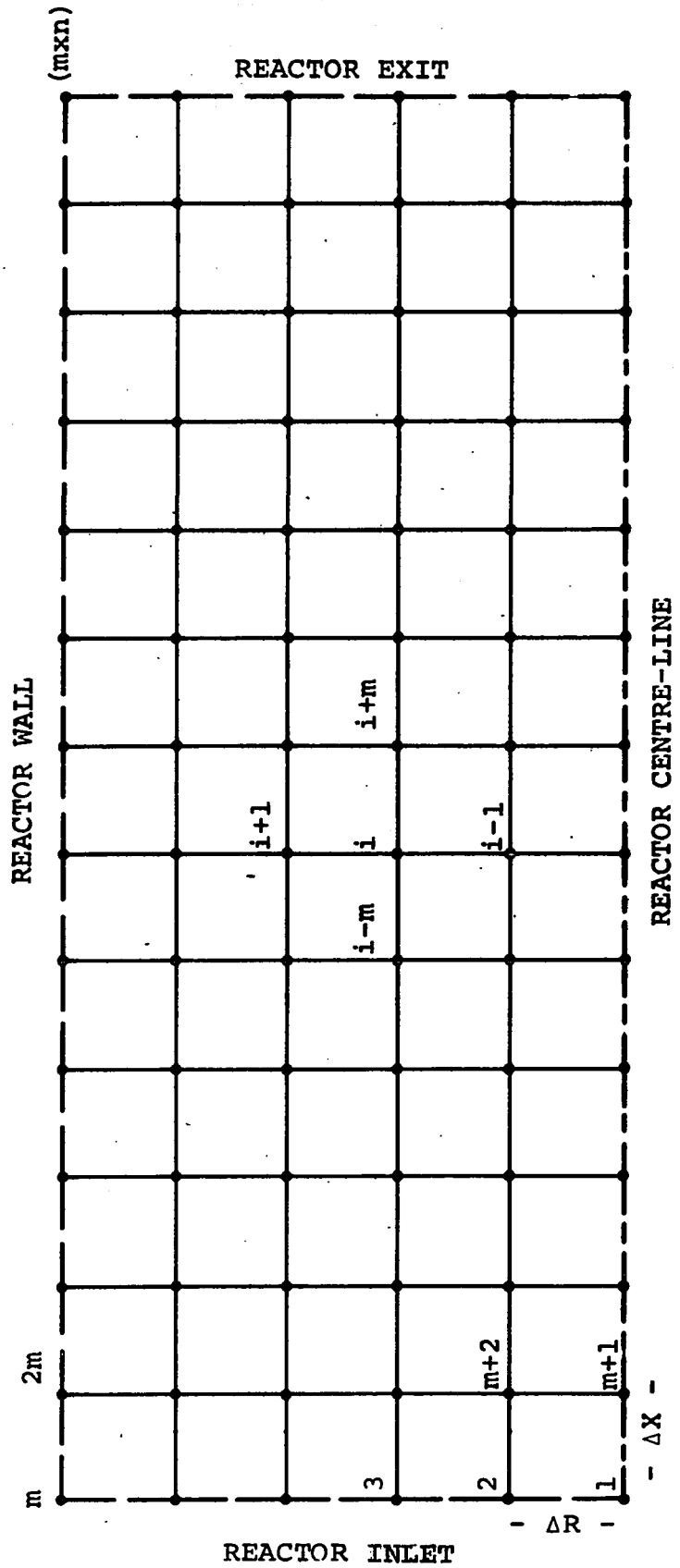


FIGURE 4 REACTOR GRID SYSTEM

the exit. The grid points are numbered from the centre-line to the wall and from the entrance to the exit; see Figure (4). It is seen that each grid point represents a cylindrical shell of length ΔX, except at the entrance and exit where they are of length $\frac{\Delta X}{2}$. If there are n longitudinal increments and m radial increments, then there will be a total of (m x n) grid points.

Now consider the cylindrical shell at grid point i whose cross-sectional area is represented by dashed lines in the plane section of Figure (5). A mass balance on the reactant about this volume increment over a time interval dt proceeds as follows:

i) Mass transferred in by axial diffusion

$$= - D_a \varepsilon_R S \left[\frac{C_i - C_{i-m}}{\Delta X}\right]$$

ii) Mass transferred out by axial diffusion

$$= - D_a \varepsilon_R S \left[\frac{C_{i+m} - C_i}{\Delta X}\right]$$

iii) Mass transferred in by radial diffusion

$$= - D_r \varepsilon_R A_o \left[\frac{C_i - C_{i+1}}{\Delta R}\right]$$

iv) Mass transferred out by radial diffusion

$$= - D_r \varepsilon_R A_i \left[\frac{C_{i-1} - C_i}{\Delta R}\right]$$

v) Mass transferred in by convection = $\varepsilon_R u S C_{i-m}$

vi) Mass transferred out by convection = ε_R u S C_i

vii) Disappearance of mass due to reaction

$$= S\Delta X(1 - \varepsilon_R)f(C,T)$$

viii) Mass accumulation or depletion

$$= S\Delta X(\varepsilon_R + (1 - \varepsilon_R)\varepsilon_P)\frac{\partial C}{\partial t}$$

Substituting these terms in a balance equation and rearranging the coefficients will yield the following:

$$\left[\frac{\varepsilon_R D_a S}{\Delta X} + \varepsilon_R\, u\, S\right] C_{i-m} + \left[\frac{\varepsilon_R D_r A_i}{\Delta R}\right] C_{i-1} + \varepsilon_R \left[\frac{-2\, D_a S}{\Delta X} - \frac{D_r A_i}{\Delta R} - \frac{D_r A_o}{\Delta R} - u\, S\right] C_i + \left[\frac{\varepsilon_R D_r A_o}{\Delta R}\right] C_{i+1} + \left[\frac{\varepsilon_r D_a S}{\Delta X}\right]$$

$$C_{i+m} = (1 - \varepsilon_R)S\Delta X f(C,T) + (\varepsilon_R + (1 - \varepsilon_R)\varepsilon_P)S\Delta X\frac{\partial C}{\partial t}$$

(V-1)

In the above expression:

$$S = \pi\left[\left(R_i + \frac{\Delta R}{2}\right)^2 - \left(R_i - \frac{\Delta R}{2}\right)^2\right]$$

$$A_o = 2\pi\left(R_i + \frac{\Delta R}{2}\right)\Delta X$$

$$A_i = 2\pi\left(R_i - \frac{\Delta R}{2}\right)\Delta X$$

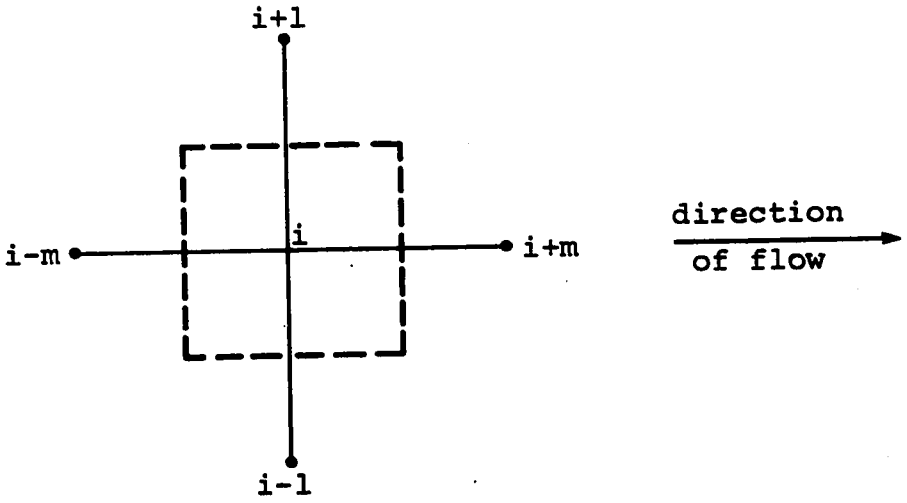


FIGURE 5 FINITE DIFFERENCE CELL IN REACTOR INTERIOR

A similar heat balance about this volume increment will yield the following equation:

$$\left[\frac{\varepsilon_R K_a S}{\Delta X} + \varepsilon_R u S \rho_f z_f\right] T_{i-m} + \left[\frac{\varepsilon_R K_r A_i}{\Delta R}\right] T_{i-1} + \varepsilon_R$$

$$\left[\frac{-2 K_a S}{\Delta X} - \frac{K_r A_i}{\Delta R} - \frac{K_r A_o}{\Delta R} - u S \rho_f z_f\right] T_i + \left[\frac{\varepsilon_R K_r A_o}{\Delta R}\right]$$

$$T_{i+1} + \left[\frac{\varepsilon_R K_a S}{\Delta X}\right] T_{i+m} = (1 - \varepsilon_R) S \Delta X \Delta Hf(C,T) +$$

$$(\varepsilon_R \rho_f z_f + (1 - \varepsilon_R) \rho_P z_P) S \Delta X \frac{\partial T}{\partial t} \qquad \text{(V-2)}$$

The following modifications to these equations must be made to account for the various boundary conditions.

i) At the entrance represented in Figure (6), diffusion of heat and mass into the entrance cells in the forward axial direction is assumed to be negligible. This has been termed a Danckwerts boundary condition, (24). Heat and mass only enter these cells by convective flow in the axial direction. Heat and mass are also assumed to diffuse in the radial directions only across the boundaries of the cell within the reactor itself. Also, chemical reaction occurs only in that part of the cell within the reactor. These assumptions are quite valid since radial and axial diffusion operate mainly due to the turbulent mixing caused by the presence of the catalyst packing. As well, chemical

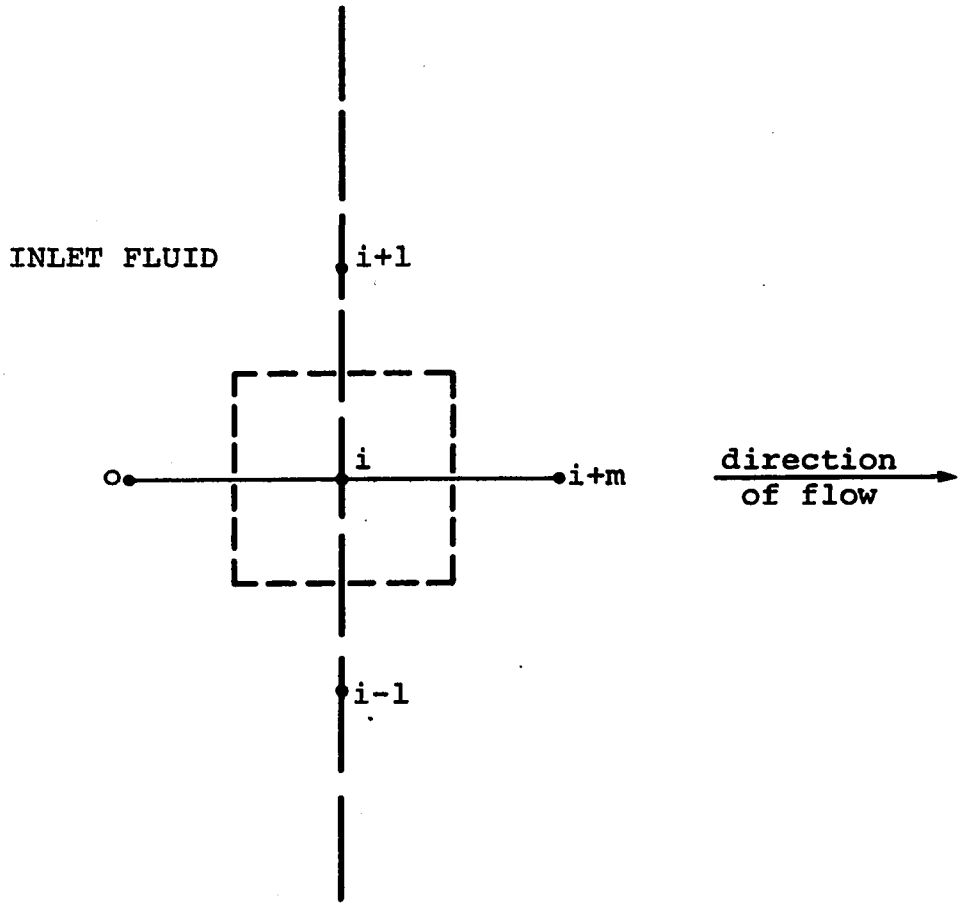


FIGURE 6 FINITE DIFFERENCE CELL AT REACTOR INLET

reaction occurs only within the catalyst particles. Therefore, the equations at this boundary will become:

$$\left[\frac{\varepsilon_R D_r A_i}{\Delta R}\right] C_{i-1} + \varepsilon_R \left[-\frac{D_a S}{\Delta X} - \frac{D_r A_i}{\Delta R} - \frac{D_r A_o}{\Delta R} - u\,S\right] C_i +$$

$$\left[\frac{\varepsilon_R D_r A_o}{\Delta R}\right] C_{i+1} + \left[\frac{\varepsilon_R D_a S}{\Delta X}\right] C_{i+m} = (1-\varepsilon_R)\, S\, \frac{\Delta X}{2}\, f(C,T)$$

$$- \varepsilon_R\, u\, S\, C_o + (\varepsilon_R + (1-\varepsilon_R)\,\varepsilon_p) S \Delta X \frac{\partial C}{\partial t}$$

and:

$$\left[\frac{\varepsilon_R K_r A_i}{\Delta R}\right] T_{i-1} + \varepsilon_R \left[-\frac{K_a S}{\Delta X} - \frac{K_r A_i}{\Delta R} - \frac{K_r A_o}{\Delta R} - u\, S \rho_f z_f\right] T_i +$$

$$\left[\frac{\varepsilon_R K_r A_o}{\Delta R}\right] T_{i+1} + \left[\frac{\varepsilon_R K_a S}{\Delta X}\right] T_{i+m} = (1-\varepsilon_R)\, S\, \frac{\Delta X}{2}\, \Delta H\, f(C,T) -$$

$$\varepsilon_R\, u\, S \rho_f z_f\, T_o + (\varepsilon_R \rho_f z_f + (1-\varepsilon_R)\rho_p z_p) Z \Delta X \frac{\partial T}{\partial t}$$

Here $$S = \pi \left[(R_i + \frac{\Delta R}{2})^2 - (R_i - \frac{\Delta R}{2})^2\right]$$

$$A_o = \pi\, \Delta X\, (R_i + \frac{\Delta R}{2})$$

$$A_i = \pi\, \Delta X\, (R_i - \frac{\Delta R}{2})$$

ii) The exit, represented in Figure (7), has essentially the same type of conditions as apply at the entrance. The difference here is that no heat or mass diffuses out of the exit cell in the positive axial direction. This is a Danckwerts boundary condition applied to the exit.

Heat and mass leave the exit cells in this direction only due to convective flow. The equations at this boundary become:

$$\left[\frac{\varepsilon_R D_a S}{\Delta X} + \varepsilon_R u S\right] C_{i-m} + \left[\frac{\varepsilon_R D_r A_i}{\Delta R}\right] C_{i-1} + \varepsilon_R$$

$$\left[-\frac{D_a S}{\Delta X} - \frac{D_r A_o}{\Delta R} - \frac{D_r A_i}{\Delta R} - u S\right] C_i + \left[\frac{\varepsilon_R D_r A_o}{\Delta R}\right] C_{i+1} =$$

$$(1 - \varepsilon_R) S \frac{\Delta X}{2} f(C,T) + (\varepsilon_R + (1 - \varepsilon_R)\varepsilon_p) S \Delta X \frac{\partial C}{\partial t}$$

and:

$$\left[\frac{\varepsilon_R K_a S}{\Delta X} + \varepsilon_R u S \rho_f z_f\right] T_{i-m} + \left[\frac{\varepsilon_R K_r A_i}{\Delta R}\right] T_{i-1} + \varepsilon_R$$

$$\left[-\frac{K_a S}{\Delta X} - \frac{K_r A_o}{\Delta R} - \frac{K_r A_i}{\Delta R} - u S \rho_f z_f\right] T_i + \left[\frac{\varepsilon_R K_r A_o}{\Delta R}\right] T_{i+1} =$$

$$(1 - \varepsilon_R) S \frac{\Delta X}{2} \Delta H f(C,T) + (\varepsilon_R \rho_f z_f + (1 - \varepsilon_R)\rho_p z_p$$

$$S \Delta X \frac{\partial T}{\partial t}$$

where S, A_o, A_i are as defined at the entrance.

iii) At the wall of the reactor represented in Figure (8), heat is conducted across the reactor wall to a constant temperature surrounding. Of coure, there is no diffusion of mass across this boundary. Here the mass and heat balances become:

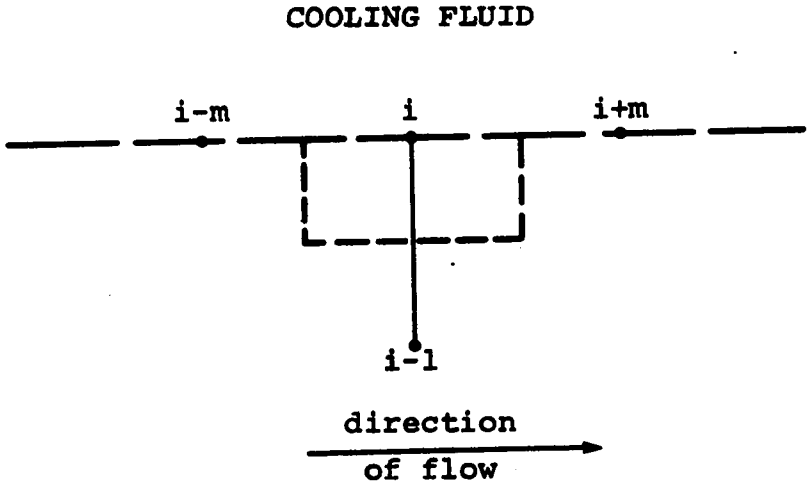


FIGURE 8 FINITE DIFFERENCE CELL AT REACTOR WALL

$$\left[\frac{\varepsilon_R D_a S}{\Delta X} + \varepsilon_R u S\right] C_{i-m} + \left[\frac{\varepsilon_R D_r A_i}{\Delta R}\right] C_{i+1} + \varepsilon_R$$

$$\left[-\frac{2D_a S}{\Delta X} - \frac{D_r A_i}{\Delta R} - u S\right] C_i + \left[\frac{D_a \varepsilon_R S}{\Delta X}\right] C_{i+m} =$$

$$(i - \varepsilon_R) S \Delta X f(C,T) + (\varepsilon_R + (1 - \varepsilon_R)\varepsilon_p) S \Delta X \frac{\partial C}{\partial t}$$

and:

$$\left[\frac{\varepsilon_R K_a S}{\Delta X} + \varepsilon_R u S \rho_f z_f\right] T_{i-m} + \left[\frac{\varepsilon_R K_r A_i}{\Delta R}\right] T_{i-1} + \varepsilon_R$$

$$\left[-\frac{2K_a S}{\Delta X} - \frac{K_r A_i}{\Delta R} - h_w A_o - u S \rho_f z_f\right] T_i + \left[\frac{K_a \varepsilon_R S}{\Delta X}\right]$$

$$T_{i+m} = (1 - \varepsilon_R) S \Delta X \Delta H f(C,T) - h_w A_o T_w + (\varepsilon_{Rf} z_f +$$

$$(1 - \varepsilon_R)\ \rho_p z_p) S \Delta X \frac{\partial T}{\partial t}$$

Here $S = \pi\left[R_o^2 - (R_o - \frac{\Delta R}{2})^2\right]$

$A_o = 2\pi R_o \Delta X$

$A_i = 2\pi (R_o - \frac{\Delta R}{2}) \Delta X$

iv) At the centre of the reactor represented in Figure (9), there is the simple condition that no heat or mass diffuses across the centre-line. Here the balances become:

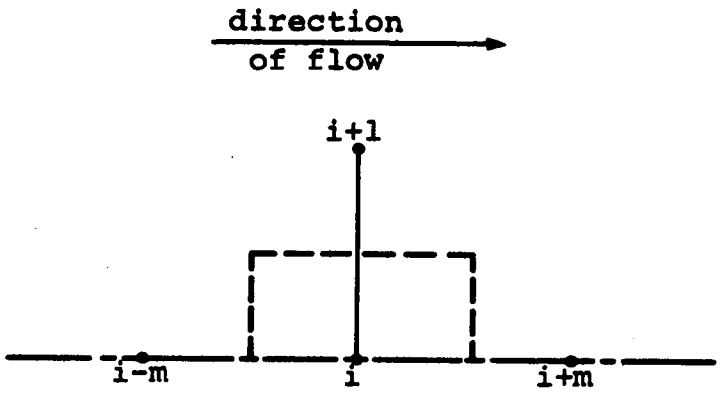


FIGURE 9 FINITE DIFFERENCE CELL AT REACTOR CENTRE-LINE

$$\left[\frac{\varepsilon_R D_a S}{\Delta X} + \varepsilon_R\, u\, S\right] C_{i-m} + \varepsilon_R \left[-\frac{2D_a S}{\Delta X} - \frac{D_r A_o}{\Delta R} - u\, S\right] C_i$$

$$+ \left[\frac{D_r A_o \varepsilon_R}{\Delta R}\right] C_{i+1} + \left[\frac{\varepsilon_R D_a S}{\Delta X}\right] C_{i+m} = (1 - \varepsilon_R)\, S\Delta X$$

$$f(C,T) + (\varepsilon_R + (1 - \varepsilon_R)\varepsilon_P) S\Delta X \frac{\partial C}{\partial t}$$

and:

$$\left[\frac{\varepsilon_R K_a S}{\Delta X} + \varepsilon_R\, U\, S\, \rho_f z_f\right] T_{i-m} + \varepsilon_R \left[-\frac{2K_a S}{\Delta X} - \frac{K_r A_o}{\Delta R} - U\, S\right.$$

$$\left.\rho_f z_f\right] T_i + \left[\frac{K_r \varepsilon_R A_o}{\Delta R}\right] T_{i+1} + \left[\frac{\varepsilon_R K_a S}{\Delta X}\right] T_{i+m} = (1 - \varepsilon_R)$$

$$S\Delta X\Delta H f(C,T) + (\varepsilon_R \rho_f z_f + (1 - \varepsilon_R)\rho_P z_P) S\Delta X \frac{\partial T}{\partial t}$$

Here $S = \frac{\pi \Delta R^2}{4}$

$A_o = \pi \Delta R\, \Delta X$

If the two sets of equations for heat and mass transport are written in order beginning with cell (1) and ending with cell (mxn), they may be summarized by the two matrix equations below:

$$\underline{A}\,\underline{C} = \underline{B}\,\underline{f}(C,T) + \underline{G}\,\frac{\partial \underline{C}}{\partial t} + \underline{s} \qquad \text{(V-3)}$$

$$\underline{U}\,\underline{T} = \underline{P}\,\underline{f}(C,T) + \underline{Y}\,\frac{\partial \underline{T}}{\partial t} + \underline{v} \qquad \text{(V-4)}$$

$\underline{A}$ and $\underline{U}$ are (mxn) x (mxn) matrices containing the diffusion and convection terms.

$\underline{B}$ is an (mxn) x (mxn) diagonal matrix containing the reaction volume terms, and $\underline{P} = \Delta H \underline{B}$.

$\underline{G}$ and $\underline{Y}$ are (mxn) x (mxn) diagonal matrices containing the transient capacity terms.

$\underline{s}$ and $\underline{v}$ are (mxn) column vectors containing the constant boundary conditions.

$\underline{C}$ and $\underline{T}$ are (mxn) column vectors containing the reactant concentrations and temperatures at each grid point.

It can be seen by examining the elements of $\underline{A}$ and $\underline{U}$, that these matrices are diagonally dominant for all grid spacings ΔX and ΔR. This is due to the choice of a backward difference approximation for the convective term.

It has been common practice in the mathematical modelling of chemical reactors, or for that matter any flow problem, to represent the convective term by a second order correct central difference approximation. If this were applied to the mass balance about the volume element in Figure (5), the following will result:

$$\text{Mass transferred in by convection} = \varepsilon_R \, u \, S \left[\frac{C_{i-m} + C_i}{2}\right]$$

$$\text{Mass transferred out by convection} = \varepsilon_R \, u \, S \left[\frac{C_i + C_{i+m}}{2}\right]$$

may be encountered in the solution of the matrix equation (V-3).

The use of a backward difference approximation for the convective term implies the assumption that the fluid in each cell is perfectly mixed. Referring to figure (5) it is easily seen that the concentration of the fluid crossing the right-hand boundary of the elemental volume is some time average of the concentration C_i, over a time interval, Δt. This is provided of course that $\Delta t < \frac{\Delta X}{u}$. The assumption of perfectly stirred grid cells does not interfere in any way with the central difference approximation to the diffusion mechanism between the grid cells. The backward difference approximation for convection is of course less accurate than the central difference approximation. However, the accuracy of the backward difference approximation could be improved by using a second order correct three point formula composed of the points i-2m, i-m, and i. This approximation will also ensure that the matrix $\underline{A}$ is monotone for all ΔX.

Now it is necessary to proceed with the time integration of the matrix equations (V-3) and (V-4). The matrices $\underline{A}$ and $\underline{U}$ are each partitioned into the matrices $\underline{A} = \underline{M} + \underline{N}$ and $\underline{U} = \underline{Q} + \underline{R}$ according to the alternating direction explicit procedure, where $\underline{M}$ and $\underline{Q}$ are lower triangular, diagonally dominant matrices and $\underline{N}$ and $\underline{R}$ are upper triangular, diagonally dominant matrices.

This procedure can be further clarified by examining the following rows of $\underline{M}$ and $\underline{N}$.

Row 1: $m_{1,1} = -\varepsilon_R u s$

$$n_{1,1} = -\frac{\varepsilon_R D_a S}{\Delta X} - \frac{\varepsilon_R D_r A_o}{\Delta R}$$

$$n_{1,2} = \frac{\varepsilon_R D_r A_o}{\Delta R}$$

$$n_{1,1+m} = \frac{\varepsilon_R D_a S}{\Delta X}$$

Row 2: $m_{2,1} = \frac{\varepsilon_R D_r A_i}{\Delta R}$

$$m_{2,2} = \frac{\varepsilon_R D_r A_i}{\Delta R} - \varepsilon_R u S$$

$$n_{2,2} = -\frac{\varepsilon_R D_a S}{\Delta X} - \frac{\varepsilon_R D_r A_o}{\Delta R}$$

$$n_{2,3} = \frac{\varepsilon_R D_r A_o}{\Delta R}$$

$$n_{2,m+1} = \frac{\varepsilon_R D_a S}{\Delta X}$$

Row i:
$m < i < ((mxn)-m+1)$

$$m_{i,i-m} = \frac{\varepsilon_R D_a S}{\Delta X} + \varepsilon_R u S$$

$$m_{i,i-1} = \frac{\varepsilon_R D_a A_i}{\Delta R}$$

$$m_{i,i} = -\frac{\varepsilon_R D_a S}{\Delta X} - \frac{\varepsilon_R D_r A_i}{\Delta R} - \varepsilon_R u S$$

$$n_{i,i} = -\frac{\varepsilon_R D_a S}{\Delta X} - \frac{\varepsilon_R D_r A_o}{\Delta R}$$

$$n_{i,i+1} = \frac{\varepsilon_R D_r A_o}{\Delta R}$$

$$n_{i,i+m} = \frac{\varepsilon_R D_a S}{\Delta X}$$

Row $(mxn)-m+1$:
$j = (mxn)-m+1$

$$m_{j,j-m} = \frac{\varepsilon_R D_a S}{\Delta X} + \varepsilon_R u S$$

$$m_{j,j-1} = 0$$

$$m_{j,j} = -\frac{\varepsilon_R D_a S}{\Delta X} - \varepsilon_R u S$$

$$n_{j,j} = -\frac{\varepsilon_R D_r A_o}{\Delta R}$$

$$n_{j,j+1} = \frac{\varepsilon_R D_r A_o}{\Delta R}$$

$$\text{Row } (mxn): \quad m_{j,j-m} = \frac{\varepsilon_R D_a S}{\Delta X} + \varepsilon_R u S \qquad n_{j,j} = 0$$
$$j = (mxn)$$

$$m_{j,j-1} = \frac{\varepsilon_R D_r A_i}{\Delta R}$$

$$m_{j,j} = -\frac{\varepsilon_R D_a S}{\Delta X} - \frac{\varepsilon_R D_r A_i}{\Delta R} - \varepsilon_R u S$$

All other elements in these rows are zero.

An examination of these coefficients shows that $\underline{M}$ and $\underline{N}$ and similarly $\underline{Q}$ and $\underline{R}$ are diagonally dominant triangular matrices.

Now if a first order correct approximation is substituted for the time derivative, the solution of the matrix equations (V-3) and (V-4) proceeds as follows.

First, an initial guess for the concentration and temperature distribution must be made. This essentially is the imposing of an arbitrary set of initial conditions. The most obvious initial guess is $\underline{C}^{(o)} = C_o$, the inlet concentration, and $\underline{T}^{(o)} = T_o$, the inlet temperature. In the following discussion, the superscript (o), refers to the initial time t_o and the superscript (n) refers to the time $t_o + n\ \Delta t$, where Δt is the time increment used in the numerical integration.

Then, using the alternating direction explicit procedure to solve for the concentrations and temperatures in the reactor at the time $t_o + \Delta t$, the matrix equations will appear as follows:

$$\left(\underline{M} - \frac{\underline{G}}{\Delta t} \right) \underline{C}^{(1)} = \left(- \underline{N} + \frac{\underline{G}}{\Delta t} \right) \underline{C}^{(o)} + \underline{B}\, \underline{f}(C,T)^{(1)} + \underline{s} \qquad \text{(V-6)}$$

$$\left(\underline{Q} - \frac{\underline{Y}}{\Delta t} \right) \underline{T}^{(1)} = \left(- \underline{R} + \frac{\underline{Y}}{\Delta t} \right) \underline{T}^{(o)} + \underline{P}\, \underline{f}(C,T) + \underline{v} \qquad \text{(V-7)}$$

As previously discussed in section III, for greater accuracy, the rate of reaction expression, $f(C,T)$, should perhaps be evaluated as an average over the time interval, Δt. However in some cases stability problems were encountered, whereas none were encountered when the rate expression was evaluated at the most advanced time step. Thus a certain degree of accuracy in the transient results was sacrificed to ensure stability of the overall solution.

Since the matrices $\underline{M} - \frac{\underline{G}}{\Delta t}$ and $\underline{Q} - \frac{\underline{Y}}{\Delta t}$ are lower triangular, the above matrix equations (V-6) and (V-7) may be solved row by row, sequentially. Examining the first row of each set of equations, it is seen that the only unknowns are $C_1^{(1)}$ and $T_1^{(1)}$. Moreover it is also seen that the two equations are coupled only by the rate expression $f(C_1,T_1)^{(1)}$. Substituting for the rate expression in (V-6), there results in matrix notation:

$$\left[\underline{M} - \frac{\underline{G}}{\Delta t}\right] \underline{C}^{(1)} = \left[-\underline{N} + \frac{\underline{G}}{\Delta t}\right] \underline{C}^{(o)} + \underline{s} + \underline{P}^{-1}\,\underline{B}$$

$$\left[\left[\underline{Q} - \frac{\underline{Y}}{\Delta t}\right] \underline{T}^{(1)} - \left[-\underline{R} + \frac{\underline{Y}}{\Delta t}\right] \underline{T}^{(o)} - \underline{v}\right] \qquad \text{(V-8)}$$

Thus in the first algebraic equation of the two matrix equations (V-6), and (V-7), $T_1^{(1)}$ is seen to be a known linear function of $C_1^{(1)}$. This relation may then be substituted into the rate expression, $f(C_1,T_1)^{(1)}$ and all that remains to be solved is one nonlinear equation in one unknown variable, $C_1^{(1)}$. A simple Newton-Raphson procedure was found to be adequate as only two or three iterations were required to reach a solution for each equation. Once $C_1^{(1)}$ has been calculated then $T_1^{(1)}$ may be calculated from the linear relationship (V-8).

Now the second algebraic equation of each of the matrix equations (V-6) and (V-7) may be solved for $C_2^{(1)}$ and $T_2^{(1)}$ in a similar manner. Since $C_1^{(1)}$ and $T_1^{(1)}$ are now known, the only unknowns in the second equations will be $C_2^{(1)}$ and $T_2^{(1)}$. This procedure is continued until the entire set of equations has been solved for $\underline{C}^{(1)}$ and $\underline{T}^{(1)}$.

Now at the next time step, $t_o + 2\,\Delta t$, the reverse sweep of the ADEP is used. In this case the following

matrix equations are solved:

$$\left(\underline{N} - \frac{\underline{G}}{\Delta t}\right) \underline{C}^{(2)} = \left(-\underline{M} + \frac{\underline{G}}{\Delta t}\right)\underline{C}^{(1)} + \underline{B}\,\underline{f}(C,T)^{(2)} + \underline{s} \qquad \text{(V-9)}$$

$$\left(\underline{R} - \frac{\underline{Y}}{\Delta t}\right) \underline{T}^{(2)} = \left(-\underline{Q} + \frac{\underline{Y}}{\Delta t}\right)\underline{T}^{(1)} + \underline{P}\,f(C,T)^{(2)} + \underline{v} \qquad \text{(V-10)}$$

Here, since the matrices, $\underline{N} - \frac{\underline{G}}{\Delta t}$ and $\underline{R} - \frac{\underline{Y}}{\Delta t}$, are upper triangular, the solution begins with the last equation, (mxn), and proceeds in the same manner as the forward sweep of the ADEP. Once $\underline{C}^{(2)}$ and $\underline{T}^{(2)}$ have been evaluated, the forward sweep of the ADEP is then used to calculate $\underline{C}^{(3)}$ and $\underline{T}^{(3)}$ and so on. This alternating type of solution is continued until a steady-state is reached. This was taken to occur when none of the elements of $\underline{C}^{(n+1)}$ and $\underline{T}^{(n+1)}$ differ in the third significant figure from their previous values of $\underline{C}^{(n)}$ and $\underline{T}^{(n)}$. This steady-state represents a feasible operating condition of the reactor. These values of $\underline{C}$ and $\underline{T}$ may now be used as a set of initial conditions and the transient response of the reactor to a step change in either inlet concentration, C_o, or inlet temperature T_o, or both, may be examined

by changing the required value and proceeding once again with the transient integration of equations (V-3) and (V-4) using the ADEP. This is continued until a new steady-state condition is achieved.

DISCUSSION OF RESULTS:

The main difference between the homogeneous model and previously developed models is the inclusion of both axial and radial diffusion in the external field of the reactor. High radial temperature gradients are present in several instances. One such case is that where the fluid must enter at a temperature high enough to cause an appreciable reaction, but where the maximum temperature in the reactor must be controlled so as not to exceed the physical limitations of the reactor. The effect of these radial gradients may be seen by examining the following case.

In this example the following parameters will serve to define the transport properties of the fluid in the packed bed reactor

$$N_{Pe_x} = 2.0$$

$$N_{Pe_r} = 11.0$$

$$N_{ST} = 2.0$$

Units of cal., gm.-moles, ^{o}K, cm., sec. were used for all parameters.

In addition: $\rho_f z_f = .0547$ $\rho_p z_p = .0672$

$\varepsilon_R = .35$ $\varepsilon_p = .543$

$T_o = 700$ $C_o = .00001$

The reaction rate expression is a Langmuir-Hinshelwood type of the specific form:

$$r' = \frac{10^8 \, e^{-12000/T} \, C}{1 + 10^5 \, C}$$

with a heat of reaction $\Delta H = -3.504 \times 10^5$

The cooling fluid temperature $T_w = 300$

The reactor length is equal to fifty particle diameters and the reactor diameter is equal to ten catalyst particle diameters. The radial and axial Peclet numbers given above, have been shown by both theoretical and experimental investigators, to be characteristic of fully developed turbulent flow in packed bed reactors. The computations for this homogeneous model were executed on an IBM 360/67 computer using a program written in FORTRAN IV. The computation time for one complete transient run was approximately six minutes. This included the determination of an initial steady-state.

First, using the parameters as designated above, the steady-state concentration and temperature profiles were calculated for this reactor. These are presented in Table (6). It is seen that most of the reaction occurs in the first half of the reactor and in the area

TABLE 6

HOMOGENEOUS MODEL

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

35.00 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.84397	0.85106	0.87997	0.94697	0.99042
1.00	0.52517	0.55638	0.67770	0.89028	0.96548
2.00	0.27530	0.33127	0.54981	0.85302	0.93709
3.00	0.14022	0.20674	0.48333	0.81865	0.90716
4.00	0.08492	0.15497	0.45575	0.78683	0.87675
5.00	0.06883	0.14305	0.44918	0.75841	0.84682
6.00	0.07235	0.15254	0.45261	0.73359	0.81816
7.00	0.08834	0.17454	0.46022	0.71211	0.79130
8.00	0.11404	0.20409	0.46923	0.69352	0.76652
9.00	0.14643	0.23771	0.47846	0.67742	0.74393
10.00	0.18603	0.27270	0.48746	0.66345	0.72352
11.00	0.22700	0.30704	0.49604	0.65132	0.70521
12.00	0.26769	0.33939	0.50412	0.64078	0.68886
13.00	0.30615	0.36899	0.51166	0.63163	0.67434
14.00	0.34125	0.39554	0.51861	0.62370	0.66149
15.00	0.37251	0.41902	0.52496	0.61683	0.65016
16.00	0.39991	0.43961	0.53071	0.61088	0.64019
17.00	0.42370	0.45754	0.53588	0.60573	0.63144
18.00	0.44424	0.47311	0.54050	0.60128	0.62378
19.00	0.46193	0.48659	0.54459	0.59743	0.61709
20.00	0.47715	0.49825	0.54821	0.59410	0.61125
21.00	0.49024	0.50832	0.55138	0.59122	0.60616
22.00	0.50150	0.51702	0.55416	0.58872	0.60172
23.00	0.51116	0.52452	0.55658	0.58656	0.59787
24.00	0.51922	0.53078	0.55862	0.58474	0.59462
25.00	0.53253	0.53414	0.55971	0.58375	0.59285

Bulk Concentration at Reactor Exit = 0.572728

TABLE 6 (continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	709.70	708.76	703.73	677.05	436.73
1.00	728.38	724.23	703.96	626.74	324.57
2.00	740.70	732.37	694.66	585.16	314.43
3.00	743.42	731.37	679.26	552.49	312.22
4.00	738.79	723.46	660.75	526.36	310.90
5.00	729.62	711.28	641.12	504.96	309.85
6.00	717.49	696.48	621.53	487.04	308.98
7.00	703.24	680.08	602.57	471.75	308.23
8.00	687.42	662.74	584.51	458.47	307.59
9.00	670.49	644.98	567.44	446.78	307.03
10.00	652.90	627.19	551.35	436.38	306.53
11.00	635.08	609.67	536.23	427.02	306.08
12.00	617.38	592.63	522.01	418.53	305.67
13.00	600.06	576.20	508.66	410.78	305.30
14.00	583.31	560.47	496.12	403.67	304.96
15.00	567.25	545.48	484.34	397.10	304.64
16.00	551.93	531.24	473.27	391.02	304.35
17.00	537.37	517.76	462.89	385.38	304.08
18.00	523.58	505.01	453.14	380.13	303.83
19.00	510.54	492.98	443.99	375.24	303.59
20.00	498.23	481.65	435.40	370.67	303.38
21.00	486.65	470.99	427.36	366.41	303.17
22.00	475.76	460.98	419.83	362.44	302.98
23.00	465.60	451.64	412.82	358.76	302.81
24.00	456.48	443.27	406.54	355.46	302.65
25.00	451.45	438.65	403.09	353.65	302.56

Bulk Temperature at Reactor Exit = 366.19

of the centre-line. Here, the heat of reaction given off is sufficient to maintain a high rate of reaction, and there is a slight temperature increase along the centre-line to a hot-spot of 743.4 ^{o}K about 3.0 cm from the entrance. As the fluid progresses through the reactor, the reactant is depleted to such a low value along the centre-line that the high rate of reaction cannot be maintained. Since heat is also being constantly drawn away from this area due to the large temperature difference between the centre-line and the wall, the temperature begins to gradually decrease. However at the reactor wall, the temperature is so low that there is a very small amount of reaction taking place and the concentration decreases slowly. The large concentration difference developed between the reactor wall and the centre-line causes a radial diffusion of reactant towards the centre of the reactor into the area of high reaction. Thus it is seen that the radial diffusion of heat towards the reactor wall is directly the cause of a counter diffusion of reactant in the opposite direction towards the reactor centre.

In the latter part of the reactor, where the temperature is not high enough to maintain a high rate of reaction, the diffusion of reactant towards the centre-line causes the reactant concentration to gradually

increase in the centre of the reactor as it progresses toward the exit. This establishes a concentration profile along the centre-line which is now opposite to the direction of fluid flow. Because of this gradient, reactant now can diffuse backwards against the convective flow into an area of higher reaction. Thus due to both axial and radial diffusion, the high reaction zone near the front of the reactor is being supplied with reactant from the low reaction, higher concentration areas of the reactor. Thus in this case, a model which did not account for radial and axial diffusion would give a rather conservative estimate of conversion.

To the above steady-state operating condition, a step increase of five percent in temperature was implemented at the reactor entrance and the transient response may be found in the Appendix. The new steady-state condition is presented in Table (7). The conversion of the system has increased from 42.7 percent to 62.9 percent, and the hotspot in the reactor has moved backwards along the centre-line to a point 2.0 cm from the entrance. Due to the increased rate of reaction the reactant is being depleted in the high reaction zone sooner and thus the temperature will begin to decrease at an earlier point in the reactor.

The transient response of the outlet concentration and temperature due to the increased rate of reaction

TABLE 7

HOMOGENEOUS MODEL

FINAL STEADY STATE CONDITIONS

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.66029	0.66853	0.71453	0.87162	0.97695
1.00	0.16547	0.18344	0.30050	0.73876	0.91808
2.00	0.03109	0.04365	0.15435	0.67281	0.85625
3.00	0.00736	0.01725	0.12415	0.62580	0.79792
4.00	0.00372	0.01474	0.13259	0.58768	0.74465
5.00	0.00436	0.01917	0.15507	0.55589	0.69679
6.00	0.00712	0.02784	0.18199	0.52934	0.65432
7.00	0.01233	0.04059	0.20853	0.50714	0.61697
8.00	0.02094	0.05746	0.23232	0.48851	0.58436
9.00	0.03390	0.07809	0.25263	0.47272	0.55602
10.00	0.05168	0.10162	0.26958	0.45924	0.53144
11.00	0.07394	0.12680	0.28367	0.44762	0.51015
12.00	0.09951	0.15233	0.29548	0.43755	0.49172
13.00	0.12676	0.17713	0.30549	0.42879	0.47574
14.00	0.15407	0.20041	0.31406	0.42118	0.46188
15.00	0.18017	0.22173	0.32147	0.41455	0.44986
16.00	0.20427	0.24090	0.32791	0.40878	0.43943
17.00	0.22598	0.25791	0.33352	0.40377	0.43038
18.00	0.24522	0.27289	0.33843	0.39942	0.42252
19.00	0.26210	0.28598	0.34272	0.39564	0.41569
20.00	0.27681	0.29739	0.34646	0.39237	0.40977
21.00	0.28957	0.30730	0.34973	0.38954	0.40464
22.00	0.30062	0.31590	0.35258	0.38709	0.40019
23.00	0.31016	0.32334	0.35507	0.38498	0.39634
24.00	0.31816	0.32959	0.35716	0.38321	0.39311
25.00	0.32248	0.33297	0.35830	0.38227	0.39138

Bulk Concentration at Reactor Exit = 0.371316

TABLE 7 (Continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	756.50	755.45	749.03	714.50	448.86
1.00	786.20	782.70	761.50	663.96	327.11
2.00	790.79	784.77	751.60	619.78	316.14
3.00	785.86	776.65	731.88	584.13	313.74
4.00	777.16	764.50	708.95	555.15	312.28
5.00	765.92	749.96	685.31	531.15	311.10
6.00	752.64	733.75	662.10	510.89	310.12
7.00	737.71	716.34	639.88	493.50	309.28
8.00	721.49	698.14	618.89	478.35	308.55
9.00	704.26	679.49	599.21	465.00	307.90
10.00	686.34	660.70	580.82	453.10	307.33
11.00	668.02	642.03	563.64	442.42	306.81
12.00	649.57	623.71	547.58	432.75	306.35
13.00	631.27	605.92	532.55	423.94	305.93
14.00	613.36	588.78	518.48	415.87	305.54
15.00	596.00	572.36	505.29	408.45	305.18
16.00	579.31	556.70	492.92	401.59	304.86
17.00	563.35	541.82	481.31	395.23	304.55
18.00	548.15	527.71	470.41	389.32	304.27
19.00	533.71	514.35	460.17	383.81	304.00
20.00	520.03	501.71	450.54	378.66	303.76
21.00	507.08	489.77	441.49	373.85	303.53
22.00	494.82	478.49	432.97	369.34	303.31
23.00	483.27	467.87	424.98	365.13	303.11
24.00	472.78	458.22	417.73	361.32	302.93
25.00	466.81	452.74	413.62	359.16	302.83

Bulk Temperature at Reactor Exit = 372.95

can be followed in Table (8). It is seen that after two seconds corresponding to one reactor residence time the outlet concentration has remained steady at a normalized value of .573. Then from this point on, the outlet concentration gradually decreases to a new steady-state value of .371. The outlet temperature responds in a much more delayed fashion. It holds steady at approximately 366.0 ^{o}K for 4.5 seconds which is well past two reactor residence times. Then it begins to rise to its steady-state value of 372.8 ^{o}K. This observation can be attributed to the following phenomena. As the heat wave progresses through the reactor it must constantly supply heat to raise the temperature of the catalyst particles and thus the full wave front is slowed down below the fluid velocity in the reactor. However the lower concentrations due to an increased rate of reaction move through the reactor at the same velocity as the fluid. In some cases where there is a significant rate of reaction in the latter stages of the reactor, the effect of the lower concentrations moving ahead of the higher temperature front can be to lower the temperatures momentarily in the latter part of the reactor due to a temporarily decreased rate of reaction. This has been shown by two recent investigators (25). However in this example the rate of reaction in the latter part of the reactor is quite negligible and the lower concentration

TABLE 8

TRANSIENT RESPONSE AT OUTLET OF HOMOGENEOUS MODEL TO A 5% INCREASE IN THE INLET TEMPERATURE

TIME (sec.)	NORMALIZED CONCENTRATION	ABSOLUTE TEMPERATURE (^{o}K)
0.5	.573	366.0
1.0	.573	365.9
1.5	.573	365.8
2.0	.573	365.8
2.5	.572	365.8
3.0	.566	365.8
3.5	.543	365.8
4.0	.503	365.9
4.5	.458	366.1
5.0	.421	366.6
5.5	.397	367.6
6.0	.383	368.7
6.5	.377	369.9
7.0	.375	371.0
7.5	.372	371.8
8.0	.371	372.4
8.5	.371	372.8

moving into this area ahead of the heat wave is not enough to show a significant decrease in reaction rate.

It is of interest to examine the effect of grid size upon the computations. In the example above, a grid size equal to one particle diameter was used. If a central difference approximation were used to describe the convective term, $u \frac{\partial C}{\partial t}$, this would be the maximum allowable grid size which will maintain stability in the numerical solution. However, using the backward difference approximation, the grid size in the axial direction was doubled to two particle diameters. The resulting initial steady-state conditions are presented in Table (9) and can be compared with Table (6). It is seen that the discrepancy in the outlet concentration is in the area of 8.0%. This discrepancy indicates that an axial grid size of two particle diameters is too large if better accuracy is to be maintained. The important point is that no stability problems were encountered in the numerical solution and the computation time was reduced by a half. This is of importance in those cases where a larger grid size than one particle diameter will not measurably affect the accuracy.

TABLE 9

HOMOGENEOUS MODEL ($\Delta X = 4\ r_o$)

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

35.00 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.77444	0.78843	0.83983	0.93754	0.98554
1.00	0.48811	0.53180	0.68372	0.89676	0.96186
2.00	0.28758	0.35559	0.59252	0.86415	0.93606
3.00	0.17925	0.26002	0.54633	0.83406	0.90930
4.00	0.13221	0.22010	0.52665	0.80663	0.88250
5.00	0.12034	0.21391	0.52109	0.78219	0.85642
6.00	0.12986	0.22789	0.52257	0.76073	0.83162
7.00	0.15397	0.25382	0.52742	0.74200	0.80845
8.00	0.18829	0.28618	0.53384	0.72571	0.78709
9.00	0.22884	0.32106	0.54092	0.71154	0.76762
10.00	0.27187	0.35574	0.54820	0.69925	0.75002
11.00	0.31433	0.38853	0.55539	0.68860	0.73422
12.00	0.35412	0.41851	0.56229	0.67938	0.72013
13.00	0.39014	0.44533	0.56878	0.67141	0.70762
14.00	0.42200	0.46897	0.57479	0.66452	0.69655
15.00	0.44975	0.48963	0.58029	0.65857	0.68681
16.00	0.47373	0.50756	0.58526	0.65344	0.67825
17.00	0.49435	0.52309	0.58972	0.64901	0.67075
18.00	0.51204	0.53650	0.59368	0.64518	0.66419
19.00	0.52721	0.54806	0.59719	0.64188	0.65847
20.00	0.54021	0.55803	0.60027	0.63903	0.65348
21.00	0.55137	0.56662	0.60297	0.63656	0.64914
22.00	0.56093	0.57401	0.60532	0.63443	0.64536
23.00	0.56905	0.58031	0.60735	0.63260	0.64211
24.00	0.57555	0.58536	0.60897	0.63111	0.63947
25.00	0.57831	0.58750	0.60965	0.63046	0.63832

Bulk Concentration at Reactor Exit = 0.620915

TABLE 9 (Continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	713.41	711.57	702.75	663.50	395.79
1.00	728.73	722.88	697.37	615.11	326.93
2.00	736.35	726.20	684.43	575.89	315.49
3.00	735.81	721.90	667.18	544.61	312.55
4.00	729.23	712.06	647.98	519.29	311.06
5.00	718.57	698.61	628.29	498.37	309.97
6.00	705.10	682.87	608.92	480.76	309.07
7.00	689.61	665.76	590.28	465.69	308.30
8.00	672.72	647.95	572.54	452.59	307.64
9.00	655.01	629.95	555.79	441.05	307.06
10.00	636.95	612.13	540.00	430.78	306.54
11.00	618.97	594.73	525.17	421.55	306.08
12.00	601.35	577.93	511.24	413.20	305.66
13.00	584.29	561.83	498.18	405.57	305.27
14.00	567.92	546.48	485.92	398.59	304.92
15.00	552.29	531.89	474.43	392.15	304.60
16.00	537.43	518.08	463.67	386.21	304.30
17.00	523.35	505.02	453.58	380.70	304.03
18.00	510.03	492.69	444.12	375.58	303.77
19.00	497.45	481.08	435.26	370.83	303.54
20.00	485.60	470.15	426.96	366.40	303.31
21.00	474.45	459.87	419.19	362.27	303.11
22.00	463.99	450.25	411.93	358.43	302.92
23.00	454.33	441.37	405.25	354.90	302.74
24.00	446.06	433.77	399.55	351.90	302.59
25.00	442.47	430.47	397.08	350.60	302.53

Bulk Temperature at Reactor Exit = 362.37

VI SURFACE RESISTANCE MODEL OF REACTOR

The surface resistance model of a packed bed chemical reactor is an extension of the homogeneous model to account for the possible resistance to heat and mass transfer between the external fluid in the reactor and the surface of the catalyst particles. The equations describing heat and mass transfer in the external field are slightly modified from the homogeneous case to the following:

$$\varepsilon_R D_a \frac{\partial^2 C}{\partial X^2} + \varepsilon_R D_r \left[\frac{\partial^2 C}{\partial R^2} + \frac{1}{R} \frac{\partial C}{\partial R}\right] - \varepsilon_R u \frac{\partial C}{\partial X} = S_v k_g (C - C_s) + \varepsilon_R \frac{\partial C}{\partial t} \qquad \text{(II-1b)}$$

$$\varepsilon_R K_a \frac{\partial^2 T}{\partial X^2} + \varepsilon_R K_r \left[\frac{\partial^2 T}{\partial R^2} + \frac{1}{R} \frac{\partial T}{\partial R}\right] - \varepsilon_R u \rho_f z_f \frac{\partial T}{\partial X} = S_v h_g (T - T_s) + \varepsilon_R \rho_f z_f \frac{\partial T}{\partial t} \qquad \text{(II-2b)}$$

The finite difference analogue of these equations is obtained in the same manner as for the homogeneous case. The only difference is that the disappearance of heat and mass from each incremental volume will be due to the diffusion across the film at the fluid-particle interface into the catalyst particles.

These terms are as follows:

Mass disappearing due to reaction = $S\Delta XS_v k_g (C-C_s)$

Heat disappearing, (appearing), due to reaction

$= S\Delta XS_v h_g (T-T_s)$

The finite difference analogue in matrix form becomes:

$$\underline{A}\,\underline{C} = \underline{w}\,(\underline{C}-\underline{C}_s) + \underline{G}\,\frac{\partial \underline{C}}{\partial t} + \underline{s} \qquad \text{(VI-1)}$$

$$\underline{U}\,\underline{T} = \underline{Z}\,(\underline{T}-\underline{T}_s) + \underline{Y}\,\frac{\partial \underline{T}}{\partial t} + \underline{v} \qquad \text{(VI-2)}$$

Now, the equations describing heat and mass transfer into the catalyst particles, plus chemical reaction are:

$$S\Delta XS_v k_g (C-C_s) = S\Delta XV_v f (C_s,T_s) + S\Delta XV_v \varepsilon_P \frac{\partial C_s}{\partial t} \qquad \text{(VI-3)}$$

and

$$S\Delta XS_v h_g (T-T_s) = S\Delta XV_v \Delta Hf (C_s,T_s) + S\Delta XV_v \rho_P z_P \frac{\partial T_s}{\partial t} \qquad \text{(VI-4)}$$

or in matrix notation:

$$\underline{W}\,(\underline{C}-\underline{C}_s) = \underline{B}_s\underline{f}\,(C_s,T_s) + \underline{G}_s\,\frac{\partial \underline{C}_s}{\partial t} \qquad \text{(VI-5)}$$

$$\underline{Z}\,(\underline{T}-\underline{T}_s) = \underline{P}_s\underline{f}\,(C_s,T_s) + \underline{Y}_s\,\frac{\partial \underline{T}_s}{\partial t} \qquad \text{(VI-6)}$$

Here, $\underline{W}$, $\underline{Z}$, $\underline{B}_s$, $\underline{P}_s$, $\underline{G}_s$, and $\underline{Y}_s$ are all diagonal matrices. The diagonal elements of $\underline{W}$ and $\underline{Z}$ are the catalyst surface areas in each reactor volume element multiplied by the mass or heat transfer coefficient.

The diagonal elements of $\underline{B}_s$ are the catalyst volumes in each reactor volume element. Again $\underline{P}_s = \Delta H \underline{B}_s$. $\underline{G}_s$ and $\underline{Y}_s$ are the transient catalyst capacity terms for the change of heat and mass within the catalyst particles.

Now, at each grid point there will be four simultaneous algebraic equations to solve for: C, T, C_s, and T_s. Again $\underline{A}$ and $\underline{U}$ are partitioned into $\underline{M} + \underline{N}$ and $\underline{Q} + \underline{R}$ as for the homogeneous case. The time derivatives in all equations are replaced by a first order finite difference approximation. In the external field equations, the terms describing diffusion from the external field to the catalyst surface may be averaged over the time step since these terms are linear.

Now, applying the forward sweep of the ADEP to all four matrix equations, there results:

$$\left(\underline{M} - \frac{\underline{G}}{\Delta t} - \frac{\underline{w}}{2}\right) \underline{C}^{(1)} = \left(-\underline{N} + \frac{\underline{G}}{\Delta t} + \frac{\underline{w}}{2}\right) \underline{C}^{(o)} - \frac{\underline{w}}{2} \underline{C}_s^{(1)} - \frac{\underline{w}}{2} \underline{C}_s^{(o)} + \underline{s} \qquad \text{(VI-7)}$$

$$\left(\underline{Q} - \frac{\underline{Y}}{\Delta t} - \frac{\underline{z}}{2}\right) \underline{T}^{(1)} = \left(-\underline{R} + \frac{\underline{Y}}{\Delta t} + \frac{\underline{z}}{2}\right) \underline{T}^{(o)} - \frac{\underline{z}}{2} \underline{T}_s^{(1)} - \frac{\underline{z}}{2} \underline{T}_s^{(o)} + \underline{v} \qquad \text{(VI-8)}$$

$$\underline{W}\, \underline{C}^{(1)} + \left(-\underline{w} - \frac{\underline{G}_s}{\Delta t}\right) \underline{C}_s^{(1)} = \frac{\underline{G}_s}{\Delta t} \underline{C}_s^{(o)} + \underline{B}_s \underline{f}\, (C_s, T_s)^{(1)} \qquad \text{(VI-9)}$$

$$\underline{Z}\,\underline{T}^{(1)} + \left[-\underline{z} - \frac{\underline{Y}_s}{\Delta t}\right] \underline{T}_s^{(1)} = \frac{\underline{Y}_s}{\Delta t}\,\underline{T}_s^{(o)} + \underline{P}_s\underline{f}\,(C_s, T_s)^{(1)} \qquad \text{(VI-10)}$$

Here it is noticed that the matrices $\left[\underline{M} - \frac{\underline{G}}{\Delta t} - \frac{\underline{W}}{2}\right]$ and $\left[\underline{Q} - \frac{\underline{Y}}{\Delta t} - \frac{\underline{z}}{2}\right]$ are lower triangular which allows the solution of each algebraic equation of (VI-7) and (VI-8) in a sequential manner.

Following the same type of procedure as for the homogeneous case, the first algebraic equation from each of the matrix equations (VI-7), (VI-8), (VI-9), and (VI-10), gives a set of four equations in four unknowns; $C_1^{(1)}$, $T_1^{(1)}$, $C_{s1}^{(1)}$, and $T_{s1}^{(1)}$. However it is seen that the first equation of (VI-7) is simply a linear relationship between $C_1^{(1)}$ and $C_{s1}^{(1)}$. Also, the first equation of (VI-8) is a linear relation between $T_1^{(1)}$ and $T_{s1}^{(1)}$. These relations may be substituted into the corresponding equations of (VI-9) and (VI-10), which now leaves two equations in two unknown variables $C_{s1}^{(1)}$ and $T_{s1}^{(1)}$. However, again by substituting for the rate expression in (VI-9) a linear relation can be found between $C_{s1}^{(1)}$ and $T_{s1}^{(1)}$. Using this relationship for $T_{s1}^{(1)}$ in the rate expression of the first equation (VI-9), all that remains is one nonlinear equation in one unknown variable, $C_{s1}^{(1)}$. This can be solved by the Newton-Raphson procedure in a few iterations. Then $T_{s1}^{(1)}$, $C_1^{(1)}$, and $T_1^{(1)}$ can be calculated by resubstitution of the calculated values into the appropriate equations.

Proceeding to the second grid point, corresponding to the second set of four algebraic equations, the only unknown variables here now are $C_2^{(1)}$, $T_2^{(1)}$, $C_{s2}^{(1)}$, and $T_{s2}^{(1)}$. These equations are solved in the same manner as those for the first grid point. This procedure is continued until the last grid point, (mxn), has been reached. Now, the entire concentration and temperature distribution, $\underline{C}^{(1)}$, $\underline{T}^{(1)}$, $\underline{C}_s^{(1)}$, and $\underline{T}_s^{(1)}$, at time $t_o + \Delta t$ is known.

To calculate the concentration and temperature distribution at the time level, $t_o + 2\Delta t$, the reverse sweep of the ADEP is used. The matrix equations to be solved now appear as follows:

$$\left(\underline{N} - \frac{\underline{G}}{\Delta t} - \frac{\underline{w}}{2}\right) \underline{C}^{(2)} = \left(-\underline{M} + \frac{\underline{G}}{\Delta t} + \frac{\underline{w}}{2}\right) \underline{C}^{(1)} - \frac{\underline{w}}{2} \underline{C}_s^{(2)} - \frac{\underline{w}}{2} \underline{C}_s^{(1)} + \underline{s} \qquad \text{(VI-11)}$$

$$\left(\underline{R} - \frac{\underline{Y}}{\Delta t} - \frac{\underline{z}}{2}\right) \underline{T}^{(2)} = \left(-\underline{Q} + \frac{\underline{Y}}{\Delta t} + \frac{\underline{z}}{2}\right) \underline{T}^{(1)} - \frac{\underline{z}}{2} \underline{T}_s^{(2)} - \frac{\underline{z}}{2} \underline{T}_s^{(1)} + \underline{v} \qquad \text{(VI-12)}$$

$$-\frac{\underline{G}_s}{\Delta t} \underline{C}_s^{(2)} = \left(\underline{w} + \frac{\underline{G}_s}{\Delta t}\right) \underline{C}_s^{(1)} - \underline{w}\, \underline{C}^{(1)} + \underline{B}_s \underline{f}\, (C_s, T_s)^{(2)} \qquad \text{(VI-13)}$$

$$-\frac{\underline{Y}_s}{\Delta t} \underline{T}_s^{(2)} = \left(\underline{z} + \frac{\underline{Y}_s}{\Delta t}\right) \underline{T}_s^{(1)} - \underline{z}\, \underline{T}^{(1)} + \underline{P}_s \underline{f}\, (C_s, T_s)^{(2)} \qquad \text{(VI-14)}$$

Here, the matrices, $\left(\underline{N} - \frac{G}{\Delta t} - \frac{W}{2}\right)$ and $\left(\underline{R} - \frac{Y}{\Delta t} - \frac{Z}{2}\right)$, are upper triangular matrices. Thus by beginning at the last grid point, (mxn), the set of equations may be solved sequentially ending up at the first grid point, using the same technique as was used in the forward sweep. This alternating procedure is then carried out until a steady-state condition is achieved. Using these steady-state values as initial conditions, a step change in the inlet condition may be implemented and the transient calculations continued until a new steady-state condition is reached.

DISCUSSION OF RESULTS:

It is of interest to compare the behavior of a packed bed reactor as predicted by the homogeneous model with that predicted by the surface resistance model. To demonstrate the difference, steady-state and transient conditions were computed for both models where the transport parameters in the external field were identical. The following case was calculated on an IBM 360/67 computer in conjunction with computer programs for each model written in FORTRAN IV. The transport parameters common to both models are:

N_{Pe_x}	= 2.0	N_{ST}	= 2.0
N_{Pe_r}	= 11.0	C_o	= .00001
$\rho_f z_f$	= .0547	T_o	= 800 ^oK
$\rho_P z_P$	= .0672	T_w	= 300 ^oK

The following two parameters will serve to define the additional transport constants for the surface resistance model.

$$N'_{STM} = .605 \qquad N'_{STH} = .895$$

The reaction rate is second order and of the following form: $r' = 10^{13} \exp\left(^{-12000}/_{T}\right) C^2$ with a heat of reaction, $\Delta H = -3.504 \times 10^5$.

The reactor length was taken as 100 r_o and the reactor diameter as 20 r_o.

Using the above parameters, the steady-state condition was calculated for each model. These are presented in Tables (10) and (11). It is seen that the homogeneous model predicts a conversion of 72.5 percent whereas the surface resistance model predicts a conversion of 45.3 percent. This very significant difference must be due to the resistance to heat and mass transfer between the catalyst and the external field. Referring to section (II) the parameters q_M and q_H may be calculated using the reactor inlet conditions. They are as follows:

$q_M = 3.7$ and $q_H = .20$

These coefficients indicate that there could be a 370 percent difference in concentration and a 20 percent difference in temperature between the external field and the catalyst. The parameter q_M is of primary importance here. If there is to be such a great difference in concentration, then the concentration in the catalyst will be quite low and the rate of reaction will be much lower than was used to calculate the above parameters. Effectively, q_H will be much lower than indicated above because it depends on the square of the catalyst concentration whereas q_M depends directly on the catalyst concentration. Therefore it might be reasonable to expect a difference in concentration between the external field and the catalyst of around 100 percent and a difference in temperature of approximately 2 percent.

The steady-state concentration of the external field and the catalyst particles along the reactor centre-line are given in Figure (10). It is seen that where there is a significant amount of reaction occurring in the first part of the reactor, there is a very wide concentration difference between the external field and the catalyst particle. As the fluid proceeds through

TABLE 10

HOMOGENEOUS MODEL

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

40.00 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.45529	0.45767	0.47435	0.59289	0.93592
1.00	0.14317	0.14778	0.18004	0.39150	0.80027
2.00	0.07491	0.08181	0.12723	0.36938	0.69058
3.00	0.05220	0.06207	0.12113	0.36864	0.60830
4.00	0.04434	0.05768	0.12962	0.36685	0.54658
5.00	0.04350	0.06054	0.14356	0.36181	0.49939
6.00	0.04700	0.06773	0.15922	0.35471	0.46248
7.00	0.05373	0.07787	0.17463	0.34680	0.43300
8.00	0.06311	0.09016	0.18879	0.33889	0.40903
9.00	0.07475	0.10393	0.20121	0.33142	0.38928
10.00	0.08825	0.11859	0.21185	0.32456	0.37282
11.00	0.10313	0.13358	0.22084	0.31838	0.35898
12.00	0.11880	0.14837	0.22840	0.31287	0.34726
13.00	0.13465	0.16255	0.23479	0.30798	0.33727
14.00	0.15013	0.17581	0.24022	0.30367	0.32874
15.00	0.16479	0.18797	0.24485	0.29989	0.32141
16.00	0.17833	0.19893	0.24884	0.29658	0.31510
17.00	0.19059	0.20870	0.25228	0.29369	0.30966
18.00	0.20153	0.21734	0.25525	0.29116	0.30496
19.00	0.21118	0.22491	0.25783	0.28897	0.30090
20.00	0.21964	0.23153	0.26007	0.28706	0.29738
21.00	0.22700	0.23729	0.26201	0.28541	0.29434
22.00	0.23340	0.24229	0.26370	0.28397	0.29170
23.00	0.23893	0.24661	0.26515	0.28272	0.28942
24.00	0.24357	0.25024	0.26637	0.28167	0.28750
25.00	0.24606	0.25219	0.26702	0.28110	0.28646

Bulk Concentration at Reactor Exit = 0.274676

TABLE 10 (Continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	834.52	833.76	828.69	792.79	471.65
1.00	852.26	849.25	831.26	736.84	332.01
2.00	852.01	845.53	812.26	681.48	319.24
3.00	845.98	835.38	787.37	636.04	316.27
4.00	836.09	821.31	760.62	599.21	314.42
5.00	823.09	804.49	733.74	569.01	312.94
6.00	807.57	785.74	707.59	543.86	311.71
7.00	790.11	765.71	682.60	522.55	310.68
8.00	771.21	744.94	658.98	504.24	309.79
9.00	751.33	723.83	636.79	488.27	309.02
10.00	730.90	702.74	616.00	474.19	308.34
11.00	710.25	681.92	596.57	461.65	307.74
12.00	689.68	661.57	578.40	450.37	307.19
13.00	669.42	641.84	561.41	440.17	306.70
14.00	649.65	622.84	545.51	430.86	306.26
15.00	630.51	604.64	530.63	422.34	305.85
16.00	612.09	587,27	516.68	414.49	305.47
17.00	594.47	570.75	503.61	407.25	305.13
18.00	577.68	555.07	491.37	400.54	304.80
19.00	561.72	540.24	479.88	394.31	304.51
20.00	546.60	526.23	469.12	388.52	304.23
21.00	532.32	513.03	459.05	383.13	303.97
22.00	518.88	500.62	449.62	378.11	303.73
23.00	506.30	489.03	440.86	373.47	303.51
24.00	494.99	478.62	433.01	369.33	303.31
25.00	488.76	472.89	428.69	367.05	303.20

Bulk Temperature at Reactor Exit = 382.63

TABLE 11

SURFACE RESISTANCE MODEL

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

40.00 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.87346	0.87444	0.87998	0.90604	0.98260
1.00	0.66696	0.67152	0.69598	0.79656	0.93709
2.00	0.52021	0.53076	0.58255	0.75611	0.89144
3.00	0.41839	0.43641	0.51737	0.73536	0.85176
4.00	0.35016	0.37609	0.48361	0.71756	0.81762
5.00	0.30699	0.34056	0.46974	0.70013	0.78777
6.00	0.28263	0.32306	0.46782	0.68355	0.76131
7.00	0.27254	0.31867	0.47235	0.66838	0.73772
8.00	0.27337	0.32375	0.47971	0.65487	0.71670
9.00	0.28260	0.33547	0.48783	0.64297	0.69799
10.00	0.29810	0.35157	0.49573	0.63255	0.68138
11.00	0.31797	0.37016	0.50303	0.62344	0.66667
12.00	0.34043	0.38972	0.50966	0.61548	0.65368
13.00	0.36387	0.40907	0.51565	0.60853	0.64222
14.00	0.38697	0.42743	0.52106	0.60247	0.63213
15.00	0.40877	0.44434	0.52595	0.59719	0.62326
16.00	0.42870	0.45959	0.53035	0.59260	0.61547
17.00	0.44653	0.47515	0.53430	0.58861	0.60965
18.00	0.46224	0.48505	0.53783	0.58515	0.60268
19.00	0.47593	0.49546	0.54097	0.58214	0.59747
20.00	0.48781	0.50452	0.54375	0.57954	0.59291
21.00	0.49806	0.51237	0.54619	0.57729	0.58894
22.00	0.50690	0.51918	0.54834	0.57534	0.58548
23.00	0.51449	0.52504	0.55022	0.57365	0.58247
24.00	0.52084	0.52995	0.55180	0.57223	0.57994
25.00	0.52423	0.53259	0.55265	0.57145	0.57856

Bulk Concentration at Reactor Exit = 0.[illegible]2823

TABLE 11 (Continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	807.67	807.01	802.72	773.06	470.98
1.00	818.77	815.80	798.59	712.45	330.89
2.00	823.66	817.04	783.95	659.83	318.20
3.00	822.85	811.92	763.50	617.35	315.37
4.00	817.06	801.78	740.23	583.15	313.64
5.00	807.09	787.87	715.99	555.20	312.27
6.00	793.77	771.24	691.85	531.94	311.14
7.00	777.88	752.75	668.46	512.20	310.18
8.00	760.09	733.10	646.16	495.19	309.36
9.00	740.99	712.82	625.09	480.30	308.64
10.00	721.09	692.35	605.29	467.13	308.00
11.00	700.81	672.02	586.72	455.34	307.43
12.00	680.50	652.09	569.32	444.71	306.92
13.00	660.46	632.75	553.01	435.06	306.46
14.00	640.90	614.11	537.72	426.22	306.04
15.00	621.99	596.27	523.39	418.11	305.65
16.00	603.83	579.26	509.94	410.62	305.29
17.00	586.49	563.10	497.32	403.69	304.96
18.00	569.99	547.77	485.47	397.25	304.65
19.00	554.33	533.28	474.35	391.26	304.36
20.00	539.51	519.59	463.91	385.67	304.09
21.00	525.50	506.67	454.11	380.46	303.84
22.00	512.28	494.50	444.91	375.58	303.61
23.00	499.87	483.08	436.31	371.05	303.39
24.00	488.65	472.76	428.56	366.96	303.20
25.00	482.34	466.97	424.21	364.68	303.09

Bulk Temperature at Reactor Exit = 379.75

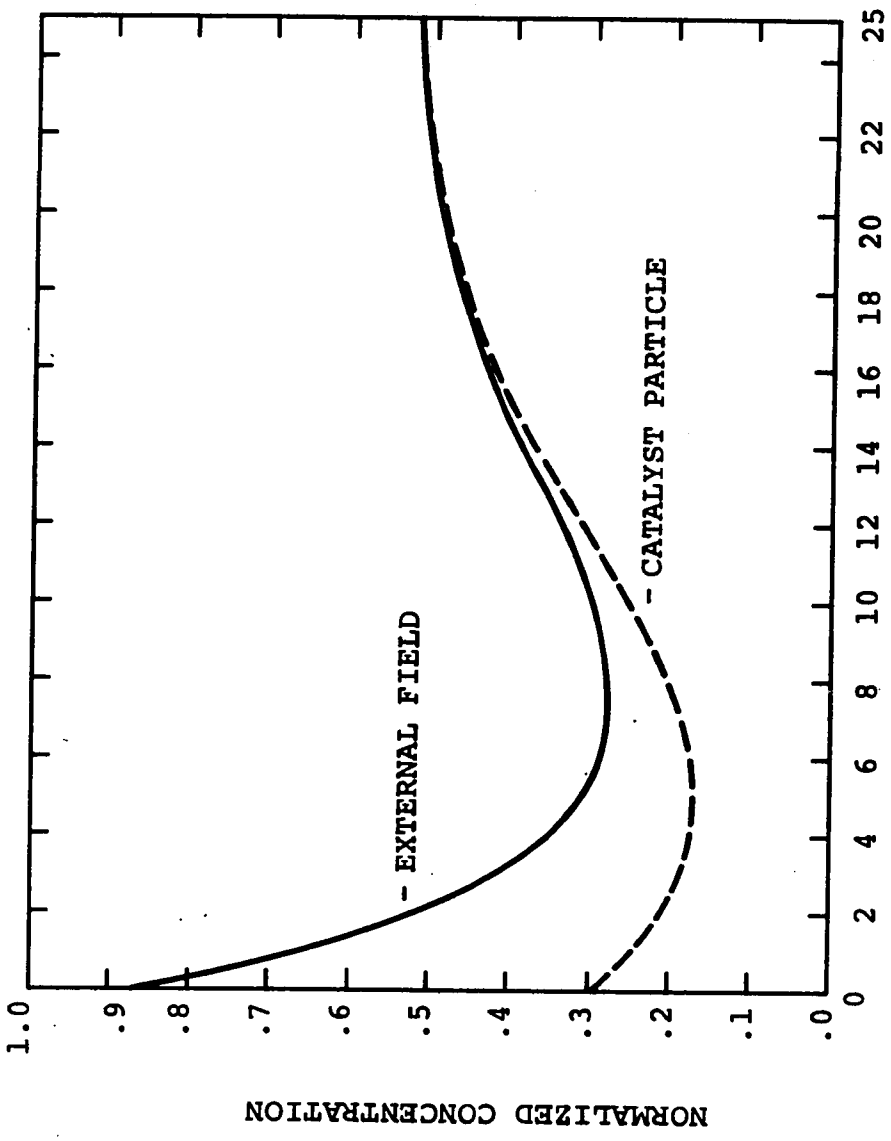


FIGURE 10 STEADY-STATE CONCENTRATION PROFILES ALONG REACTOR CENTRE-LINE

the reactor it is cooled by the wall temperature and the rate of reaction decreases causing less and less of a concentration difference across the catalyst surface. Again, it is noticed that the concentration along the centre-line increases in the latter stages of the reactor due to radial diffusion of reactant from the high concentration zone along the reactor wall. At no point in the reactor was the catalyst temperature more than $25^{o}K$ above the external field temperature, thus verifying earlier predictions. Because of the high resistance to mass transfer at the catalyst surface the reactant cannot flow freely into the catalyst. Much of it is carried through the reactor by convective flow to the exit, thereby reducing the conversion. Thus, in this case, if a reactor model neglected the resistance to transport at the catalyst surface it would predict a conversion which would be much higher than would actually be realized.

A step increase of five percent in the inlet temperature was implemented and the transient response of both models was followed. A detailed account of the transient response of the surface resistance model may be found in the appendix. The response of the outlet concentration and temperature for both models is given in Table (12) for purposes of comparison. The greatest difference is noted in the response of the outlet

temperature. In the homogeneous model, the heat wave travels through the reactor much more slowly than the fluid velocity because much of the heat is absorbed by the catalyst packing. It is not until after five seconds or two and one half reactor times have elapsed that the temperature begins to rise due to the inlet temperature increase and the higher rate of reaction. However in the surface resistance model there is a finite resistance to heat transfer between the external field and the catalyst particles. Thus as the fluid progresses through the reactor, some of the heat is absorbed by the catalyst, but this transfer is not instantaneous because of the resistance to heat transfer. Thus, the heat wave continues to move through the reactor at the same velocity as the fluid, although its size is being gradually diminished. This has the effect of smoothing out the heat wave as it passes through the reactor. Thus after one reactor residence time there will be a gradual increase in the outlet temperature as the leading edge of the heat front reaches the exit. The temperature will continue to increase as the heat wave gradually affects the exit condition. Both models show the outlet concentration beginning to decrease after approximately one reactor residence time.

TABLE 12

TRANSIENT RESPONSE OF REACTOR OUTLET

	SURFACE RESISTANCE		HOMOGENEOUS	
TIME (SEC.)	NORMALIZED CONCEN.	ABSOLUTE TEMP. (^{o}K)	NORMALIZED CONCEN.	ABSOLUTE TEMP. (^{o}K)
0.0	.563	379.8	.275	382.6
0.5	.563	379.7	.275	382.4
1.0	.563	379.7	.275	382.2
1.5	.563	379.7	.275	382.2
2.0	.560	379.8	.275	382.1
2.5	.548	380.3	.274	382.1
3.0	.528	381.4	.271	382.1
3.5	.509	382.8	.263	382.1
4.0	.498	384.2	.249	382.2
4.5	.492	385.2	.234	382.4
5.0	.490	385.9	.223	382.9
5.5	.489	386.2	.217	383.8
6.0	.489	386.4	.213	384.8
6.5	.489	386.4	.212	385.8
7.0			.211	386.7
7.5			.210	387.3
8.0			.210	387.7
8.5			.210	388.0

VII INTERNAL RESISTANCE MODEL OF REACTOR

This model of a packed bed reactor is a further extension of the surface resistance model to include those conditions where concentration and temperature gradients may be developed within the individual catalyst particles. The heat and mass transfer equations for the external field are the same as those for the surface resistance model, (II-1b) and (II-2b). The equations describing heat and mass transfer to the catalyst are as given in section II:

$$S_v k_g (C-C_s) + D_P S_v \left.\frac{\partial C_P}{\partial r}\right|_{r=r_o} = f(C_s,T_s)\Big|_{r=r_o} + \varepsilon_P \left.\frac{\partial C_s}{\partial t}\right|_{r=r_o} \qquad \text{(II-6c)}$$

$$S_v h_g (T-T_s) + K_P S_v \left.\frac{\partial T_P}{\partial r}\right|_{r=r_o} = \Delta Hf(C_s,T_s)\Big|_{r=r_o} + \rho_P z_P \left.\frac{\partial T_s}{\partial t}\right|_{r=r_o} \qquad \text{(II-7c)}$$

The equations describing heat and mass transfer within the catalyst particles were also given in section II:

$$D_P \left[\frac{\partial^2 C_P}{\partial r^2} + \frac{2}{r}\frac{\partial C_P}{\partial r}\right] = f(C_P,T_P) + \varepsilon_P \frac{\partial C_P}{\partial t} \qquad \text{(II-8)}$$

$$K_p \left[\frac{\partial^2 T_p}{\partial r^2} + \frac{2}{r}\frac{\partial T_p}{\partial r}\right] = \Delta Hf(C_p, T_p) + \rho_p z_p \frac{\partial T_p}{\partial t} \quad \text{(II-9)}$$

Equations (II-1b) and (II-2b) are finite differenced as in the surface resistance model, giving the two matrix equations:

$$\underline{A}\,\underline{C} = \underline{W}(\underline{C}-\underline{C_s}) + \underline{G}\frac{\partial \underline{C}}{\partial t} + \underline{s} \quad \text{(VI-1)}$$

$$\underline{U}\,\underline{T} = \underline{Z}(\underline{T}-\underline{T_s}) + \underline{Y}\frac{\partial \underline{T}}{\partial t} + \underline{v} \quad \text{(VI-2)}$$

Now, as shown in section IV, the catalyst particle is divided into ℓ volume increments. The finite difference analogue to equations (II-8) and (II-9) is given by applying a heat and mass balance about the outside volume increment. Referring to Figure (11), the mass balance becomes:

i) Mass in by diffusion = $4\pi r_o^2 k_g (C-C_s)$

ii) Mass out by diffusion = $-D_p 4\pi \left[\frac{r_o + r_1}{2}\right]^2 (C_{P1}-C_s)$

iii) Disappearance of mass due to reaction

$$= \frac{4}{3}\pi\left[r_o^3 - \left[\frac{r_o + r_1}{2}\right]^3\right] f(C_s, T_s)$$

iv) Transient accumulation = $\varepsilon_p \frac{4}{3}\pi\left[r_o^3 - \left[\frac{r_o + r_1}{2}\right]^3\right]$

$$\frac{\partial C_s}{\partial t}$$

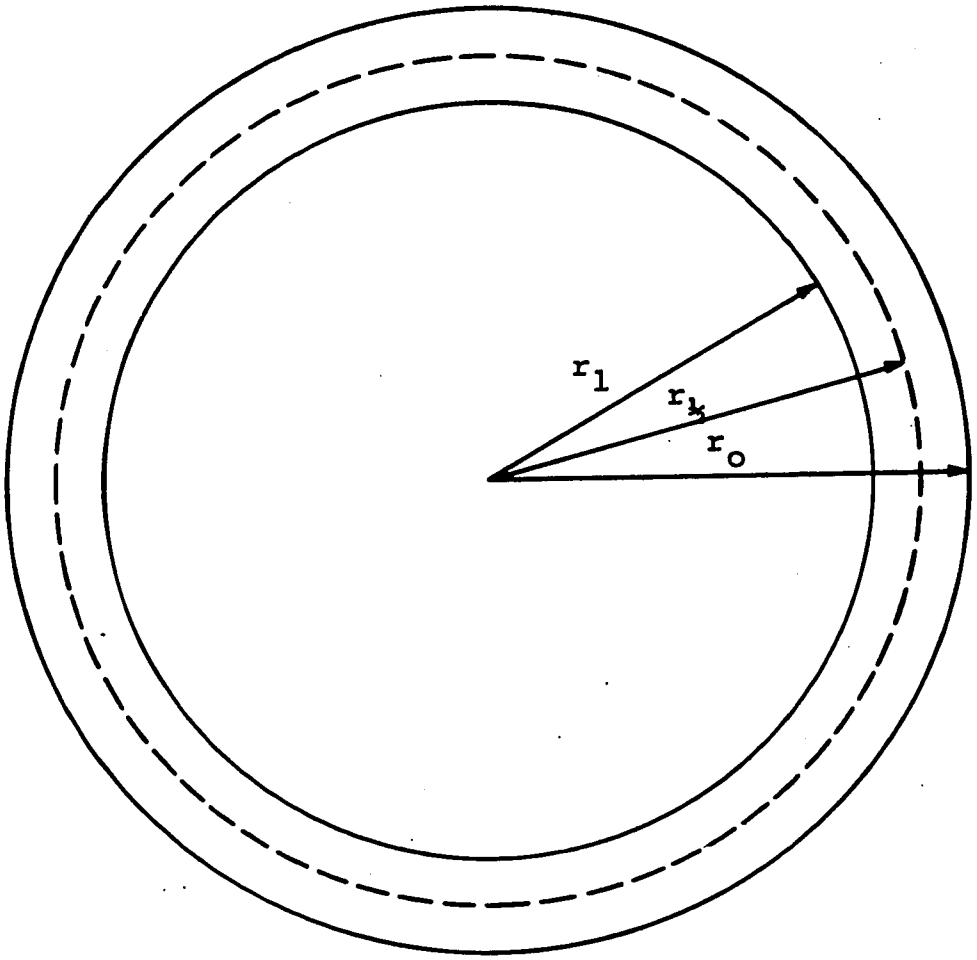


FIGURE 11 ELEMENTAL SHELL VOLUME NEXT TO CATALYST SURFACE

Substituting these terms into a transient mass balance and rearranging the terms yields

$$\{w(C-C_s) = a_s(C_s-C_{pl}) + b_s f(C_s,T_s) + g_s \frac{\partial C_s}{\partial t} \}_i \quad \text{(VII-1)}$$

Here the subscript, i, indicates that this equation is written for the i^{th} volume increment in the reactor. This type of equation applies to the surface conditions within each volume increment. For the heat balance on this outside catalyst volume increment, there results:

$$\{z(T-T_s) = u_s(T_s-T_{pl}) + p_s f(C_s,T_s) + y_s \frac{\partial T_s}{\partial t} \}_i \quad \text{(VII-2)}$$

In these equations:

$$a_s = D_p \pi (r_o + r_1)^2$$

$$u_s = K_p \pi (r_o + r_1)^2$$

$$b_s = \frac{4}{3} \pi \left[r_o^3 - \left(\frac{r_o + r_1}{2} \right)^3 \right]$$

$$p_s = \Delta H b_s$$

$$g_s = \epsilon_p b_s$$

$$y_s = \rho_p z_p b_s$$

Replacing the time derivative by a first order approximation, the forward sweep of the ADEP becomes at $t_o + \Delta t$:

$$\{ wC^{(1)} - \left[w + \frac{g_s}{\Delta t}\right] C_s^{(1)} = \left[a_s - \frac{g_s}{\Delta t}\right] C_s^{(o)} - a_s C_{Pl}^{(o)} + b_s f(C_s,T_s)^{(1)} \}_i \qquad \text{(VII-3)}$$

$$\{ zT^{(1)} - \left[z + \frac{y_s}{\Delta t}\right] T_s^{(1)} = \left[u_s - \frac{y_s}{\Delta t}\right] T_s^{(o)} - u_s T_{Pl}^{(o)} + p_s f(C_s,T_s)^{(1)} \}_i \qquad \text{(VII-4)}$$

The backward sweep of the ADEP becomes:

$$\{a_s C_{Pl}^{(2)} - \left[a_s - \frac{g_s}{\Delta t}\right] C_s^{(2)} = \left[w - \frac{g_s}{\Delta t}\right] C_s^{(1)} - wC^{(1)} + b_s f(C_s,T_s)^{(2)} \}_i \qquad \text{(VII-5)}$$

$$\{u_s T_{Pl}^{(2)} - \left[u_s - \frac{y_s}{\Delta t}\right] T_s^{(2)} = \left[z - \frac{y_s}{\Delta t}\right] T_s^{(1)} - zT^{(1)} + p_s f(C_s,T_s)^{(2)} \}_i \qquad \text{(VII-6)}$$

For the catalyst particle itself, mass and heat balances are written for each volume increment as shown in section IV, with the inclusion of transient capacity terms. In matrix notation these heat and mass balances for the catalyst in each reactor volume

element become:

$$\{\ \underline{A}_P\ \underline{C}_P = \underline{B}_P\ \underline{f}\ (C_P, T_P) + \underline{G}_P \frac{\partial \underline{C}_P}{\partial t} + \underline{s}'_P\ \}_i \qquad \text{(VII-7)}$$

$$\{\ \underline{U}_P\ \underline{T}_P = \underline{P}_P\ \underline{f}\ (C_P, T_P) + \underline{Y}_P \frac{\partial \underline{T}_P}{\partial t} + \underline{v}'_P\ \}_i \qquad \text{(VII-8)}$$

The column vectors $\underline{s}'_P$ and $\underline{v}'_P$ are not constant vectors. The first algebraic equation in each of the matrix equations, (VII-7) and (VII-8), represent a mass and heat balance about the catalyst volume increment closest to the surface. This balance includes diffusion and conduction from the surface increment of the catalyst, and the surface conditions are not constant. The elements of $\underline{s}'_P$ then are:

$$s'_{P1} = - D_P \pi\ (r_o + r_1)^2\ C_s$$

$$s'_{Pj} = 0,\ j = 2, \ldots, \ell$$

Similarly

$$v'_{P1} = - K_P \pi\ (r_o + r_1)^2\ T_s$$

$$v'_{Pj} = 0,\ j = 2, \ldots, \ell$$

The matrices $\underline{A}_P$ and $\underline{U}_P$ can be partitioned into two matrices respectively where $\underline{A}_P = \underline{M}_P + \underline{N}_P$ and $\underline{U}_P = \underline{Q}_P + \underline{R}_P$ according to the ADEP.

If the transient terms are replaced by a first order finite difference expression, the forward sweep of the ADEP time integration of the matrix equations becomes:

$$\{ \quad -\underline{s}'_P{}^{(1)} + \left[\underline{M}_P - \frac{\underline{G}_P}{\Delta t}\right] \underline{C}_P^{(1)} = \left[-\underline{N}_P + \frac{\underline{G}_P}{t}\right] \underline{C}_P^{(o)}$$

$$+ \underline{B}_P \underline{f} (C_P, T_P)^{(1)} \}_i \qquad \text{(VII-9)}$$

$$\{ \quad -\underline{v}'_P{}^{(1)} + \left[\underline{Q}_P - \frac{\underline{Y}_P}{\Delta t}\right] \underline{T}_P^{(1)} = \left[-\underline{R}_P + \frac{\underline{Y}_P}{\Delta t}\right] \underline{T}_P^{(o)}$$

$$+ \underline{P}_P f (C_P, T_P)^{(1)} \}_i \qquad \text{(VII-10)}$$

and the reverse sweep of the ADEP becomes:

$$\{ \quad \left[\underline{N}_P - \frac{\underline{G}_P}{\Delta t}\right] \underline{C}_P^{(2)} = \left[-\underline{M}_P + \frac{\underline{G}_P}{\Delta t}\right] \underline{C}_P^{(1)} + \underline{s}'_P{}^{(1)}$$

$$+ \underline{B}_P \underline{f} (C_P, T_P)^{(2)} \}_i \qquad \text{(VII-11)}$$

$$\{ \quad \left[\underline{R}_P - \frac{\underline{Y}_P}{\Delta t}\right] \underline{T}_P^{(2)} = \left[-\underline{Q}_P + \frac{\underline{Y}_P}{\Delta t}\right] \underline{T}_P^{(1)} + \underline{v}'_P{}^{(1)}$$

$$+ \underline{P}_P \underline{f} (C_P, T_P)^{(2)} \}_i \qquad \text{(VII-12)}$$

Now, choosing initial condition for $\underline{C}$, $\underline{T}$, $\underline{C}_s$, $\underline{T}_s$, $\{\underline{C}_P\}_i$, $\{\underline{T}_P\}_i$, the alternating direction explicit procedure can be used to integrate these equations in the time domain.

Beginning at the first grid point, the first algebraic equations of the matrix equations, (VI-5) and (VI-6), are solved simultaneously with equations, (VII-3) and (VII-4), written for that grid point. This will yield $T_1^{(1)}$, $C_1^{(1)}$, $T_{s1}^{(1)}$ and $C_{s1}^{(1)}$. Then the matrix equations, (VII-9) and (VII-10), are solved, beginning at the outside increment of the catalyst, for

$\{\underline{C}_p\}_i^{(1)}$ and $\{\underline{T}_p\}_i^{(1)}$. Then, proceeding to the second grid point in the reactor, the second algebraic equations of (VI-5) and (VI-6) are solved simultaneously with equations, (VII-3) and (VII-4), written at the second grid point. This will yield $C_2^{(1)}$, $T_2^{(1)}$, $C_{s2}^{(1)}$, and $T_{s2}^{(1)}$. Following this, the matrix equations, (VII-9) and (VII-10), are solved for $\{\underline{C}_p\}_2^{(1)}$ and $\{\underline{T}_p\}_2^{(1)}$. This procedure is continued until the conditions at $t_o + \Delta t$ have been calculated for every grid point in the reactor.

To solve for the reactor conditions at $t_o + 2\Delta t$, the reverse sweep of the ADEP is used. Beginning at the last grid point, (mxn), the matrix equations (VII-11) and (VII-12) are solved for $\{\underline{C}_p\}_{(mxn)}^{(2)}$ and $\{\underline{T}_p\}_{(mxn)}^{(2)}$. This computation is begun at the centre of the catalyst particle. Then the last algebraic equations of the matrix equations, (VI-9) and (VI-10), are solved simultaneously with equations, (VII-11) and (VII-12), written for the last grid point, (mxn). This will yield $C_{(mxn)}^{(2)}$, $T_{(mxn)}^{(2)}$, $C_{s(mxn)}^{(2)}$, $T_{s(mxn)}^{(2)}$. This procedure is continued at grid point (mxn-1) and onwards through the reactor, ending up at the first grid point, to give the reactor conditions at $t_o + 2\Delta t$.

The forward sweep of the ADEP is then repeated to calculate the conditions at $t_o + 3\Delta t$. This alternating procedure is carried out until an initial feasible steady-state condition is achieved. A step change in the inlet

conditions may then be introduced and the transient conditions may then be calculated by a continuation of this alternating procedure until a new steady-state is achieved.

This above procedure is very time consuming. For a reactor with 255 grid points, the time required on an IBM 360/67 computer to reach both the initial and final steady-states was between one and two hours. This was for a highly reactive case and computing times beyond this range are not expected.

Several factors have a direct effect on the computing time. They are the number of reactor grid points, the number of catalyst grid points, and the time step. If the course of some investigation should require several runs using the internal resistance model, some preliminary work should be done to determine the set of parameters which will give the required accuracy in the results.

The corresponding homogeneous reactor model could be run with different grid spacings to determine which minimum number of grid points is necessary in the reactor to yield an acceptable degree of accuracy. Then the catalyst particle model itself should be subjected to the same type of analysis to determine how many grid points are necessary to adequately represent the conditions within the catalyst.

It has been found that a time step of $\Delta t > \frac{\Delta X}{u}$ should not be used in calculating the reactor external field if accuracy in the transient results is to be maintained. However, this is not true in the computation of the transient conditions within the catalyst particles. In many cases the catalyst particles respond much more slowly to a change in boundary conditions than does the reactor. How much more slowly may be approximately determined by comparing the transient response of a single catalyst particle with that of the homogeneous model of the reactor. On the basis of this comparison it may be desirable to use a time step several times larger than the reactor time step, in the computation of the catalyst transient conditions.

Suppose it is decided that the time step for the catalyst particle is to be three times larger than the time step for the reactor external field. This innovation may be incorporated into the alternating direction scheme as follows:

i) $\underline{T}^{(o)}$, $\underline{C}^{(o)}$, $\underline{T}_s^{(o)}$, $\underline{C}_s^{(o)}$, $\{\underline{T}_p\}_i^{(o)}$ $\{\underline{C}_p\}_i^{(o)}$ are known.

ii) Compute $\underline{T}^{(1)}$, $\underline{C}^{(1)}$, $\underline{T}_s^{(1)}$ $\underline{C}_s^{(1)}$ using the forward sweep of the ADEP.

iii) Compute $\underline{T}^{(2)}$, $\underline{C}^{(2)}$, $\underline{T}_s^{(2)}$, $\underline{C}_s^{(2)}$ using the reverse sweep of the ADEP.

iv) Compute $\underline{T}^{(3)}$, $\underline{C}^{(3)}$, $\underline{T}_s^{(3)}$, $\underline{C}_s^{(3)}$, $\{\underline{T}_p\}_i^{(3)}$, $\{\underline{C}_p\}_i^{(3)}$ using the forward sweep of the ADEP.

v) Compute $\underline{T}^{(4)}$, $\underline{C}^{(4)}$, $\underline{T}_s^{(4)}$, $\underline{C}_s^{(4)}$, $\{\underline{T}_p\}_i^{(6)}$, $\{\underline{C}_p\}_i^{(6)}$ using the reverse sweep of the ADEP.

vi) Compute $\underline{T}^{(5)}$, $\underline{C}^{(5)}$, $\underline{T}_s^{(5)}$, $\underline{C}_s^{(5)}$ using the forward sweep of the ADEP.

vii) Compute $\underline{T}^{(6)}$, $\underline{C}^{(6)}$, $\underline{T}_s^{(6)}$, $\underline{C}_s^{(6)}$ using the reverse sweep of the ADEP.

Now, all conditions at $t_o + 6\Delta t$ are known.

This above sequence is then continued until steady-state is reached. The ratio of the catalyst particle time step to the reactor external field time step may be varied throughout a transient run. A smaller ratio would be used immediately after the step change in the inlet conditions and a larger one would be used as steady-state is approached.

DISCUSSION OF RESULTS:

As previously mentioned, the use of the internal resistance model is warranted in those cases where it is expected that the resistance to heat and mass transfer within the catalyst particle will play a significant role in determining the overall behavior of packed bed reactors. This may best be demonstrated by comparing the transient response of the surface resistance model and the internal resistance model with the same distur-

bance on the inlet conditions.

The following parameters will be used for this discussion:

N_{Pe_X}	=	2.0	N_1	=	705
N_{Pe_r}	=	8.2	N_2	=	1225
N_{ST}	=	2.0	N'_{Sh}	=	66.5
N'_{STH}	=	.895	N'_{Nu}	=	55.3
N'_{STM}	=	.605	T_w	=	300
C_o	=	.00001	T_o	=	600

These parameters characterizing transport in the external field and across the particle surface will be identical for both models. An additional set of parameters must be specified for the catalyst particles being considered in the internal resistance model. They are:

$$\beta = -0.6 \quad ; \quad \gamma = 20.0 \quad ; \quad \Psi = 0.5$$

Specifically, the form of the rate of reaction expression will be:

$$r' = 10^7 \exp\left(^{-12000}/_{T}\right) C$$

At this point it may be mentioned that these catalyst parameters yield multiple steady-state solutions within the catalyst particles. This has been

shown by McGuire and Lapidus, (14), to have an overriding effect upon the overall stability of this packed bed reactor. Applying the criteria established in section (II) it is seen that with $\beta = -0.6$, the temperature difference between the catalyst centre and surface may be as much as 60 percent of the absolute temperature at the catalyst surface. This would certainly indicate that the internal resistance model would best describe the reactor behavior.

Using the numerical techniques previously discussed, programs written in FORTRAN IV were run on an IBM 360/67 computer to calculate the reactor steady-state conditions corresponding to the above set of parameters for both models. The reactor was considered to be fifty particle diameters long and ten particle diameters wide. The steady-state concentration and temperature distributions in the external field are listed in Tables (13) and (14). It is seen that very little reaction is occurring and there is no appreciable difference between the steady-state conditions yielded by these models.

Next a step change corresponding to a five percent increase in temperature at the inlet was introduced and the transient response of both models was calculated until a new steady-state was achieved. A detailed account of the transient response of the internal resistance

TABLE 13

INTERNAL RESISTANCE MODEL

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

30.0 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.99923	0.99928	0.99946	0.99979	0.99996
1.00	0.99790	0.99813	0.99879	0.99960	0.99985
2.00	0.99706	0.99748	0.99851	0.99948	0.99974
3.00	0.99668	0.99722	0.99842	0.99936	0.99963
4.00	0.99665	0.99721	0.99840	0.99927	0.99952
5.00	0.99681	0.99834	0.99841	0.99918	0.99942
6.00	0.99706	0.99752	0.99845	0.99912	0.99933
7.00	0.99733	0.99771	0.99849	0.99906	0.99925
8.00	0.99758	0.99789	0.99853	0.99902	0.99919
9.00	0.99781	0.99805	0.99857	0.99899	0.99913
10.00	0.99799	0.99819	0.99861	0.99896	0.99908
11.00	0.99815	0.99831	0.99865	0.99894	0.99904
12.00	0.99828	0.99841	0.99868	0.99892	0.99901
13.00	0.99839	0.99849	0.99872	0.99891	0.99898
14.00	0.99848	0.99857	0.99874	0.99891	0.99897
15.00	0.99856	0.99863	0.99877	0.99891	0.99895
16.00	0.99863	0.99868	0.99880	0.99891	0.99895
17.00	0.99868	0.99873	0.99882	0.99891	0.99894
18.00	0.99873	0.99877	0.99884	0.99891	0.99894
19.00	0.99878	0.99881	0.99886	0.99892	0.99894
20.00	0.99882	0.99884	0.99889	0.99893	0.99895
21.00	0.99885	0.99887	0.99891	0.99894	0.99896
22.00	0.99889	0.99890	0.99893	0.99896	0.99897
23.00	0.99892	0.99893	0.99895	0.99897	0.99898
24.00	0.99895	0.99896	0.99897	0.99899	0.99899
25.00	0.99897	0.99898	0.99899	0.99900	0.99900

Bulk Concentration at Reactor Exit = 0.998994

TABLE 13 (Continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	599.85	599.24	595.77	575.64	404.27
1.00	598.11	595.46	582.20	527.43	320.91
2.00	593.42	587.94	564.16	490.50	312.69
3.00	585.67	577.30	544.85	462.82	310.46
4.00	575.29	564.48	525.84	441.53	309.04
5.00	562.94	550.31	507.84	424.66	307.95
6.00	549.31	535.50	491.11	410.96	307.06
7.00	534.97	520.54	475.70	399.55	306.33
8.00	520.41	505.80	461.56	389.88	305.71
9.00	505.98	491.52	448.62	381.54	305.17
10.00	491.92	477.85	436.76	374.25	304.71
11.00	478.40	464.90	425.89	367.80	304.30
12.00	465.54	452.69	415.92	362.05	303.93
13.00	453.38	441.25	406.77	356.88	303.60
14.00	441.96	430.56	398.36	352.21	303.31
15.00	431.27	420.61	390.62	347.97	303.04
16.00	421.30	411.37	383.50	344.11	302.79
17.00	412.02	402.79	376.95	340.58	302.57
18.00	403.41	394.84	370.91	337.34	302.36
19.00	395.42	387.48	365.34	334.38	302.18
20.00	388.02	380.67	360.21	331.66	302.00
21.00	381.16	374.38	355.48	329.15	301.84
22.00	374.83	368.56	351.12	326.85	301.70
23.00	368.99	363.20	347.11	324.73	301.57
24.00	363.79	358.44	343.54	322.85	301.45
25.00	360.90	355.78	341.56	321.81	301.38

Bulk Temperature at Reactor Exit = 326.81

TABLE 14

SURFACE RESISTANCE MODEL

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

30.00 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.99942	0.99945	0.99957	0.99981	0.99996
1.00	0.99840	0.99853	0.99898	0.99963	0.99985
2.00	0.99767	0.99795	0.99872	0.99952	0.99974
3.00	0.99729	0.99768	0.99862	0.99941	0.99963
4.00	0.99718	0.99762	0.99858	0.99932	0.99953
5.00	0.99726	0.99768	0.99858	0.99924	0.99944
6.00	0.99743	0.99781	0.99859	0.99917	0.99935
7.00	0.99763	0.99795	0.99861	0.99911	0.99927
8.00	0.99782	0.99809	0.99864	0.99906	0.99920
9.00	0.99800	0.99821	0.99866	0.99902	0.99914
10.00	0.99814	0.99831	0.99868	0.99898	0.99908
11.00	0.99827	0.99840	0.99870	0.99895	0.99904
12.00	0.99836	0.99847	0.99872	0.99892	0.99900
13.00	0.99844	0.99853	0.99873	0.99890	0.99896
14.00	0.99851	0.99858	0.99874	0.99888	0.99893
15.00	0.99856	0.99862	0.99875	0.99887	0.99891
16.00	0.99860	0.99865	0.99876	0.99885	0.99889
17.00	0.99864	0.99867	0.99876	0.99884	0.99887
18.00	0.99866	0.99869	0.99876	0.99883	0.99885
19.00	0.99868	0.99871	0.99877	0.99882	0.99884
20.00	0.99870	0.99872	0.99877	0.99881	0.99882
21.00	0.99871	0.99873	0.99877	0.99880	0.99881
22.00	0.99872	0.99874	0.99877	0.99879	0.99880
23.00	0.99873	0.99874	0.99876	0.99879	0.99879
24.00	0.99873	0.99874	0.99876	0.99878	0.99878
25.00	0.99873	0.99874	0.99876	0.99877	0.99878

Bulk Concentration at Reactor Exit = 0.998766

TABLE 14 (Continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	599.72	599.12	595.70	575.63	404.27
1.00	597.77	595.19	582.05	527.40	320.91
2.00	592.99	587.60	564.00	490.45	312.69
3.00	585.24	576.97	544.69	462.77	310.46
4.00	574.90	564.17	525.68	441.47	309.04
5.00	562.60	550.04	507.68	424.60	307.94
6.00	549.01	535.25	490.96	410.90	307.06
7.00	534.72	520.32	475.56	399.50	306.32
8.00	520.19	505.61	461.44	389.83	305.70
9.00	505.78	491.35	448.51	381.49	305.17
10.00	491.75	477.71	436.66	374.20	304.70
11.00	478.26	464.77	425.81	367.76	304.29
12.00	465.42	452.59	415.85	362.02	303.93
13.00	453.30	441.17	406.72	356.86	303.60
14.00	441.90	430.52	398.33	352.20	303.31
15.00	431.25	420.60	390.62	347.97	303.04
16.00	421.33	411.39	383.53	344.12	302.79
17.00	412.10	402.87	377.01	340.61	302.57
18.00	403.56	394.98	371.02	337.40	302.37
19.00	395.66	387.70	365.51	334.47	302.18
20.00	388.27	381.00	360.46	331.79	302.01
21.00	381.66	374.84	355.83	329.34	301.86
22.00	375.51	369.18	351.59	327.10	301.71
23.00	369.89	364.03	347.73	325.06	301.59
24.00	364.96	359.50	344.34	323.28	301.47
25.00	362.27	357.03	342.50	322.30	301.41

Bulk Temperature at Reactor Exit = 327.42

model may be found in the appendix; however the difference in the response of the two models can be seen by examining the outlet concentration and temperature throughout the transient run. These figures are presented in Table (15).

The surface resistance model indicated that the increase in the inlet temperature caused a slight increase in the rate of chemical reaction. However most of the increased heat of reaction passed across the small resistance at the catalyst surface and was quickly diffused toward the reactor wall. As a result, the new steady state was achieved very rapidly. The internal resistance model showed an entirely different behavior. During the first five seconds the outlet showed a slight increase in reactivity within the reactor. Then the outlet concentration began to fall sharply to a conversion of approximately fifty percent before gradually rising until a final steady-state conversion of 43.3 percent was achieved. Previously, the conversion had been only about 0.1 percent. During the transient response the outlet temperature rose from 325.3^{o}K to a high of 413.4^{o}K before settling out at a steady-state value of 403.5^{o}K. The new steady-state conditions are given in Table (16).

The reactor response given by the internal resistance model may be attributed to the inclusion of the

TABLE 15

TRANSIENT RESPONSE OF REACTOR OUTLET TO A 5% INCREASE IN THE INLET TEMPERATURE

	INTERNAL RESISTANCE		SURFACE RESISTANCE	
TIME (SEC.)	NORMALIZED CONCEN.	ABSOLUTE TEMP. (^{o}K)	NORMALIZED CONCEN.	ABSOLUTE TEMP.(^{o}K)
0.0	.999	326.8	.999	327.4
1.0	.999	327.6	.999	327.0
2.0	.999	328.0	.999	327.0
3.0	.998	328.7	.998	327.8
4.0	.998	329.2	.997	329.0
5.0	.990	330.1	.997	329.2
6.0	.957	332.7		
7.0	.886	339.3		
8.0	.786	350.4		
9.0	.679	365.4		
10.0	.586	381.2		
11.0	.530	395.0		
12.0	.503	405.1		
13.0	.497	411.0		
14.0	.501	413.4		
16.0	.521	412.3		
18.0	.539	406.4		
20.0	.550	405.1		
24.0	.561	404.5		
28.0	.565	403.9		
32.0	.567	403.6		
36.0	.567	403.5		
40.0	.568	403.5		

TABLE 16

INTERNAL RESISTANCE MODEL

FINAL STEADY STATE CONDITIONS

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.93936	0.94278	0.95546	0.99379	0.99812
1.00	0.79453	0.80689	0.86927	0.97627	0.99124
2.00	0.67012	0.69553	0.79249	0.95178	0.97893
3.00	0.56315	0.59927	0.72731	0.92307	0.96152
4.00	0.47776	0.52188	0.67350	0.89225	0.93992
5.00	0.41260	0.46236	0.63005	0.86085	0.91525
6.00	0.36444	0.41801	0.59567	0.82993	0.88860
7.00	0.32986	0.38592	0.56901	0.80020	0.86098
8.00	0.30595	0.36360	0.54883	0.77215	0.83320
9.00	0.29047	0.34912	0.53406	0.74606	0.80595
10.00	0.28176	0.34100	0.52378	0.72210	0.77971
11.00	0.27869	0.33821	0.51724	0.68084	0.73169
12.00	0.28050	0.34003	0.51384	0.68084	0.73169
13.00	0.28675	0.34599	0.51324	0.66357	0.71037
14.00	0.29726	0.35592	0.51573	0.64862	0.69104
15.00	0.31196	0.36965	0.52132	0.63598	0.67378
16.00	0.33042	0.38609	0.52554	0.62517	0.65854
17.00	0.35195	0.40433	0.52895	0.61583	0.64515
18.00	0.37580	0.42377	0.53209	0.60774	0.63342
19.00	0.40140	0.44433	0.53534	0.60079	0.62320
20.00	0.42808	0.46516	0.53888	0.59491	0.61433
21.00	0.45396	0.48292	0.54245	0.58999	0.60670
22.00	0.47528	0.49767	0.54585	0.58590	0.60018
23.00	0.49226	0.50981	0.54893	0.58252	0.59466
24.00	0.50548	0.51951	0.55158	0.57981	0.59012
25.00	0.51229	0.52457	0.55302	0.57839	0.58772

Bulk Concentration at Reactor Exit = 0.566475

TABLE 16 (Continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	668.58	665.70	653.70	606.94	414.89
1.00	758.00	747.20	693.03	564.23	323.80
2.00	831.39	809.19	721.27	537.28	315.59
3.00	890.27	858.00	740.21	521.74	314.05
4.00	932.34	892.08	751.51	512.94	313.41
5.00	959.03	912.82	756.41	507.76	313.05
6.00	973.00	922.57	755.96	504.25	312.81
7.00	976.95	923.65	751.04	501.22	312.62
8.00	973.16	917.97	742.41	497.98	312.42
9.00	963.39	907.00	730.73	494.17	312.18
10.00	948.94	891.85	716.57	489.61	311.90
11.00	930.73	873.32	700.42	484.27	311.57
12.00	909.39	851.97	682.68	478.17	311.20
13.00	885.31	828.17	663.61	471.37	310.78
14.00	858.69	802.13	643.06	463.89	310.32
15.00	829.68	774.01	621.11	455.79	309.82
16.00	798.64	744.60	600.64	447.44	309.30
17.00	766.07	714.53	581.33	439.07	308.77
18.00	732.52	684.25	562.89	430.83	308.26
19.00	698.41	653.85	545.08	422.76	307.75
20.00	664.20	623.90	527.83	414.89	307.26
21.00	631.16	596.58	511.32	407.26	306.78
22.00	601.68	571.85	495.68	399.91	306.31
23.00	575.70	549.54	481.04	392.92	305.87
24.00	553.37	530.02	467.88	386.53	305.47
25.00	541.15	519.26	460.51	382.92	305.24

Bulk Temperature at Reactor Exit = 403.63

transport properties of the catalyst particles within the reactor model. The initial temperature increase caused a higher rate of reaction inside the catalyst. However, the increased heat of reaction could not be conducted to the catalyst surface quickly enough and thus the temperature inside the catalyst continued to increase. The high mass diffusion coefficient within the catalyst allowed a rather liberal flow of reactant into the catalyst and a high reaction rate was maintained until finally the heat produced by the reaction equalled the rate at which it was being conducted from the catalyst. The heat released from the catalyst particle during this process is passed through the external field to those particles surrounding it and a sort of chain reaction is experienced on down through the reactor until there is not enough reactant to maintain a sufficiently high rate of reaction. It is noticed that the outlet condition overshoots its steady-state value and the conversion decreases slightly towards the end of the transient. This is due to the fact that initially the reactant concentration is very high throughout the whole reactor. This high concentration combines with the high temperatures which are produced to yield a very high degree of reactivity. As the reactor is gradually depleted of reactant the high rate of reaction cannot be sustained. This slight decrease in

reaction rate is indicated at the outlet by a decrease in conversion and a corresponding decrease in the outlet temperature.

The effect of the particle internal temperature gradients can be seen more clearly by following the transient response of the temperature in the external field, on the catalyst surface and at the centre of the catalyst for a selected grid point. Using the seventh grid point down the centre-line as an example; Figure (12) shows how these temperatures are affected by the step increase in the inlet temperature. This temperature increase is carried by convection down the reactor and within 1.0 seconds the external field temperature has increased by approximately five percent, carrying it even higher than the temperatures within the catalyst. This causes a higher rate of reaction and the temperature at the centre of the catalyst begins to gradually climb. Then after a time of 3.0 seconds, heat released by the now highly reactive particles in the area of the reactor closer to the entrance, reaches this grid point causing a sharp increase in the temperature of the external field. This additional heat is all that is required to move the catalyst to a highly reactive state. The temperature at the centre of the catalyst shoots up very rapidly until at a time of about 7.0 seconds there is a temperature difference between the

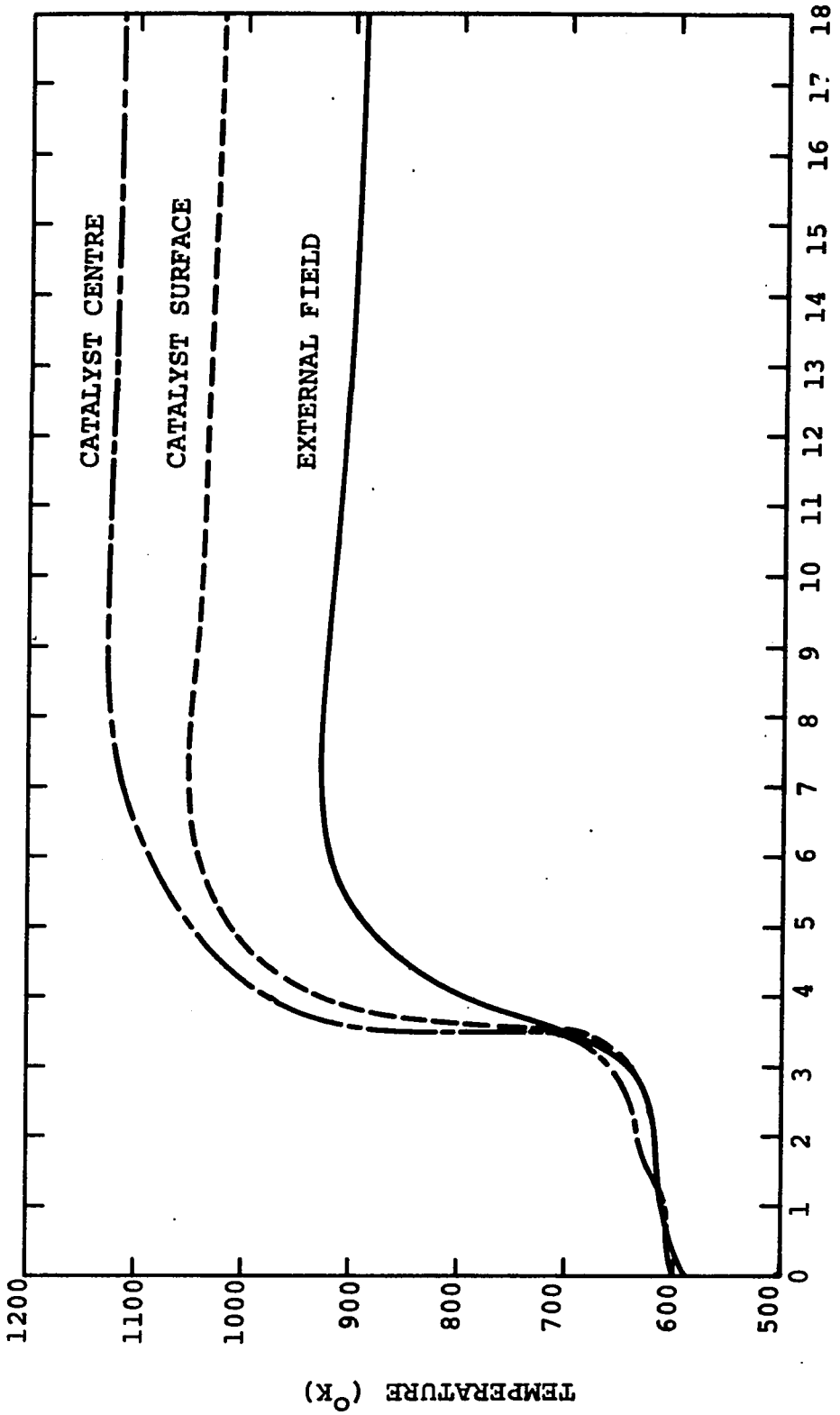


FIGURE 12 TRANSIENT RESPONSE OF TEMPERATURES 3.0 CM FROM ENTRANCE ALONG REACTOR CENTRE-LINE

external field and the catalyst centre of 200°K. From this point on the temperatures begin a very gradual decrease to their new steady-state values. This decrease in temperature before reaching steady-state is caused by a slightly decreased rate of reaction due to the lower reactant concentration now being carried by the external fluid into this area.

The delayed effect of the temperature increase on down the reactor may be seen by following the transient response of the external field temperature of the first and the eleventh grid points down the reactor centre-line. These temperatures are shown in Figure (13). It is seen that the convection mechanism carries the initial temperature increase to the latter grid point rather quickly. At the first grid point the temperature, affected by the high temperatures in the catalyst, begins to rise sharply at a time about 2.0 seconds after the step change was implemented. The temperature at the grid point 5.0 cm from the entrance doesn't begin to rise rapidly until after 4.0 seconds. This is a delay of 2.0 seconds between these two grid points where the convective flow requires only 0.5 seconds to traverse this distance. Thus it is seen that the transport resistance of the catalyst particles imposes a time delay on the system which is in addition to the delay caused by the

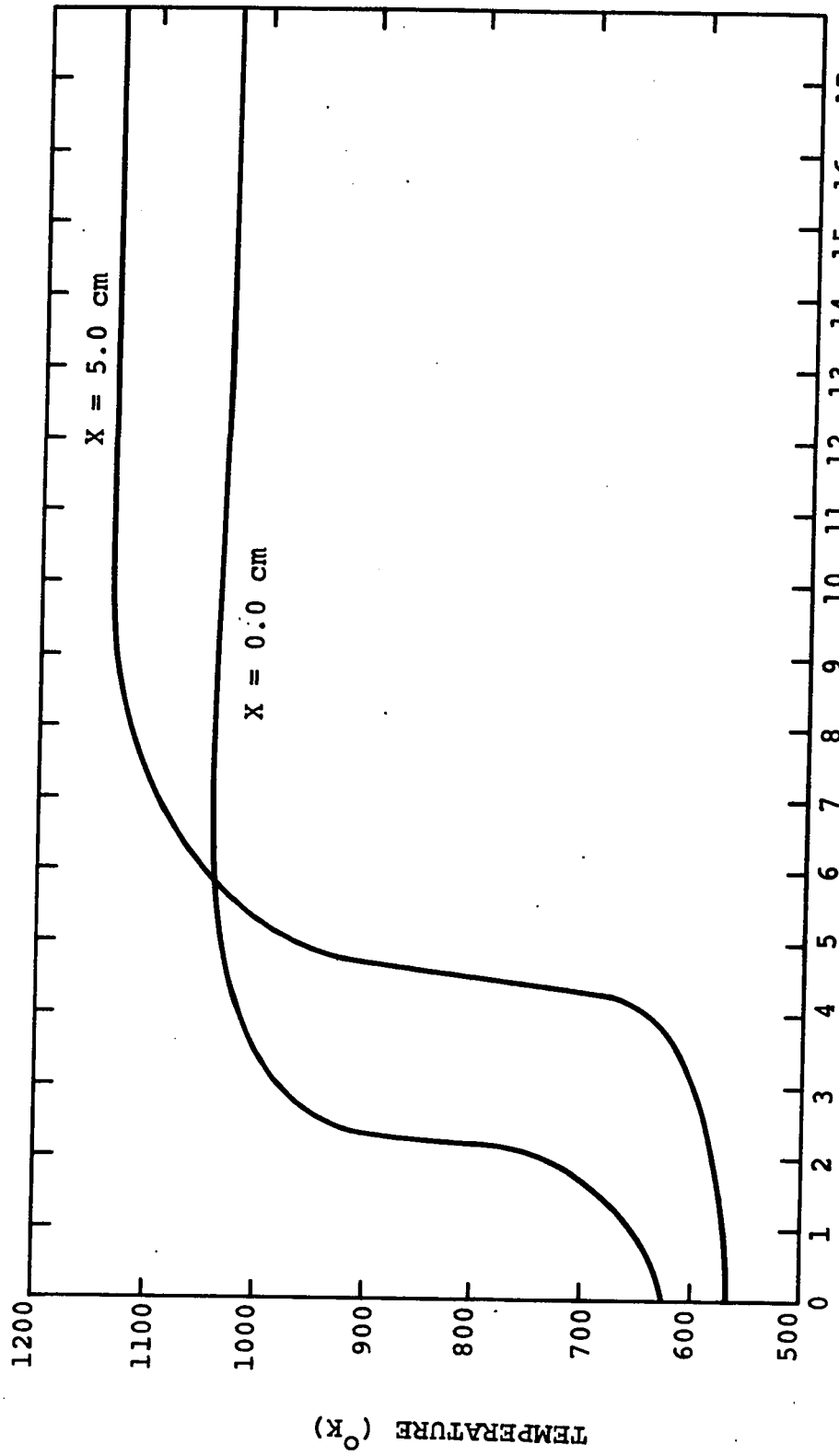
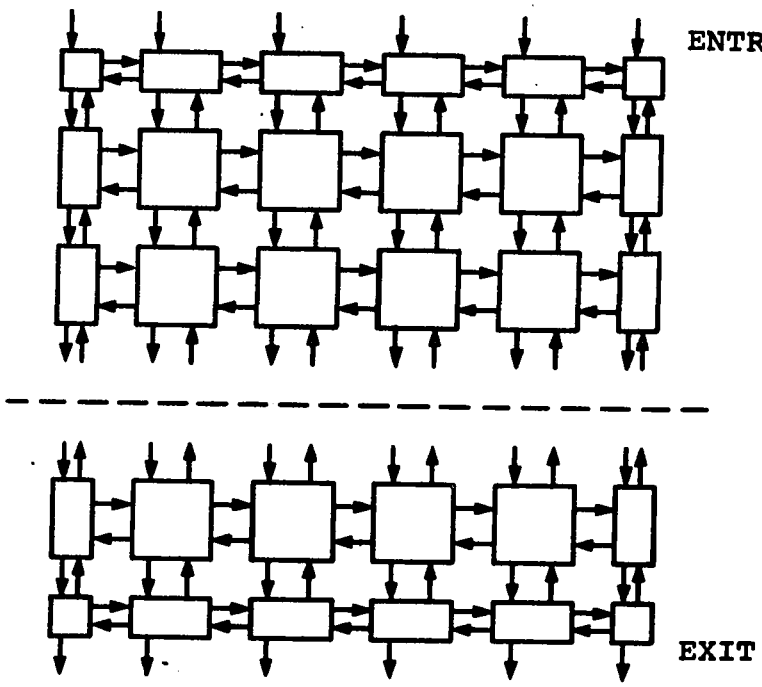


FIGURE 13 TRANSIENT RESPONSE OF TEMPERATURE AT CATALYST CENTRE AT SELECTED AXIAL POSITIONS ALONG CENTRE-LINE

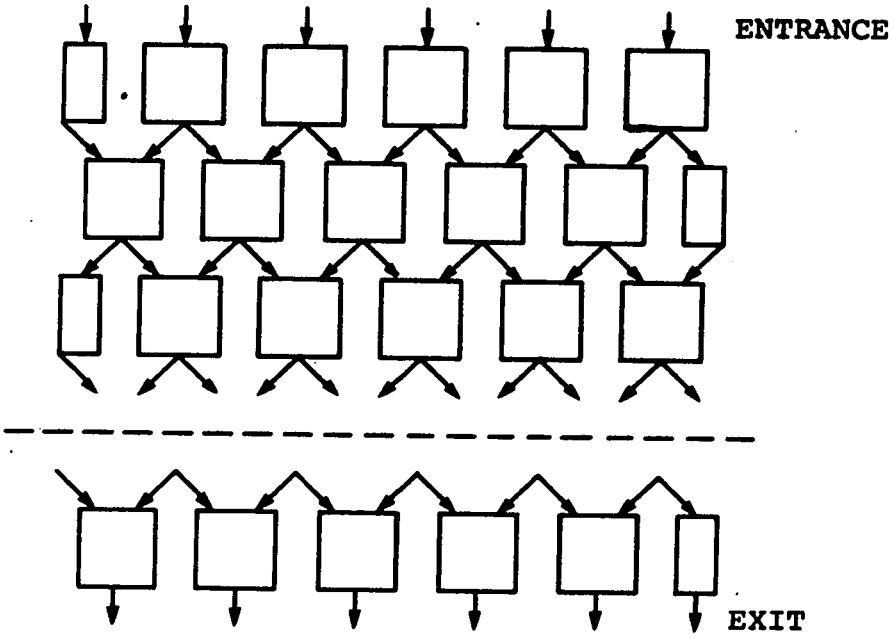
heat capacity of the bed and the convective flow. This is verified by examining the transient response of the outlet temperature in Table (15). The temperature doesn't begin to rise due to the increased reactivity until after 7.0 seconds which corresponds to three and one half reactor residence times.

In the internal resistance model, convection in the external field has been approximated by a backward difference formulation and the effective radial and axial diffusion is considered to depend directly on the temperature and concentration gradients according to Fick's first law of diffusion. A finite stage model presented by Deans and Lapidus,(14), considered radial and axial diffusion to be the result of the perfect mixing of a selected two dimensional array of continuous stirred tank reactors, each element in the array having the diameter of a catalyst particle. A diagramatic representation of these two models is shown in Figure (14). Mass and heat transfer can occur along any of the paths in the indicated directions. Using the finite stage model and the same set of transport parameters used here, McGuire and Lapidus, (14), have presented results for a five percent increase in the inlet temperature. Figure (15) shows the final steady-state external field temperature distribution along the reactor

FIGURE 14 REPRESENTATIONS OF TRANSPORT IN REACTOR EXTERNAL FIELD



i) CONVECTION WITH FICK'S DIFFUSION MODEL



ii) MIXING CELL MODEL

centre-line obtained from the finite stage model and the internal resistance model described here. It is seen that the temperature in the finite stage model initially is lower than in the internal resistance model. However it rises rapidly and reaches a hotspot of 1230^{o}K approximately 8.5 cm from the entrance. The internal resistance model predicts a hotspot of 975^{o}K about 7.0 cm from the entrance and then drops gradually to a temperature of 540^{o}K at the exit. The much higher temperatures in the finite stage model are to be expected. Due to the nature of the mixing cell concept, the effect of the cooling fluid cannot influence the centre-line temperature until a distance down the centre-line equal to the reactor diameter has been reached. The higher temperature in the first centimeter of the reactor predicted by the internal resistance model is due to the backward diffusion of heat from the hotspot in the reactor. This phenomena is not present in the finite stage model due to the initial value nature of the mixing cell approximation. Also it has been previously noted that there is a considerable concentration difference between the reactor wall and the reactor centre-line. Again, the finite stage model does not allow the radial diffusion of reactant to affect the centre-line conditions until a distance down the centre-line of one reactor diameter has been reached. Nor

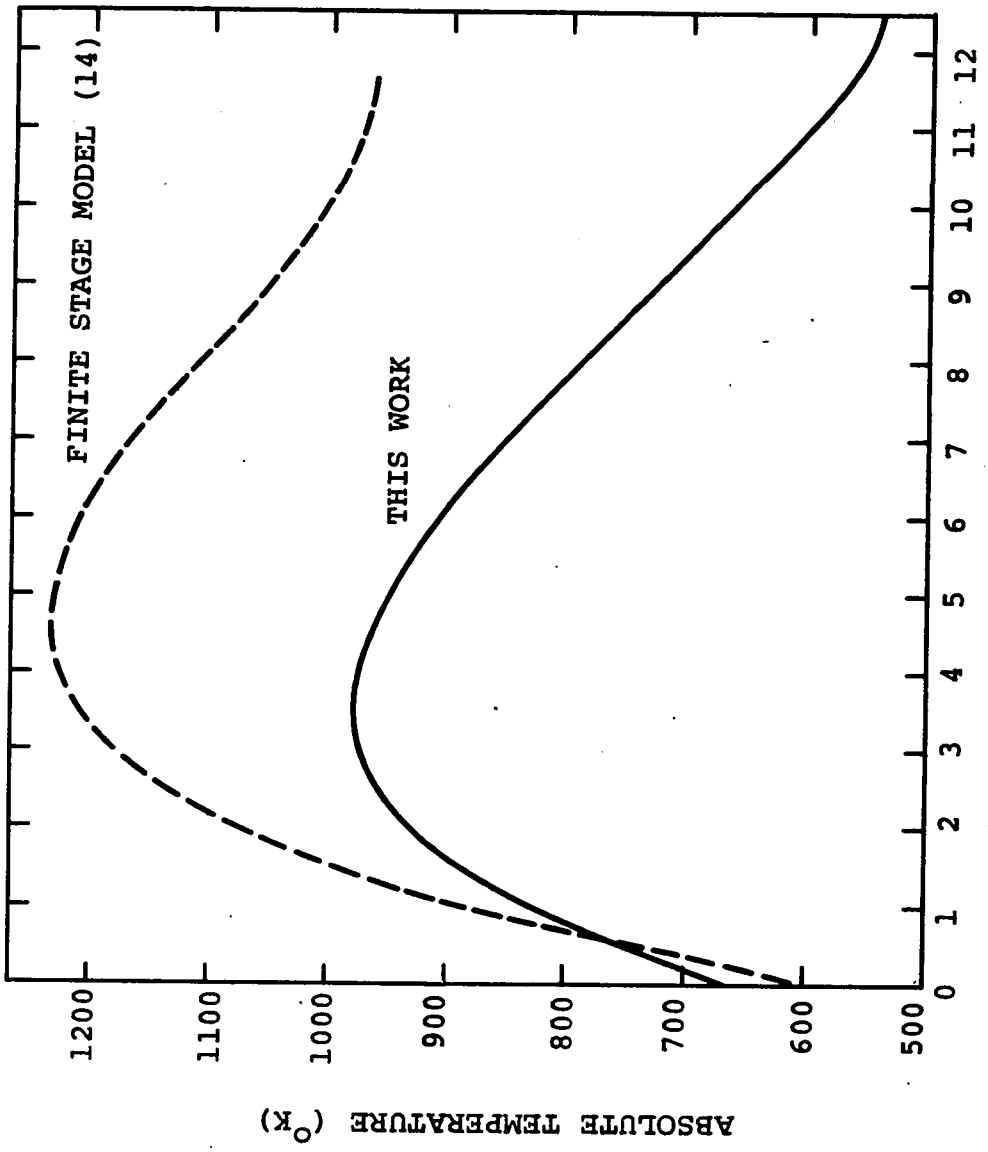


FIGURE 15 COMPARISON OF CENTRE-LINE TEMPERATURE AT STEADY-STATE WITH THAT GIVEN BY FINITE STAGE MODEL

will it allow the backward diffusion of reactant along a concentration gradient which is opposite to the direction of convective flow. Thus the finite stage model will indicate higher temperatures and lower concentrations along the reactor centre-line than would the internal resistance model. The combined effect of this on the overall conversion of a particular system is difficult to predict since the higher temperatures increase the rate of reaction, whereas the lower concentrations would decrease the rate of reaction.

Mathematical models of chemical reactors have been used primarily in design to study the stability of a reactor under the influence of an external disturbance upon the system. In the case presented above, a five percent increase in the inlet temperature was imposed on the reactor. If the inlet temperature were to be reduced to its original value and the reactor returns to its initial steady-state condition, then the reactor may be considered stable under this particular disturbance. This temperature reduction was carried out and the resulting steady-state condition is presented in Table (17). It is seen that the conversion has decreased from 43.3 percent to 27.7 percent but the reactor has not moved anywhere near the low reactive state where it originally started. This is due to the fact that the catalyst particles in the high reaction zone of the reactor maintained

TABLE 17

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.96158	0.96339	0.97084	0.99628	0.99884
1.00	0.87669	0.88521	0.91661	0.98514	0.99454
2.00	0.78548	0.80498	0.86933	0.96973	0.98680
3.00	0.69766	0.72977	0.82860	0.95168	0.97585
4.00	0.62099	0.66452	0.79381	0.93217	0.96223
5.00	0.55880	0.61145	0.76451	0.91205	0.94657
6.00	0.51119	0.57062	0.74033	0.89195	0.92952
7.00	0.47672	0.54093	0.72096	0.87238	0.91167
8.00	0.45362	0.52103	0.70610	0.85373	0.89357
9.00	0.44031	0.50970	0.69565	0.83637	0.87570
10.00	0.43565	0.50616	0.69024	0.82068	0.85852
11.00	0.43896	0.51001	0.69114	0.80708	0.84243
12.00	0.44935	0.51958	0.69123	0.79516	0.82763
13.00	0.46567	0.53331	0.69085	0.78453	0.81415
14.00	0.48680	0.55015	0.69078	0.77505	0.80191
15.00	0.51176	0.56946	0.69142	0.76667	0.79089
16.00	0.54000	0.59153	0.69308	0.75938	0.78104
17.00	0.58086	0.61546	0.69583	0.75318	0.77233
18.00	0.60159	0.63481	0.69902	0.74800	0.76473
19.00	0.62589	0.65070	0.70226	0.74371	0.75817
20.00	0.64464	0.66371	0.70532	0.74017	0.75255
21.00	0.65939	0.67434	0.70809	0.73726	0.74778
22.00	0.67115	0.68306	0.71054	0.73488	0.74376
23.00	0.68060	0.69019	0.71267	0.73293	0.74040
24.00	0.68808	0.69590	0.71443	0.73137	0.73767
25.00	0.69196	0.69889	0.71538	0.73057	0.73624

Bulk Concentration at Reactor Exit = 0.723535

TABLE 17 (Continued)

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	624.25	622.49	614.23	577.84	404.39
1.00	675.91	667.87	634.67	536.17	321.41
2.00	728.74	710.91	646.21	507.84	313.71
3.00	776.37	747.61	652.03	489.53	312.05
4.00	814.19	775.61	653.93	477.51	311.22
5.00	840.60	794.20	652.78	469.29	310.67
6.00	856.14	803.96	649.00	463.25	310.27
7.00	862.22	806.03	642.82	458.32	309.95
8.00	860.38	801.58	634.39	453.82	309.66
9.00	851.97	791.61	623.73	449.29	309.38
10.00	837.93	776.79	610.42	444.36	309.07
11.00	818.86	757.48	593.64	438.75	308.73
12.00	795.48	734.82	577.85	432.72	308.36
13.00	768.61	709.89	562.87	426.54	307.97
14.00	739.05	683.41	548.25	420.30	307.58
15.00	707.48	655.81	533.72	414.05	307.19
16.00	674.30	626.97	519.12	407.77	306.80
17.00	639.97	597.48	504.43	401.48	306.40
18.00	606.27	571.41	490.04	395.21	306.01
19.00	577.17	548.09	476.25	389.04	305.62
20.00	552.13	527.16	463.18	383.04	305.25
21.00	530.18	508.31	450.91	377.26	304.88
22.00	510.69	491.26	439.45	371.76	304.54
23.00	493.27	475.83	428.83	366.56	304.21
24.00	478.10	462.29	419.34	361.85	303.91
25.00	469.75	454.80	414.05	359.21	303.75

Bulk Temperature at Reactor Exit = 373.60

their high state of reaction even though their surface temperature dropped by approximately $30^{o}K$. Because the catalyst particles can exist at two steady-state conditions with the same boundary condition, the instability of the chemical reactor under this positive temperature perturbation is linked to the behavior of the catalyst. This same investigation was carried out in more depth by McGuire and Lapidus, (14), who discussed the effect of the size and time of duration of the external disturbance.

In this example, the parameters describing heat and mass transport in the external field are representative of turbulent flow in a packed bed reactor. The physical constants associated with these parameters are given in the Appendix. The parameters chosen to describe the catalyst were selected from a very narrow range which will yield multiple steady states. The heat of reaction of $\Delta H = -3.504 \times 10^{6}$ cal/gm-mole is far beyond the range of typical exothermic reactions. Influencing the choice of these parameters was the desire to examine the effect of a highly nonlinear temperature dependent rate of reaction, with possible multiple steady state conditions within the catalyst. However, in the majority of cases, a stability analysis is geared to the determination of the limits beyond which a boundary perturbation will cause the temperature to increase beyond an acceptable level in the reactor or catalyst.

VIII CONCLUSIONS

The partial differential equations describing heat and mass transfer within a packed bed chemical reactor can be finite differenced in both the spatial and time domains, and the resulting system of nonlinear algebraic equations can be solved by an alternating direction explicit procedure. Because of the nonlinear nature of these equations, the stability of this procedure cannot be guaranteed. However, if the criteria for stability in the corresponding linear problem are followed in the formulation of the nonlinear case, and if the nonlinear terms are computed at the most advanced time step, then the stability problem may be minimized. In the examples used to demonstrate the behavior of the three proposed models, no stability problems were encountered.

The alternating direction explicit procedure has proven to be an efficient tool in the numerical solution of nonlinear equations of this type. Integration in the time domain can be accomplished by solving sequentially a series of nonlinear algebraic equations even though the model has been formulated as a boundary value problem. Previously the problem had to be formulated as an initial value problem to allow this type of solution.

The three mathematical models of a packed bed reactor indicate the varying degrees of complexity by which this type of reactor may be represented. For a particular case, an examination of the parameters involved should dictate the choice of which model will best represent the reactor within a given degree of accuracy, and yet require the least computational effort.

The internal resistance model perhaps represents the greatest degree of sophistication in simulating the behavior of a packed bed reactor thus far. In many cases, the use of a model of this degree of complexity would not be warranted. In a particular investigation, the degree of certainty with which the diffusion parameters within the external field, across the surface film of the catalyst, and within the catalyst are known, may not be very high. Thus the use of rather uncertain parameters would negate the added precision that this detailed model affords. This field of parameter investigation may have to be updated before the internal resistance model can be used to full advantage.

In those cases where the conduction and diffusion parameters are well enough defined, the internal resistance model could be employed in the field of reactor design. Its substitution as a laboratory model would help to circumvent scale-up problems. The excessive computing time required in the use of this complex model eliminates it from use in the field of control. However,

if a simpler control model were postulated, the results of several simulation runs on the internal resistance model could be used to determine the appropriate control constants.

A comparison between the internal resistance model and a similar model using the mixing cell concept to simulate diffusion in the external field showed a difference in the predicted hotspot of the reactor of approximately 200^{o}K. This discrepancy was due to the different radial diffusion mechanisms assumed for each model. The sensitivity of this particular example to the radial transport of heat is indicated by the fact that a change in the radial Peclet number from 8.2 to 11.0 caused an increase in the hotspot of approximately 100^{o}K.

The most serious limitation on the use of these models is the assumption of a constant molar density. A constance density is a reasonable assumption only in the case of a liquid system or, in the case of gases where the reactor approaches isothermal operation. The inclusion of a temperature dependent density would necessitate the solution of three or more coupled nonlinear algebraic equations at each grid point since an additional momentum balance would have to be included. This could be avoided by computing the density at the previous time step; however this procedure may influence the numerical stability.

NOMENCLATURE

SCALARS:

A'	-	rate expression constant in exponential term $e^{-A'/T}$
A_o	-	reactor wall surface area
C	-	concentration of reactant in external field
C_p	-	reactant concentration inside the catalyst
C_s	-	reactant concentration on surface of catalyst
D_a	-	axial mass diffusion coefficient
D_r	-	radial mass diffusion coefficient
D_p	-	mass diffusion coefficient within catalyst
$f(C,T)$	-	rate of reaction expression
h_g	-	heat transfer coefficient between external field and catalyst
h_w	-	heat transfer coefficient at reactor wall
ΔH	-	heat of reaction
K_a	-	axial thermal conductivity coefficient
K_r	-	radial thermal conductivity coefficient
K_p	-	thermal conductivity within catalyst
k_g	-	mass transfer coefficient between external field and catalyst
k_o	-	constant in rate of reaction expression
L	-	reactor length
m	-	number of reactor radial grid points
n	-	number of reactor axial grid points
R	-	distance in radial direction of reactor

R_o - reactor radius

r - distance from centre of catalyst

r_o - catalyst radius

S_v - external surface area of catalyst per unit volume of reactor

T - temperature of external field

T_p - temperature within catalyst

T_s - temperature on catalyst surface

T_w - temperature at reactor wall

t - time

u - bulk linear velocity of fluid

V_v - volume of catalyst per unit volume of reactor

X - distance along axial direction of reactor

z_f - heat capacity of fluid

z_p - heat capacity of catalyst

GREEK LETTERS:

$$\alpha = \frac{-\Delta H A' C_o D_p}{K_p T_o^2} \text{ ; second order reaction}$$

$$\beta = \frac{-C_o \Delta H D_p}{K_p T_o}$$

$$\gamma = \frac{A'}{T_o}$$

$$\Psi = r_o \sqrt{\frac{K_o e^{-A'/T_o}}{D_p}} \text{ ; first order reaction}$$

$$\Psi = r_o \sqrt{\frac{K_o e^{-A'/T_o} C_o}{D_P}} \quad ; \quad \text{second order reaction}$$

$$\Psi = r_o \sqrt{\frac{k_o e^{-A'/T_o}}{D_P C_o}} \quad ; \quad \text{L-H reaction}$$

Δt, ΔX, ΔR, Δr - increments in t, X, R, and r respectively

ε_R - porosity of packed bed

ε_P - porosity of catalyst

η - catalyst effectiveness factor

$\rho(A)$ - spectral radius of matrix $\underline{A}$

ρ_f - density of fluid

ρ_P - density of catalyst

$$\Phi = r_o \sqrt{\frac{f(C,T)}{D_P C}}$$

ω = acceleration parameter

ω_b = optimum acceleration parameter

DIMENSIONLESS GROUPS:

$$N_1 = \frac{2 r_o u \rho_P z_P}{K_P}$$

$$N_2 = \frac{2 r_o u}{D_P}$$

$$N_{Pe_x} = \frac{2 r_o u}{D_a}$$

$$N_{Pe_r} = \frac{2 r_o u}{D_r}$$

$$N_{ST} = \frac{h_w}{u\ \rho_f\ z_f}$$

$$N'_{Nu} = \frac{2\ h_g\ r_o}{K_P}$$

$$N'_{Sh} = \frac{2\ k_g\ r_o}{D_P}$$

$$N'_{STM} = \frac{6\ k_g\ (1 - \varepsilon_R)}{u\ \varepsilon_R}$$

$$N'_{STH} = \frac{6\ h_g\ (1 - \varepsilon_R)}{u\rho_f\ z_f\ \varepsilon_R}$$

$$q_H = \frac{r_o\ \eta\ \Delta H\ f(C_s, T_s)}{3\ h_g\ T_s}$$

$$q_M = \frac{r_o\ \eta\ f(C_s, T_s)}{3\ k_g\ C_s}$$

SUBSCRIPTS:

a	-	axial direction
f	-	external fluid
i	-	i'th element of vector
i,j	-	i'th row and j'th column of matrix
o	-	value at boundary
P	-	catalyst particle
R	-	reactor packed bed
r	-	radial direction
s	-	surface of catalyst particle
w	-	reactor wall

SUPERSCRIPTS:

n	-	n'th iteration or time step
*	-	true solution of algebraic equations

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A P P E N D I X

APPENDIX A

COMPUTER PROGRAM FOR CATALYST PARTICLE:

This section illustrates the use of the computer program which calculates the steady-state concentration and temperature profiles and the effectiveness factor for various catalyst geometries, under a particular set of parameters. The program is coded in FORTRAN IV for an IBM 360/67 computer. Input data was entered on punched cards and the results were printed on an IBM high-speed printer.

The input variables are defined at the beginning of the program source listing. They must be punched on cards in the order given in this list. As an illustration of this procedure Table A-1 gives the input data which was used to produce the results given in this section.

Besides these input variables, a FORTRAN statement of the reaction rate expression must be included in the source program at the beginning of:

i) MAINLINE PROGRAM

ii) SUBROUTINE RETI

iii) SUBROUTINE ETARG

Also, a FORTRAN statement of the derivative of the rate expression with respect to concentration must be included at the beginning of SUBROUTINE RETI. In deriving

this expression it must be remembered that, at steady state, the temperature is a known linear function of concentration. The proper place for these statements is indicated in the source listing of the program. For the first order reaction used in this section the rate of reaction definition was given by:

```
F(CC,TT) = (1.0E+08)*EXP(-23844./(1.987*TT))*CC
```

and its derivative was given by:

```
FD(CC,TT) = (1.0E+08)*EXP(-23844./(1.987*TT))*(1.+
            CC*(23844./(1.987*(TT**2)))*(DH*D/TC))
```

where CC and TT are dummy variables referring to concentration and temperature respectively.

Table A-2 is the set of results given in computer output form for the input parameters of Table A-1.

TABLE A-1

INPUT DATA FOR STEADY-STATE CATALYST PROGRAM

INPUT CARD

```
          (TO)                 (CO)                 (D)
 1  bbbb.60000000E+03bbb.10000000E-02bbb.20900000E-02

          (TC)                 (DH)                 (RO)
 2  bbbb.50000000E-03bb-.86200000E+05bbb.10000000E+01

          (EL)                 (EK)
 3  bbbb.50000000E-05bbb.10000000E-02

          (OMS)    (OML)    (OMC)    (NIC)
 4  bbb1.7500bb1.7500bb1.7500bbbbb1

                   (RRE(I))
 5  b(1.0E+08)*EXP(-23844./(1.987*T))*C
```

TABLE A-2

RESULTS FROM PROGRAM FOR

STEADY-STATE CATALYST

SPHERICAL CATALYST PARTICLE 30 INCREMENTS

PHYSICAL , THERMODYNAMIC AND KINETIC DATA

ALL UNITS ARE IN CM.,SEC.,CAL.,GM.-MOLES,DEGREES KELVIN

PARTICLE RADIUS	1.000000
SURFACE CONCENTRATION	0.001000
SURFACE TEMPERATURE	600.000000
MASS DIFFUSIVITY	0.002090
THERMAL CONDUCTIVITY	0.000500
HEAT OF REACTION	-86200.000000
NO. OF INCREMENTS	30
SURFACE REACTION RATE	0.000206
AVERAGE REACTION RATE	0.000666
EFFECTIVENESS FACTOR	3.233084
ACCELERATION FACTOR	1.750000

RATE OF REACTION = (1.0E+08)*EXP(-23844./(1.987*T))*C

CATALYST STEADY STATE CONDITIONS

ITERATION NO. 77

RADIUS	NORMALIZED CONCENTRATION	ABSOLUTE TEMPERATURE
1.000	1.00000	600.00
1.000	0.99374	602.26
1.000	0.98747	604.51
1.000	0.97495	609.02
1.000	0.94991	618.05
0.999	0.89981	636.10
0.998	0.79970	672.17
0.996	0.60146	743.60
0.992	0.25036	870.11
0.984	0.01249	955.82
0.969	0.00006	960.30
0.938	0.00000	960.32
0.875	0.00000	960.32
0.750	0.00000	960.32
0.500	0.00000	960.32
0.0	0.00000	960.32

SLAB CATALYST PARTICLE 30 INCREMENTS

PHYSICAL , THERMODYNAMIC AND KINETIC DATA

ALL UNITS ARE IN CM.,SEC.,CAL.,GM.-MOLES,DEGREES KELVIN

PARTICLE RADIUS	1.000000
SURFACE CONCENTRATION	0.001000
SURFACE TEMPERATURE	600.000000
MASS DIFFUSIVITY	0.002090
THERMAL CONDUCTIVITY	0.000500
HEAT OF REACTION	-86200.000000
NO. OF INCREMENTS	30
SURFACE REACTION RATE	0.000206
AVERAGE REACTION RATE	0.000225
EFFECTIVENESS FACTOR	1.092734
ACCELERATION FACTOR	1.750000

RATE OF REACTION = (1.0E+08)*EXP(-23844./(1.987*T))*C

CATALYST STEADY STATE CONDITIONS

ITERATION NO. 49

RADIUS	NORMALIZED CONCENTRATION	ABSOLUTE TEMPERATURE
1.000	1.00000	600.00
1.000	0.99364	602.29
1.000	0.98727	604.59
1.000	0.97455	609.17
1.000	0.94910	618.34
0.999	0.89824	636.67
0.998	0.79676	673.23
0.996	0.59642	745.42
0.992	0.24465	872.16
0.984	0.01200	955.99
0.969	0.00005	960.30
0.938	0.00000	960.32
0.875	0.00000	960.32
0.750	0.00000	960.32
0.500	0.00000	960.32
0.0	0.00000	960.32

CYLINDRICAL CATALYST PARTICLE 30 INCREMENTS

PHYSICAL , THERMODYNAMIC AND KINETIC DATA

ALL UNITS ARE IN CM.,SEC.,CAL.,GM.-MOLES,DEGREES KELVIN

PARTICLE RADIUS	1.000000
SURFACE CONCENTRATION	0.001000
SURFACE TEMPERATURE	600.000000
MASS DIFFUSIVITY	0.002090
THERMAL CONDUCTIVITY	0.000500
HEAT OF REACTION	-86200.000000
NO. OF INCREMENTS	30
SURFACE REACTION RATE	0.000206
AVERAGE REACTION RATE	0.000447
EFFECTIVENESS FACTOR	2.170429
ACCELERATION FACTOR	1.750000

RATE OF REACTION = (1.0E+08)*EXP(-23844./(1.987*T))*C

CATALYST STEADY STATE CONDITIONS

ITERATION NO. 51

RADIUS	NORMALIZED CONCENTRATION	ABSOLUTE TEMPERATURE
1.000	1.00000	600.00
1.000	0.99369	602.27
1.000	0.98738	604.55
1.000	0.97475	609.10
1.000	0.94950	618.19
0.999	0.89902	636.38
0.998	0.79822	672.70
0.996	0.59893	744.51
0.992	0.24749	871.14
0.984	0.01224	955.90
0.969	0.00005	960.30
0.938	0.00000	960.32
0.875	0.00000	960.32
0.750	0.00000	960.32
0.500	0.00000	960.32
0.0	0.00000	960.32

A-3

PROGRAM FOR STEADY-STATE CATALYST

SOURCE LISTING

```
C          ***** DEFINITION OF INPUT VARIABLES *****
C
C
C     TO       INLET TEMPERATURE
C
C     CO       INLET CONCENTRATION
C
C     D        MASS DIFFUSIVITY INSIDE CATALYST
C
C     TC       CATALYST THERMAL CONDUCTIVITY
C
C     DH       HEAT OF REACTION
C
C     RO       CATALYST RADIUS
C
C     EL       RELATIVE ERROR IN CONCENTRATION BETWEEN SUC-
C              CEEDING ITERATIONS AT ASSUMED STEADY-STATE
C
C     EK       ABSOLUTE ERROR IN TEMPERATURE BETWEEN SUCCEED-
C              ING ITERATIONS AT ASSUMED STEADY-STATE
C
C     OMS      ACCELERATION FACTOR FOR SPHERICAL CASE
C
C     OML      ACCELERATION FACTOR FOR SLAB CASE
C
C     OMC      ACCELERATION FACTOR FOR CYLINDRICAL CASE
C
C     NIC      NO. OF COPIES OF RESULTS REQUIRED
C
C     RRE(I)   REACTION RATE EXPRESSION (NOT MORE THAN 72
C              CHARACTERS)
```

```
C      ***** PROGRAM FOR CATALYST EFFECTIVENESS FACTOR *****
C
C
C                    ***** MAINLINE PROGRAM *****
C
C      THIS MAINLINE CONTROLS THE COMPUTATIONS AND CALLS THE
C      NECESSARY SUBROUTINES . IT ALSO READS IN THE INPUT PAR-
C      AMETERS AND WRITES OUT THE RESULTS .
C
       COMMON R(60),B(60),C(60),S(60),T(60),X(60),WS(61),QR(
      161),SC(61),ST(61),TN(60),CN(60),SN(60),XN(60),RN(60),
      2CON(60),A1(60),A2(60),A3(60),A4(60),AVRR,RO,CO,TO,AO,
      3UO,D,TC,DH,OM,OMS,OML,OMC,L,LL,LK,NR,IC,N
       DIMENSION RRE(20)
C
C      THE FOLLOWING EXPRESSION DEFINES THE RATE OF REACTION
C
       F(CC,TT)=(1.0E+08)*EXP(-23844./(1.987*TT))*CC
C
C      READ IN THE INPUT PARAMETERS
C
       READ (5,10) TO,CO,D,TC,DH,RO,EL,EK
    10 FORMAT (1X,3E16.8/1X,3E16.8)
       READ (5,511) OMS,OML,OMC,NIC
   511 FORMAT (1X,3F8.4,I6)
       READ (5,901) (RRE(I),I=1,20)
   901 FORMAT (20A4)
       CNORM=1.0
       L=30
   400 CALL EREHPS
       GO TO 405
   401 CALL BALS
       GO TO 405
   402 CALL DNILYC
   405 IF (L.EQ.60) GO TO 710
       DO 40 J=1,L
       TN(J)=TC
       CN(J)=CO
       T(J)=TO
    40 C(J)=CO
       GO TO 720
   710 C(1)=(CO+CN(1))/2.
       DO 730 I=2,L,2
       K=I/2
   730 C(I)=CN(K)
       DO 740 I=3,LL,2
   740 C(I)=(C(I+1)+C(I-1))/2.
       DO 750 I=1,L
   750 T(I)=TO-(DH*D/TC)*(CO-C(I))
       DO 760 I=1,L
```

```
      CN(I)=C(I)
  760 TN(I)=T(I)
  720 N=0
   51 CALL RETI
  230 N=N+1
      DO 21 I=1,L
C
C     COMPARE THE SOLUTION AT THE (N+1)'TH ITERATION WITH
C     THE SOLUTION AT THE N'TH ITERATION
C
      IF (ABS((S(I)-CN(I))/CN(I)).GT.EL) GO TO 31
      IF (ABS(X(I)-TN(I)).GT.EK) GO TO 31
   21 CONTINUE
      GO TO 61
   31 DO 41 I=1,L
      T(I)=X(I)
      C(I)=S(I)
      TN(I)=X(I)
   41 CN(I)=S(I)
      GO TO 51
C
C     WRITE OUT THE RESULTS
C
   61 CONTINUE
      DO 3 JL=1,NIC
      IF (L.EQ.60) GO TO 64
      DO 92 I=1,L
      CON(I)=S(I)/CO
   92 CONTINUE
   54 WRITE (6,25) N
   25 FORMAT (1H1////' ',12X,'CATALYST STEADY STATE CONDITI'
     1,'ONS'/'-',12X,'ITERATION NO.',I6/'-',12X,'RADIUS',13X
     2,'NORMALIZED',13X,'ABSOLUTE'/' ',30X,'CONCENTRATION',
     310X,'TEMPERATURE'/'0')
      WRITE (6,81) RO,CNORM,TO
   81 FORMAT ('0',12X,F6.3,10X,F11.5,15X,F8.2)
      DO 74 I=2,L,2
   74 WRITE (6,81) R(I),CON(I),X(I)
      GO TO 3
   64 CONTINUE
      DO 5 I=1,L
      CON(I)=S(I)/CO
    5 CONTINUE
      WRITE (6,25) N
      WRITE (6,44) RO,CNORM,TO
   44 FORMAT (' ',12X,F6.3,10X,F11.5,15X,F8.2)
      DO 94 I=2,L,2
   94 WRITE (6,44) R(I),CON(I),X(I)
    3 CONTINUE
   84 RRS=F(CO,TO)
```

```
      CALL ETARG
      ETA=AVRR/RRS
      DO 4 JL=1,NIC
      IF (NR.NE.1) GO TO 601
      WRITE (6,602) L
  602 FORMAT (1H1////' ',12X,'SPHERICAL CATALYST PARTICLE',
     110X,I3,' INCREMENTS')
      GO TO 606
  601 IF (NR.NE.2) GO TO 603
      WRITE (6,604) L
  604 FORMAT (1H1////' ',12X,'SLAB CATALYST PARTICLE',10X,I3
     1,' INCREMENTS')
      GO TO 606
  603 WRITE (6,607) L
  607 FORMAT (1H1////' ',12X,'CYLINDRICAL CATALYST PARTICLE'
     1,10X,I3,' INCREMENTS')
  606 WRITE (6,16) RO,CO,TO,D,TC,DH,L,RRS,AVRR,ETA,OM
      WRITE (6,902) (RRE(I),I=1,20)
    4 CONTINUE
   16 FORMAT ('-',12X,'PHYSICAL , THERMODYNAMIC AND KINETIC'
     1,' DATA'/'-',12X,'ALL UNITS ARE IN CM.,SEC.,CAL.,GM.-'
     2,'MOLES,DEGREES KELVIN'/'-',12X,'PARTICLE RADIUS',25X,
     3F16.6/'0',12X,'SURFACE CONCENTRATION',19X,F16.6/'0',
     412X,'SURFACE TEMPERATURE',21X,F16.6/'0',12X,'MASS DIF'
     5,'FUSIVITY',24X,F16.6/'0',12X,'THERMAL CONDUCTIVITY',
     620X,F16.6/'0',12X,'HEAT OF REACTION',24X,F16.6/'-',12X
     7,'NO. OF INCREMENTS',23X,I9/'-',12X,'SURFACE REACTION'
     8,' RATE',19X,F16.6/'0',12X,'AVERAGE REACTION RATE',19X
     9,F16.6/'0',12X,'EFFECTIVENESS FACTOR',20X,F16.6/'0',
     112X,'ACCELERATION FACTOR',21X,F16.6)
  902 FORMAT ('-',12X,'RATE OF REACTION = ',20A4)
      IF (L.EQ.60) GO TO 700
      L=60
      IF (NR.EQ.1) GO TO 400
      IF (NR.EQ.2) GO TO 401
      GO TO 402
  700 L=30
      IF (NR.EQ.1) GO TO 401
      IF (NR.EQ.2) GO TO 402
      STOP
      END
```

```
C                ***** SUBROUTINE RETI *****
C
      SUBROUTINE RETI
C
C     THIS SUBROUTINE CALCULATES THE CONCENTRATION AND THE
C     TEMPERATURE PROFILES WITHIN THE CATALYST PARTICLE AT
C     THE (N+1)'TH ITERATION USING PSOR AS APPLIED TO NON-
C     LINEAR EQUATIONS
C
      COMMON R(60),B(60),C(60),S(60),T(60),X(60),WS(61),QR(
     161),SC(61),ST(61),TN(60),CN(60),SN(60),XN(60),RN(60),
     2CCN(60),A1(60),A2(60),A3(60),A4(60),AVRR,RO,CO,TO,AO,
     3UO,D,TC,DH,OM,OMS,OML,OMC,L,LL,LK,NR,IC,N
C
C     THE FOLLOWING EXPRESSIONS DEFINE THE RATE OF REACTION
C     AND IT'S DERIVATIVE WITH RESPECT TO CONCENTRATION
C
      F(CC,TT)=(1.0E+08)*EXP(-23844./(1.987*TT))*CC
      FS(CC,TT)=(1.0E+08)*(EXP(-23844./(1.987*TT)))*(1.+CC*
     1(23844./(1.987*(TT**2.))))*(DH*D/TC))
      S(1)=C(1)
      SN(1)=C(1)
      X(1)=T(1)
C
C     NEWTON RAPHSON ITERATION AT FIRST GRID POINT INSIDE
C     THE CATALYST
C
   40 FUN=-A3(1)*C(1)-A4(1)*C(2)+AO+A2(1)*S(1)-B(1)*F(S(1),
     1X(1))
      DER=-A2(1)+B(1)*FS(S(1),X(1))
      S(1)=S(1)+FUN/DER
      X(1)=TO-(DH*D/TC)*(CO-S(1))
      IF (ABS((S(1)-SN(1))/S(1)).GT.0.0005) GO TO 30
      GO TO 80
   30 SN(1)=S(1)
      GO TO 40
   80 DO 50 I=2,LL
      IF (N.GT.0) GO TO 404
      S(I)=S(I-1)
      SN(I)=S(I-1)
      X(I)=X(I-1)
      GO TO 110
  404 S(I)=C(I)
      SN(I)=C(I)
      X(I)=T(I)
C
C     NEWTON RAPHSON ITERATION AT INTERIOR GRID POINTS OF
C     THE CATALYST
C
  110 FUN=-A3(I)*C(I)-A4(I)*C(I+1)+A1(I)*S(I-1)+A2(I)*S(I)-
```

```
     1B(I)*F(S(I),X(I))
      DER=-A2(I)+B(I)*FS(S(I),X(I))
      S(I)=S(I)+FUN/DER
      IF (S(I).GT.(1.1*CO)) GO TO 85
      IF (S(I).LT.0.) GO TO 29
      X(I)=TO-(DH*D/TC)*(CO-S(I))
      IF (ABS((S(I)-SN(I))/S(I)).GT.0.0005) GO TO 90
      GO TO 50
   29 IJ=I
      DO 22 J=IJ,L
      S(J)=0.
      X(J)=TO-DH*D*CO/TC
   22 CONTINUE
      GO TO 99
   85 S(I)=0.
      X(I)=TO-DH*D*CO/TC
      SN(I)=S(I)
      GO TO 110
   90 SN(I)=S(I)
      GO TO 110
   50 CONTINUE
      IF (N.GT.0) GO TO 406
      S(L)=S(LL)
      SN(L)=S(LL)
      X(L)=X(LL)
      GO TO 70
  406 S(L)=C(L)
      SN(L)=C(L)
      X(L)=T(L)
C
C     NEWTON RAPHSON ITERATION AT THE GRID POINT IN THE
C     CENTRE OF THE CATALYST
C
   70 FUN=-A3(L)*C(L)+A1(L)*S(LL)+A2(L)*S(L)-B(L)*F(S(L),
     1X(L))
      DER=-A2(L)+B(L)*FS(S(L),X(L))
      S(L)=S(L)+FUN/DER
      IF (S(I).GT.(1.1*CO)) GO TO 75
      IF (S(L).LT.0.) GO TO 39
      X(L)=TO-(DH*D/TC)*(CO-S(L))
      IF (ABS((S(L)-SN(L))/S(L)).GT.0.0005) GO TO 60
      GO TO 99
   75 S(L)=0.
      X(L)=TO-DH*D*CO/TC
      SN(L)=S(L)
      GO TO 70
   39 S(L)=0.
      X(L)=TO-DH*D*CO/TC
      GO TO 99
   60 SN(L)=S(L)
```

```
      GO TO 70
   99 RETURN
      END
```

```
C                ***** SUBROUTINE ETARG *****
C
      SUBROUTINE ETARG
C
C     THIS SUBROUTINE COMPUTES THE AVERAGE RATE OF REACTION
C     WITHIN THE CATALYST USING A THIRD ORDER CORRECT INTE-
C     GRATING PROCEDURE
C
      COMMON R(60),B(60),C(60),S(60),T(60),X(60),WS(61),QR(
     161),SC(61),ST(61),TN(60),CN(60),SN(60),XN(60),RN(60),
     2CON(60),A1(60),A2(60),A3(60),A4(60),AVRR,RO,CO,TO,AO,
     3UO,D,TC,DH,OM,OMS,OML,OMC,L,LL,LK,NR,IC,N
C
C     THE FOLLOWING EXPRESSION DEFINES THE RATE OF REACTION
C
      F(CC,TT)=(1.0E+08)*EXP(-23844./(1.987*TT))*CC
      DOUBLE PRECISION W(61),SR(61),G(4,5),H(4,5),P(4,5),SS,Y
      AVRR=0.0
      SR(1)=DBLE(RO)
      SC(1)=CO
      ST(1)=TO
      IF (L.EQ.60) GO TO 700
      DO 701 I=2,7
      J=2*(I-1)
      SR(I)=DBLE(R(J))
      SC(I)=C(J)
  701 ST(I)=T(J)
      DO 702 I=8,25
      SR(I)=DBLE(R(I+5))
      SC(I)=C(I+5)
  702 ST(I)=T(I+5)
      NO=25
      GO TO 703
  700 DO 704 I=2,7
      J=4*(I-1)
      SR(I)=DBLE(R(J))
      SC(I)=C(J)
  704 ST(I)=T(J)
      DO 705 I=8,43
      SR(I)=DBLE(R(I+17))
      SC(I)=C(I+17)
  705 ST(I)=T(I+17)
      NO=43
C
C     COMPUTATION OF INTEGRATING COEFFICIENTS
C
  703 IL=0
  177 DO 166 I=1,4
      M=IL+I
      G(1,I)=1.0D+00
```

```
      G(2,I)=SR(M)
      G(3,I)=SR(M)**2.
  166 G(4,I)=SR(M)**3.
      G(1,5)=SR(IL+1)-SR(IL+4)
      G(2,5)=(SR(IL+1)**2.-SR(IL+4)**2.)/2.
      G(3,5)=(SR(IL+1)**3.-SR(IL+4)**3.)/3.
      G(4,5)=(SR(IL+1)**4.-SR(IL+4)**4.)/4.
      GO TO 111
  133 DO 134 I=1,3
      M=IL+I
      G(1,I)=1.0D+00
      G(2,I)=SR(M)
      G(3,I)=SR(M)**2.
  134 G(4,I)=SR(M)**3.
      G(1,4)=1.0D+00
      G(2,4)=0.0D+00
      G(3,4)=0.0D+00
      G(4,4)=0.0D+00
      G(1,5)=SR(IL+1)
      G(2,5)=(SR(IL+1)**2.)/2.
      G(3,5)=(SR(IL+1)**3.)/3.
      G(4,5)=(SR(IL+1)**4.)/4.
  111 M=4
      N=5
      MX=M-1
      DO 170 K=1,MX
      KK=K+1
      KL=K
      Y=G(K,K)
      DO 140 I=K,M
      IF (ABS(Y).GE.ABS(G(I,K))) GO TO 140
      Y=G(I,K)
      KL=I
  140 CONTINUE
      DO 150 J=K,N
      H(K,J)=G(KL,J)
  150 G(KL,J)=G(K,J)
      DO 160 J=K,N
  160 G(K,J)=H(K,J)
      DO 270 I=KK,M
      DO 270 J=K,N
  270 P(I,J)=G(I,J)-(G(K,J)*G(I,K))/G(K,K)
      DO 170 I=KK,M
      DO 170 J=K,N
  170 G(I,J)=P(I,J)
      W(M)=G(M,N)/G(M,M)
      DO 180 J=2,M
      MM=M-J+1
      JJ=J-1
      SS=0.0D+00
```

```
      DO 190 I=1,JJ
      NN=N-I
      SS=SS+G(MM,NN)*W(NN)
  190 CONTINUE
      W(MM)=(G(MM,N)-SS)/G(MM,MM)
  180 CONTINUE
      DO 909 I=1,4
      M=IL+I
      WS(I)=SNGL(W(I))
C
C     COMPUTATION OF AVERAGE REACTION RATE
C
  909 QR(M)=SNGL(SR(M))
      DO 181 I=1,4
      M=IL+I
      IF (NR.NE.1) GO TO 300
      IF (M.EQ.NO) GO TO 185
      AVRR=AVRR+WS(I)*F(SC(M),ST(M))*QR(M)**2.
      GO TO 181
  300 IF (NR.NE.2) GO TO 301
      AVRR=AVRR+WS(I)*F(SC(M),ST(M))
      GO TO 181
  301 AVRR=AVRR+WS(I)*F(SC(M),ST(M))*QR(M)
  181 CONTINUE
  185 IL=IL+3
      IF (IL.EQ.(NO-1)) GO TO 198
      IF (IL.EQ.(NO-4)) GO TO 133
      GO TO 177
  198 IF (NR.NE.1) GO TO 310
      AVRR=AVRR*3./RO**3.
      GO TO 199
  310 IF (NR.NE.2) GO TO 311
      AVRR=AVRR/RO
      GO TO 199
  311 AVRR=AVRR*2./RO**2.
  199 RETURN
      END
```

```
C                ***** SUBROUTINE EREHPS *****
C
      SUBROUTINE EREHPS
C
C     THIS SUBROUTINE CALCULATES THE COEFFICIENTS OF THE EQ
C     UATIONS DESCRIBING HEAT AND MASS TRANSFER WITHIN A
C     SPHERICAL CATALYST PARTICLE
C
      COMMON R(60),B(60),C(60),S(60),T(60),X(60),WS(61),QR(
     161),SC(61),ST(61),TN(60),CN(60),SN(60),XN(60),RN(60),
     2CON(60),A1(60),A2(60),A3(60),A4(60),AVRR,RO,CO,TO,AO,
     3UO,D,TC,DH,OM,OMS,OML,OMC,L,LL,LK,NR,IC,N
      IF (L.EQ.60) GO TO 22
      OM=OMS
   22 NR=1
      SL=L
      LL=L-1
      LK=L+1
      R(L)=0.
      IF (L.EQ.60) GO TO 20
   40 LJ=L-2
      DO 60 I=2,LJ,2
      KL=L-I
   60 R(KL)=(RO-R(KL+2))/2.+R(KL+2)
      DO 70 I=3,LL,2
   70 R(I)=(R(I+1)+R(I-1))/2.
      R(1)=(R(2)+RO)/2.
      GO TO 50
   20 DO 600 I=1,30
  600 RN(I)=R(I)
      R(1)=(RO+RN(1))/2.
      DO 601 I=2,L,2
      K=I/2
  601 R(I)=RN(K)
      DO 602 I=3,LL,2
  602 R(I)=(R(I+1)+R(I-1))/2.
   50 DP=-((D/4.)*((R(1)+R(2)))**2.)/(R(1)-R(2))
      DQ=-((D/4.)*((R(1)+RO))**2.)/(RO-R(1))
      A1(1)=0.
      A2(1)=DP+DQ
      A3(1)=(1.-OM)*(DP+DQ)
      A4(1)=OM*DP
      AO=-CO*OM*DQ
      B(1)=OM*(1./24.)*((R(1)+RO)**3.-(R(2)+R(1))**3.)
      DO 30 I=2,LL
      DP=-(D/4.)*((R(I)+R(I+1))**2.)/(R(I)-R(I+1))
      DQ=-(D/4.)*((R(I)+R(I-1))**2.)/(R(I-1)-R(I))
      A2(I)=DP+DQ
      A1(I)=-OM*DQ
      A3(I)=(1.-OM)*(DP+DQ)
```

```
      A4(I)=OM*DP
   30 B(I)=OM*(1./24.)*((R(I)+R(I-1))**3.-(R(I+1)+R(I))**3.)
      DP=-(D/4.)*R(LL)
      A2(L)=DP
      A1(L)=-OM*DP
      A3(L)=(1.-OM)*DP
      A4(L)=0.
      B(L)=OM*(1./24.)*R(LL)**3.
      RETURN
      END
```

```
C                ***** SUBROUTINE BALS *****
C
      SUBROUTINE BALS
C
C     THIS SUBROUTINE CALCULATES THE COEFFICIENTS OF THE EQ
C     UATIONS DESCRIBING HEAT AND MASS TRANSFER WITHIN A
C     SLAB CATALYST PARTICLE
C
      COMMON R(60),B(60),C(60),S(60),T(60),X(60),WS(61),QR(
     161),SC(61),ST(61),TN(60),CN(60),SN(60),XN(60),RN(60),
     2CON(60),A1(60),A2(60),A3(60),A4(60),AVRR,RO,CO,TO,AO,
     3UO,D,TC,DH,OM,OMS,OML,OMC,L,LL,LK,NR,IC,N
      IF (L.EQ.60) GO TO 22
      OM=OML
   22 NR=2
      SL=L
      LL=L-1
      LK=L+1
      R(L)=0.
      IF (L.EQ.60) GO TO 20
   40 LJ=L-2
      DO 60 I=2,LJ,2
      KL=L-I
   60 R(KL)=(RO-R(KL+2))/2.+R(KL+2)
      DO 70 I=3,LL,2
   70 R(I)=(R(I+1)+R(I-1))/2.
      R(1)=(R(2)+RO)/2.
      GO TO 50
   20 DO 600 I=1,30
  600 RN(I)=R(I)
      R(1)=(RO+RN(1))/2.
      DO 601 I=2,L,2
      K=I/2
  601 R(I)=RN(K)
      DO 602 I=3,LL,2
  602 R(I)=(R(I+1)+R(I-1))/2.
   50 DP=-D/(R(1)-R(2))
      DQ=-D/(RO-R(1))
      A1(1)=0.
      A2(1)=DP+DQ
      A3(1)=(1.-OM)*(DP+DQ)
      A4(1)=OM*DP
      AO=-CO*OM*DQ
      B(1)=OM*((RO+R(1))/2.-(R(1)+R(2))/2.)
      DO 30 I=2,LL
      DP=-D/(R(I)-R(I+1))
      DQ=-D/(R(I-1)-R(I))
      A2(I)=DP+DQ
      A1(I)=-OM*DQ
      A3(I)=(1.-OM)*(DP+DQ)
```

```
      A4(I)=OM*DP
   30 B(I)=OM*((R(I-1)+R(I))/2.-(R(I)+R(I+1))/2.)
      DP=-D/R(LL)
      A2(L)=DP
      A1(L)=-CM*DP
      A3(L)=(1.-OM)*DP
      A4(L)=0.
      B(L)=OM*R(LL)/2.
      RETURN
      END
```

```
C                ***** SUBROUTINE DNYLIC *****
C
      SUBROUTINE DNILYC
C
C     THIS SUBROUTINE CALCULATES THE COEFFICIENTS OF THE EQ
C     UATIONS DESCRIBING HEAT AND MASS TRANSFER WITHIN A
C     CYLINDRICAL CATALYST PARTICLE
C
      COMMON R(60),B(60),C(60),S(60),T(60),X(60),WS(61),QR(
     161),SC(61),ST(61),TN(60),CN(60),SN(60),XN(60),RN(60),
     2CON(60),A1(60),A2(60),A3(60),A4(60),AVRR,RO,CO,TO,AO,
     3UO,D,TC,DH,OM,OMS,OML,OMC,L,LL,LK,NR,IC,N
      IF (L.EQ.60) GO TO 22
      OM=OMC
   22 NR=3
      SL=L
      LL=L-1
      LK=L+1
      R(L)=0.
      IF (L.EQ.60) GO TO 20
   40 LJ=L-2
      DO 60 I=2,LJ,2
      KL=L-I
   60 R(KL)=(RO-R(KL+2))/2.+R(KL+2)
      DO 70 I=3,LL,2
   70 R(I)=(R(I+1)+R(I-1))/2.
      R(1)=(R(2)+RO)/2.
      GO TO 50
   20 DO 600 I=1,30
  600 RN(I)=R(I)
      R(1)=(RO+RN(1))/2.
      DO 601 I=2,L,2
      K=I/2
  601 R(I)=RN(K)
      DO 602 I=3,LL,2
  602 R(I)=(R(I+1)+R(I-1))/2.
   50 DP=-D*(R(1)+R(2))/(R(1)-R(2))
      DQ=-D*(R(1)+RO)/(RO-R(1))
      A1(1)=0.
      A2(1)=DP+DQ
      A3(1)=(1.-OM)*(DP+DQ)
      A4(1)=OM*DP
      AO=-CO*CM*DQ
      B(1)=OM*(1./4.)*((RO+R(1))**2.-(R(1)+R(2))**2.)
      DO 30 I=2,LL
      DP=-D*(R(I)+R(I+1))/(R(I)-R(I+1))
      DQ=-D*(R(I)+R(I-1))/(R(I-1)-R(I))
      A2(I)=DP+DQ
      A1(I)=-CM*DQ
      A3(I)=(1.-OM)*(DP+DQ)
```

```
      A4(I)=OM*DP
   30 B(I)=OM*(1./4.)*((R(I)+R(I-1))**2.-(R(I)+R(I+1))**2.)
      DP=-D
      A2(L)=DP
      A1(L)=-OM*DP
      A3(L)=(1.-OM)*DP
      A4(L)=0.
      B(L)=OM*(1./4.)*R(LL)**2.
      RETURN
      END
```

APPENDIX B

COMPUTER PROGRAM FOR HOMOGENEOUS MODEL OF A PACKED-BED REACTOR:

This section illustrates the use of the computer program which calculates the transient response of the homogeneous model of a packed-bed reactor to a step change in the inlet conditions. The program is coded in FORTRAN IV for an IBM 360/67 computer. Input data was entered on punched cards and the transient conditions were printed out at designated time intervals on an IBM high-speed printer.

The input variables are defined at the beginning of the program source listing. They must be punched on cards in the order given in this list. Table B-1 presented the input data used for the example in this section in the form it is to be punched on cards.

In addition, a FORTRAN statement of the reaction rate expression must be included in the source program at the beginning of SUBROUTINE RETI. Also a FORTRAN statement of the derivative of the rate expression with respect to concentration must be included at the beginning of this subroutine. The correct place for these statements is indicated in the source listing of the program. For the Langmuir-Hinshelwood reaction type used in this section,

the rate of reaction definition was given by:

```
F(Q,Z) = (1.0E+08)*EXP(-12000./Z)*Q/(1.0+(1.0E+05)*Q)
```

The derivative was given by:

```
FD(Q,Z,W) = (1.0E+08)*EXP(-12000./Z)*91.0/((1.0+
            (1.0E+05)*Q)**Z)+(Q/(1.0+(1.0E+05)*Q))*
            (12000./(Z**2))*W)
```

where Q,Z, and W are dummy variables referring to concentration, temperature, and the derivative of the temperature with respect to temperature. This derivative is not constant, but is computed by the program at each time interval.

Table B-2 is a set of transient results given in computer output form, for the input parameters of Table B-1.

TABLE B-1

INPUT DATA FOR HOMOGENEOUS MODEL PROGRAM

INPUT CARD

```
                (RO)                (SO)                (CO)                (TO)
1       bbbb.20000000E+01bbb.25000000E+02bbb.10000000E-04bbb.70000000E+03
            (RADIFF)            (RRDIFF)            (RACOND)            (RRCOND)
2       bbbb.31500000E+01bbb.57300000E+00bbb.17640000E+00bbb.32100000E-01
                (BVEL)              (DELH)              (TW)              (DTHETA)
3       bbbb.12600000E+02bb-.35040000E+06bbb.30000000E+03bbb.20000000E-01
                (RHTCP)             (RDEN)              (RPOR)              (WHTC)
4       bbbb.21860000E+02bbb.25000000E-02bbb.35000000E+00bbb.11300000E+01
                 (DT)                (DC)              (CHTCP)             (CDEN)
5       bbbb.35000000E+02bbb.00000000E+00bbb.60000000E+01bbb.11200000E-01
               (CPOR)               (EC)                (ET)                (ES)
6       bbbb.5430000E+00bbb.10000000E-04bbb.50000000E-01bbb.10000000E-01
                (EX)
7       bbbb.50000000E+00
                 (M)    (N)    (NPI)  (NPK)   (NO)
8       bbbbbb4bbbb50bbbb25bbbb25bbbbb1
                      (RRE(I))
9       b(10**8)*EXP(-20/T)*C/(1+(10**5)*C)
```

TABLE B-2

RESULTS FROM PROGRAM FOR HOMOGENEOUS REACTOR MODEL

PHYSICAL , THERMODYNAMIC AND KINETIC DATA

ALL UNITS ARE IN CM.,SEC.,CAL.,GM.-MOLES,DEGREES KELVIN

REACTOR LENGTH	25.000000
REACTOR RADIUS	2.000000
RADIAL DIFFUSION COEFFICIENT	0.573000
AXIAL DIFFUSION COEFFICIENT	3.150000
FLUID HEAT CAPACITY	21.859985
FLUID DENSITY	0.002500
COOLING FLUID TEMPERATURE	300.000000
BULK FLUID LINEAR VELOCITY	12.599999
INLET REACTANT CONCENTRATION	0.000010
INLET FLUID TEMPERATURE	700.000000
REACTOR VOID FRACTION	0.350000
CATALYST HEAT CAPACITY	6.000000
CATALYST DENSITY	0.011200
CATALYST VOID FRACTION	0.543000
HEAT TRANSFER COEFF AT REACTOR WALL	1.129999
HEAT OF REACTION	-350400.000000
ITERATION TIME STEP	0.020000
NO. OF RADIAL POINTS	5
NO. OF AXIAL POINTS	51

RATE OF REACTION = (10**8)*EXP(-20/T)*C/(1+(10**5)*C)

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

35.00 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.84397	0.85106	0.87997	0.94697	0.99042
1.00	0.52517	0.55638	0.67770	0.89028	0.96548
2.00	0.27530	0.33127	0.54981	0.85302	0.93709
3.00	0.14022	0.20674	0.48333	0.81865	0.90716
4.00	0.08492	0.15497	0.45575	0.78683	0.87675
5.00	0.06883	0.14305	0.44918	0.75841	0.84682
6.00	0.07235	0.15254	0.45261	0.73359	0.81816
7.00	0.08834	0.17454	0.46022	0.71211	0.79130
8.00	0.11404	0.20409	0.46923	0.69352	0.76652
9.00	0.14743	0.23771	0.47846	0.67742	0.74393
10.00	0.18603	0.27270	0.48746	0.66345	0.72352
11.00	0.22700	0.30704	0.49604	0.65132	0.70521
12.00	0.26769	0.33939	0.50412	0.64078	0.68886
13.00	0.30615	0.36899	0.51166	0.63163	0.67434
14.00	0.34125	0.39554	0.51861	0.62370	0.66149
15.00	0.37251	0.41902	0.52496	0.61683	0.65016
16.00	0.39991	0.43961	0.53071	0.61088	0.64019
17.00	0.42370	0.45754	0.53588	0.60573	0.63144
18.00	0.44424	0.47311	0.54050	0.60128	0.62378
19.00	0.46193	0.48659	0.54459	0.59743	0.61709
20.00	0.47715	0.49825	0.54821	0.59410	0.61125
21.00	0.49024	0.50832	0.55138	0.59122	0.60616
22.00	0.50150	0.51702	0.55416	0.58872	0.60172
23.00	0.51116	0.52452	0.55658	0.58656	0.59787
24.00	0.51922	0.53078	0.55862	0.58474	0.59462
25.00	0.52353	0.53414	0.55971	0.58375	0.59285

BULK CONCENTRATION AT REACTOR EXIT = 0.572728

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	709.70	708.76	703.73	677.05	436.73
1.00	728.38	724.23	703.96	626.74	324.57
2.00	740.70	732.37	694.66	585.16	314.43
3.00	743.42	731.37	679.26	552.49	312.22
4.00	738.79	723.46	660.75	526.36	310.90
5.00	729.62	711.28	641.12	504.96	309.85
6.00	717.49	696.48	621.53	487.04	308.98
7.00	703.24	680.08	602.57	471.75	308.23
8.00	687.42	662.74	584.51	458.47	307.59
9.00	670.49	644.98	567.44	446.78	307.03
10.00	652.90	627.19	551.35	436.38	306.53
11.00	635.08	609.67	536.23	427.02	306.08
12.00	617.38	592.63	522.01	418.53	305.67
13.00	600.06	576.20	508.66	410.78	305.30
14.00	583.31	560.47	496.12	403.67	304.96
15.00	567.25	545.48	484.34	397.10	304.64
16.00	551.93	531.24	473.27	391.02	304.35
17.00	537.37	517.76	462.89	385.38	304.08
18.00	523.58	505.01	453.14	380.13	303.83
19.00	510.54	492.98	443.99	375.24	303.59
20.00	498.23	481.65	435.40	370.67	303.38
21.00	486.65	470.99	427.36	366.41	303.17
22.00	475.76	460.98	419.83	362.44	302.98
23.00	465.60	451.64	412.82	358.76	302.81
24.00	456.48	443.27	406.54	355.46	302.65
25.00	451.45	438.65	403.09	353.65	302.56

BULK TEMPERATURE AT REACTOR EXIT = 366.19

ITERATION NO. 25 TIME = 0.5000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.72509	0.73434	0.77727	0.89764	0.98477
1.00	0.30550	0.33668	0.48397	0.81881	0.94972
2.00	0.14064	0.18572	0.40504	0.80087	0.92090
3.00	0.08576	0.14097	0.40704	0.78916	0.89602
4.00	0.06661	0.13044	0.42349	0.77317	0.87089
5.00	0.06319	0.13492	0.43764	0.75310	0.84433
6.00	0.07071	0.15008	0.44903	0.73183	0.81727
7.00	0.08789	0.17386	0.45923	0.71159	0.79103
8.00	0.11392	0.20391	0.46898	0.69339	0.76645
9.00	0.14741	0.23767	0.47841	0.67739	0.74391
10.00	0.18603	0.27269	0.48745	0.66344	0.72352
11.00	0.22699	0.30704	0.49604	0.65132	0.70521
12.00	0.26769	0.33939	0.50412	0.64078	0.68886
13.00	0.30615	0.36899	0.51166	0.63163	0.67434
14.00	0.34125	0.39554	0.51861	0.62370	0.66149
15.00	0.37251	0.41902	0.52496	0.61683	0.65016
16.00	0.39991	0.43961	0.53071	0.61088	0.64019
17.00	0.42370	0.45754	0.53588	0.60574	0.63144
18.00	0.44425	0.47311	0.54050	0.60129	0.62379
19.00	0.46195	0.48660	0.54460	0.59744	0.61710
20.00	0.47717	0.49826	0.54822	0.59411	0.61126
21.00	0.49026	0.50835	0.55140	0.59123	0.60617
22.00	0.50153	0.51706	0.55419	0.58875	0.60175
23.00	0.51120	0.52456	0.55662	0.58660	0.59791
24.00	0.51929	0.53085	0.55868	0.58479	0.59467
25.00	0.52362	0.53422	0.55978	0.58382	0.59292

BULK CONCENTRATION AT REACTOR EXIT = 0.572800

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	747.81	746.76	740.92	710.17	448.66
1.00	762.48	758.35	736.60	650.56	326.49
2.00	758.26	750.54	712.93	597.64	315.10
3.00	749.32	737.83	686.41	557.35	312.48
4.00	740.17	725.10	662.82	527.79	310.97
5.00	729.84	711.58	641.58	505.29	309.87
6.00	717.51	696.52	621.61	487.10	308.98
7.00	703.24	680.08	602.59	471.75	308.23
8.00	687.42	662.74	584.51	458.47	307.59
9.00	670.49	644.98	567.44	446.78	307.03
10.00	652.90	627.19	551.35	436.38	306.53
11.00	635.08	609.67	536.23	427.02	306.08
12.00	617.38	592.63	522.01	418.53	305.67
13.00	600.06	576.20	508.66	410.78	305.30
14.00	583.31	560.47	496.12	403.67	304.96
15.00	567.25	545.48	484.34	397.10	304.64
16.00	551.92	531.24	473.27	391.02	304.35
17.00	537.36	517.74	462.88	385.38	304.08
18.00	523.55	504.99	453.12	380.12	303.83
19.00	510.49	492.94	443.95	375.22	303.59
20.00	498.16	481.58	435.35	370.64	303.38
21.00	486.53	470.88	427.28	366.37	303.17
22.00	475.58	460.81	419.71	362.38	302.98
23.00	465.33	451.40	412.64	358.66	302.80
24.00	456.09	442.92	406.28	355.33	302.64
25.00	450.94	438.19	402.75	353.47	302.55

BULK TEMPERATURE AT REACTOR EXIT = 365.97

ITERATION NO. 50 TIME = 1.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.67630	0.68506	0.73134	0.87877	0.97956
1.00	0.19592	0.21775	0.34811	0.76289	0.92929
2.00	0.05006	0.07056	0.22114	0.71778	0.88283
3.00	0.02041	0.04304	0.21677	0.69572	0.84638
4.00	0.01875	0.05045	0.26058	0.68642	0.81996
5.00	0.02825	0.07419	0.31823	0.68431	0.80088
6.00	0.04616	0.10800	0.37189	0.68422	0.78545
7.00	0.07172	0.14736	0.41449	0.68239	0.77062
8.00	0.10411	0.18877	0.44543	0.67734	0.75482
9.00	0.14197	0.22982	0.46710	0.66943	0.73798
10.00	0.18331	0.26899	0.48247	0.65985	0.72078
11.00	0.22577	0.30546	0.49403	0.64983	0.70405
12.00	0.26718	0.33877	0.50337	0.64022	0.68842
13.00	0.30597	0.36877	0.51140	0.63144	0.67418
14.00	0.34119	0.39547	0.51852	0.62364	0.66144
15.00	0.37249	0.41900	0.52493	0.61681	0.65014
16.00	0.39991	0.43960	0.53071	0.61088	0.64018
17.00	0.42370	0.45754	0.53588	0.60573	0.63144
18.00	0.44425	0.47311	0.54050	0.60128	0.62379
19.00	0.46195	0.48660	0.54460	0.59744	0.61710
20.00	0.47717	0.49827	0.54822	0.59411	0.61126
21.00	0.49027	0.50835	0.55141	0.59124	0.60618
22.00	0.50154	0.51707	0.55420	0.58875	0.60175
23.00	0.51122	0.52458	0.55664	0.58661	0.59792
24.00	0.51931	0.53087	0.55869	0.58481	0.59468
25.00	0.52365	0.53425	0.55981	0.58384	0.59294

BULK CONCENTRATION AT REACTOR EXIT = 0.572826

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	754.21	753.14	746.84	713.47	448.81
1.00	779.61	775.93	754.38	660.31	326.93
2.00	779.21	772.82	738.11	612.07	315.77
3.00	767.44	757.67	710.42	571.54	313.14
4.00	751.89	738.37	679.77	538.08	311.46
5.00	735.66	718.50	650.96	511.14	310.15
6.00	719.75	699.40	625.85	489.82	309.11
7.00	703.88	681.05	604.18	472.81	308.29
8.00	687.54	663.00	585.03	458.82	307.61
9.00	670.49	645.04	567.58	446.88	307.03
10.00	652.89	627.20	551.39	436.40	306.53
11.00	635.07	609.67	536.23	427.02	306.08
12.00	617.37	592.62	522.01	418.53	305.67
13.00	600.06	576.20	508.66	410.78	305.30
14.00	583.31	560.47	496.12	403.67	304.96
15.00	567.25	545.48	484.33	397.10	304.64
16.00	551.92	531.23	473.27	391.02	304.35
17.00	537.35	517.74	462.88	385.37	304.08
18.00	523.54	504.98	453.11	380.12	303.83
19.00	510.47	492.92	443.94	375.21	303.59
20.00	498.12	481.55	435.33	370.63	303.37
21.00	486.48	470.83	427.24	366.35	303.17
22.00	475.50	460.74	419.65	362.35	302.98
23.00	465.21	451.28	412.55	358.62	302.80
24.00	455.91	442.75	406.16	355.26	302.64
25.00	450.70	437.97	402.58	353.38	302.55

BULK TEMPERATURE AT REACTOR EXIT = 365.86

ITERATION NO. 100 TIME = 2.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.66157	0.66984	0.71586	0.87219	0.97717
1.00	0.16783	0.18608	0.30420	0.74073	0.91904
2.00	0.03248	0.04560	0.15947	0.67667	0.85869
3.00	0.00823	0.01909	0.13188	0.63241	0.80289
4.00	0.00476	0.01771	0.14566	0.59859	0.75371
5.00	0.00657	0.02531	0.17671	0.57341	0.71217
6.00	0.01256	0.04056	0.21505	0.55643	0.67890
7.00	0.02485	0.06462	0.25528	0.54710	0.65411
8.00	0.04618	0.09790	0.29484	0.54458	0.63748
9.00	0.07802	0.13905	0.33284	0.54766	0.62804
10.00	0.11941	0.18532	0.36897	0.55477	0.62429
11.00	0.16729	0.23355	0.40278	0.56416	0.62435
12.00	0.21772	0.28081	0.43356	0.57408	0.62626
13.00	0.26705	0.32480	0.46058	0.58305	0.62836
14.00	0.31257	0.36404	0.48338	0.59008	0.62948
15.00	0.35277	0.39780	0.50185	0.59476	0.62904
16.00	0.38714	0.42610	0.51632	0.59713	0.62699
17.00	0.41592	0.44942	0.52738	0.59762	0.62363
18.00	0.43978	0.46849	0.53573	0.59674	0.61940
19.00	0.45952	0.48411	0.54206	0.59502	0.61476
20.00	0.47593	0.49699	0.54694	0.59289	0.61008
21.00	0.48966	0.50774	0.55079	0.59065	0.60561
22.00	0.50126	0.51678	0.55392	0.58849	0.60150
23.00	0.51110	0.52446	0.55652	0.58650	0.59781
24.00	0.51927	0.53083	0.55865	0.58477	0.59464
25.00	0.52364	0.53424	0.55980	0.58383	0.59293

BULK CONCENTRATION AT REACTOR EXIT = 0.572814

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	756.31	755.26	748.85	714.42	448.85
1.00	785.62	782.11	760.90	663.66	327.09
2.00	789.56	783.54	750.31	619.04	316.10
3.00	783.28	774.07	729.27	582.61	313.67
4.00	772.23	759.60	704.09	552.38	312.15
5.00	757.53	741.62	677.22	526.61	310.89
6.00	739.86	720.99	650.06	504.18	309.80
7.00	720.05	698.68	623.71	484.50	308.85
8.00	699.10	675.81	599.07	467.31	308.02
9.00	677.92	653.39	576.70	452.45	307.30
10.00	657.20	632.12	556.77	439.72	306.69
11.00	637.32	612.29	539.13	428.83	306.16
12.00	618.43	593.89	523.44	419.43	305.71
13.00	600.51	576.75	509.30	411.19	305.32
14.00	583.48	560.69	496.38	403.84	304.96
15.00	567.30	545.55	484.43	397.16	304.64
16.00	551.93	531.26	473.30	391.04	304.35
17.00	537.35	517.74	462.88	385.38	304.08
18.00	523.54	504.98	453.11	380.12	303.83
19.00	510.46	492.92	443.94	375.21	303.59
20.00	498.11	481.54	435.32	370.63	303.37
21.00	486.45	470.80	427.22	366.34	303.17
22.00	475.45	460.69	419.62	362.33	302.98
23.00	465.13	451.21	412.50	358.59	302.80
24.00	455.78	442.64	406.08	355.22	302.64
25.00	450.53	437.81	402.47	353.33	302.55

BULK TEMPERATURE AT REACTOR EXIT = 365.79

ITERATION NO. 150 TIME = 2.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.66040	0.66865	0.71465	0.87166	0.97697
1.00	0.16568	0.18368	0.30084	0.73892	0.91816
2.00	0.03122	0.04382	0.15482	0.67314	0.85646
3.00	0.00744	0.01743	0.12490	0.62640	0.79836
4.00	0.00383	0.01506	0.13399	0.58873	0.74549
5.00	0.00462	0.01991	0.15766	0.55770	0.69832
6.00	0.00785	0.02961	0.18645	0.53239	0.65697
7.00	0.01429	0.04447	0.21559	0.51214	0.62140
8.00	0.02560	0.06507	0.24284	0.49638	0.59151
9.00	0.04357	0.09139	0.26765	0.48471	0.56711
10.00	0.06912	0.12253	0.29047	0.47686	0.54807
11.00	0.10164	0.15698	0.31211	0.47272	0.53421
12.00	0.13926	0.19320	0.33336	0.47222	0.52535
13.00	0.17974	0.23003	0.35485	0.47522	0.52119
14.00	0.22117	0.26670	0.37687	0.48144	0.52128
15.00	0.26220	0.30267	0.39940	0.49041	0.52500
16.00	0.30187	0.33747	0.42214	0.50142	0.53150
17.00	0.33946	0.37057	0.44454	0.51365	0.53983
18.00	0.37432	0.40142	0.46593	0.52618	0.54898
19.00	0.40593	0.42948	0.48565	0.53816	0.55801
20.00	0.43392	0.45434	0.50319	0.54890	0.56619
21.00	0.45809	0.47578	0.51820	0.55796	0.57300
22.00	0.47848	0.49379	0.53059	0.56513	0.57821
23.00	0.49532	0.50856	0.54046	0.57045	0.58181
24.00	0.50872	0.52023	0.54798	0.57413	0.58404
25.00	0.51638	0.52695	0.55247	0.57654	0.58567

BULK CONCENTRATION AT REACTOR EXIT = 0.565523

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	756.49	755.43	749.01	714.50	448.86
1.00	786.15	782.65	761.45	663.94	327.10
2.00	790.67	784.65	751.48	619.71	316.14
3.00	785.57	776.37	731.61	583.97	313.74
4.00	776.53	763.88	708.36	554.83	312.26
5.00	764.64	748.70	684.16	530.53	311.08
6.00	750.25	731.41	660.02	509.78	310.07
7.00	733.63	712.35	636.43	491.66	309.19
8.00	715.01	691.84	613.63	475.54	308.41
9.00	694.76	670.30	591.75	460.99	307.71
10.00	673.35	648.26	570.93	447.79	307.07
11.00	651.44	626.32	551.34	435.81	306.50
12.00	629.73	605.08	533.12	424.99	305.98
13.00	608.83	584.98	516.41	415.28	305.51
14.00	589.16	566.29	501.22	406.63	305.10
15.00	570.91	549.11	487.51	398.94	304.73
16.00	554.07	533.36	475.13	392.10	304.40
17.00	538.53	518.91	463.90	385.97	304.11
18.00	524.14	505.58	453.64	380.42	303.84
19.00	510.76	493.21	444.19	375.36	303.60
20.00	498.24	481.66	435.44	370.70	303.38
21.00	486.50	470.86	427.27	366.37	303.17
22.00	475.47	460.71	419.63	362.34	302.98
23.00	465.12	451.21	412.50	358.59	302.80
24.00	455.77	442.62	406.06	355.21	302.64
25.00	450.50	437.79	402.45	353.32	302.55

BULK TEMPERATURE AT REACTOR EXIT = 365.78

ITERATION NO. 200 TIME = 3.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.66030	0.66853	0.71453	0.87162	0.97696
1.00	0.16548	0.18344	0.30051	0.73877	0.91808
2.00	0.03110	0.04366	0.15438	0.67283	0.85626
3.00	0.00737	0.01726	0.12421	0.62584	0.79796
4.00	0.00373	0.01477	0.13272	0.58777	0.74472
5.00	0.00439	0.01925	0.15535	0.55607	0.69693
6.00	0.00721	0.02806	0.18252	0.52965	0.65458
7.00	0.01261	0.04114	0.20945	0.50770	0.61744
8.00	0.02169	0.05866	0.23382	0.48946	0.58518
9.00	0.03564	0.08044	0.25493	0.47428	0.55737
10.00	0.05518	0.10570	0.27302	0.46169	0.53363
11.00	0.08011	0.13324	0.28870	0.45138	0.51358
12.00	0.10917	0.16172	0.30264	0.44319	0.49693
13.00	0.14054	0.19003	0.31549	0.43704	0.48348
14.00	0.17250	0.21746	0.32778	0.43295	0.47309
15.00	0.20385	0.24372	0.33996	0.43099	0.46569
16.00	0.23399	0.26887	0.35244	0.43123	0.46125
17.00	0.26286	0.29312	0.36553	0.43376	0.45974
18.00	0.29061	0.31678	0.37948	0.43858	0.46108
19.00	0.31748	0.34010	0.39439	0.44563	0.46513
20.00	0.34366	0.36322	0.41027	0.45472	0.47164
21.00	0.36919	0.38612	0.42693	0.46553	0.48022
22.00	0.39398	0.40865	0.44408	0.47762	0.49039
23.00	0.41774	0.43047	0.46127	0.49044	0.50155
24.00	0.43972	0.45083	0.47773	0.50325	0.51296
25.00	0.45504	0.46530	0.49013	0.51369	0.52267

BULK CONCENTRATION AT REACTOR EXIT = 0.502939

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	756.50	755.45	749.03	714.50	448.86
1.00	786.19	782.70	761.50	663.96	327.11
2.00	790.78	784.76	751.60	619.77	316.14
3.00	785.84	776.62	731.86	584.11	313.74
4.00	777.10	764.43	708.89	555.12	312.28
5.00	765.77	749.81	685.18	531.08	311.10
6.00	752.31	733.43	661.83	510.75	310.11
7.00	737.07	715.72	639.35	493.23	309.26
8.00	720.30	697.00	617.96	477.87	308.52
9.00	702.23	677.55	597.69	464.20	307.86
10.00	683.07	657.61	578.45	451.86	307.27
11.00	663.10	637.43	560.15	440.59	306.73
12.00	642.63	617.27	542.74	430.21	306.23
13.00	622.05	597.41	526.18	420.59	305.77
14.00	601.75	578.11	510.50	411.68	305.34
15.00	582.11	559.61	495.75	403.43	304.94
16.00	563.41	542.12	482.00	395.85	304.58
17.00	545.86	525.78	469.29	388.91	304.25
18.00	529.56	510.65	457.63	382.60	303.95
19.00	514.54	496.75	446.98	376.89	303.67
20.00	500.74	484.01	437.28	371.71	303.43
21.00	488.06	472.32	428.42	367.00	303.20
22.00	476.39	461.58	420.32	362.72	303.00
23.00	465.64	451.70	412.89	358.80	302.81
24.00	456.04	442.88	406.27	355.33	302.64
25.00	450.65	437.93	402.56	353.38	302.55

BULK TEMPERATURE AT REACTOR EXIT = 365.85

ITERATION NO. 250 TIME = 4.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.66029	0.66853	0.71453	0.87162	0.97695
1.00	0.16547	0.18344	0.30050	0.73876	0.91808
2.00	0.03110	0.04365	0.15435	0.67281	0.85625
3.00	0.00736	0.01725	0.12415	0.62580	0.79792
4.00	0.00372	0.01474	0.13259	0.58768	0.74465
5.00	0.00436	0.01917	0.15509	0.55590	0.69680
6.00	0.00713	0.02786	0.18204	0.52936	0.65434
7.00	0.01236	0.04065	0.20862	0.50719	0.61701
8.00	0.02104	0.05762	0.23250	0.48860	0.58444
9.00	0.03416	0.07844	0.25293	0.47290	0.55616
10.00	0.05226	0.10228	0.27007	0.45954	0.53170
11.00	0.07506	0.12792	0.28444	0.44811	0.51058
12.00	0.10141	0.15410	0.29664	0.43834	0.49241
13.00	0.12966	0.17971	0.30720	0.43002	0.47684
14.00	0.15817	0.20400	0.31652	0.42303	0.46357
15.00	0.18565	0.22653	0.32494	0.41729	0.45240
16.00	0.21135	0.24719	0.33273	0.41276	0.44316
17.00	0.23496	0.26605	0.34012	0.40943	0.43576
18.00	0.25655	0.28337	0.34736	0.40734	0.43013
19.00	0.27638	0.29946	0.35466	0.40655	0.42627
20.00	0.29483	0.31467	0.36228	0.40714	0.42419
21.00	0.31230	0.32936	0.37042	0.40920	0.42395
22.00	0.32920	0.34388	0.37930	0.41282	0.42558
23.00	0.34580	0.35845	0.38904	0.41804	0.42908
24.00	0.36192	0.37289	0.39946	0.42466	0.43427
25.00	0.37351	0.38358	0.40798	0.43115	0.43999

BULK CONCENTRATION AT REACTOR EXIT = 0.420584

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	756.50	755.45	749.03	714.50	448.86
1.00	786.20	782.70	761.50	663.96	327.11
2.00	790.79	784.77	751.60	619.78	316.14
3.00	785.86	776.65	731.88	584.13	313.74
4.00	777.16	764.50	708.95	555.15	312.28
5.00	765.91	749.95	685.30	531.15	311.10
6.00	752.61	733.71	662.08	510.88	310.12
7.00	737.64	716.27	639.82	493.47	309.28
8.00	721.32	697.98	618.76	478.29	308.54
9.00	703.94	679.18	598.98	464.88	307.90
10.00	685.75	660.14	580.40	452.89	307.32
11.00	667.01	641.09	562.95	442.06	306.80
12.00	647.96	622.23	546.48	432.18	306.32
13.00	628.83	603.69	530.91	423.09	305.89
14.00	609.86	585.58	516.12	414.65	305.48
15.00	591.22	567.99	502.07	406.77	305.10
16.00	573.06	551.01	488.71	399.40	304.75
17.00	555.54	534.69	476.03	392.48	304.42
18.00	538.76	519.13	464.04	386.00	304.11
19.00	522.84	504.40	452.78	379.96	303.82
20.00	507.86	490.57	442.25	374.34	303.55
21.00	493.87	477.68	432.49	369.16	303.30
22.00	480.91	465.75	423.48	364.40	303.08
23.00	469.00	454.79	415.24	360.05	302.87
24.00	458.43	445.08	407.94	356.21	302.69
25.00	452.40	439.55	403.79	354.03	302.58

BULK TEMPERATURE AT REACTOR EXIT = 366.64

ITERATION NO. 300 TIME = 5.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.66029	0.66853	0.71453	0.87162	0.97696
1.00	0.16547	0.18344	0.30050	0.73876	0.91808
2.00	0.03109	0.04365	0.15435	0.67281	0.85625
3.00	0.00736	0.01725	0.12415	0.62580	0.79792
4.00	0.00372	0.01474	0.13259	0.58768	0.74465
5.00	0.00436	0.01917	0.15507	0.55589	0.69679
6.00	0.00712	0.02784	0.18199	0.52934	0.65432
7.00	0.01233	0.04059	0.20853	0.50714	0.61697
8.00	0.02095	0.05747	0.23234	0.48851	0.58437
9.00	0.03393	0.07813	0.25266	0.47274	0.55603
10.00	0.05176	0.10170	0.26963	0.45926	0.53146
11.00	0.07410	0.12696	0.28377	0.44767	0.51020
12.00	0.09981	0.15261	0.29564	0.43764	0.49179
13.00	0.12726	0.17756	0.30574	0.42895	0.47587
14.00	0.15481	0.20104	0.31444	0.42143	0.46211
15.00	0.18122	0.22261	0.32203	0.41495	0.45022
16.00	0.20568	0.24210	0.32873	0.40939	0.43999
17.00	0.22783	0.25951	0.33469	0.40468	0.43122
18.00	0.24760	0.27499	0.34006	0.40075	0.42376
19.00	0.26515	0.28874	0.34497	0.39756	0.41751
20.00	0.28071	0.30101	0.34955	0.39510	0.41238
21.00	0.29459	0.31205	0.35394	0.39335	0.40832
22.00	0.30711	0.32212	0.35826	0.39235	0.40531
23.00	0.31855	0.33147	0.36266	0.39214	0.40336
24.00	0.32890	0.34008	0.36713	0.39274	0.40249
25.00	0.33545	0.34570	0.37050	0.39402	0.40297

BULK CONCENTRATION AT REACTOR EXIT = 0.383284

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	756.50	755.45	749.03	714.50	448.86
1.00	786.20	782.70	761.50	663.96	327.11
2.00	790.79	784.77	751.60	619.78	316.14
3.00	785.86	776.65	731.88	584.13	313.74
4.00	777.16	764.50	708.95	555.15	312.28
5.00	765.92	749.96	685.31	531.15	311.10
6.00	752.64	733.75	662.10	510.89	310.12
7.00	737.71	716.34	639.87	493.50	309.28
8.00	721.47	698.13	618.88	478.35	308.55
9.00	704.23	679.46	599.19	464.99	307.90
10.00	686.26	660.62	580.77	453.08	307.33
11.00	667.86	641.88	563.53	442.37	306.81
12.00	649.29	623.45	547.39	432.65	306.34
13.00	630.80	605.48	532.23	423.78	305.92
14.00	612.59	588.08	517.97	415.61	305.53
15.00	594.83	571.30	504.51	408.05	305.16
16.00	577.60	555.15	491.78	401.00	304.83
17.00	560.97	539.66	479.72	394.40	304.51
18.00	544.95	524.80	468.26	388.20	304.21
19.00	529.58	510.58	457.38	382.36	303.94
20.00	514.87	497.00	447.05	376.85	303.67
21.00	500.85	484.08	437.27	371.66	303.42
22.00	487.56	471.85	428.04	366.78	303.19
23.00	475.06	460.36	419.40	362.23	302.97
24.00	463.76	449.97	411.60	358.13	302.78
25.00	457.13	443.88	407.04	355.74	302.66

BULK TEMPERATURE AT REACTOR EXIT = 368.72

ITERATION NO. 350 TIME = 6.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.66029	0.66853	0.71453	0.87162	0.97696
1.00	0.16547	0.18344	0.30050	0.73876	0.91808
2.00	0.03110	0.04365	0.15435	0.67281	0.85625
3.00	0.00736	0.01725	0.12415	0.62580	0.79792
4.00	0.00372	0.01474	0.13259	0.58768	0.74465
5.00	0.00436	0.01917	0.15507	0.55589	0.69679
6.00	0.00712	0.02784	0.18199	0.52934	0.65432
7.00	0.01233	0.04059	0.20853	0.50714	0.61697
8.00	0.02094	0.05746	0.23232	0.48851	0.58436
9.00	0.03390	0.07810	0.25263	0.47273	0.55602
10.00	0.05169	0.10162	0.26958	0.45924	0.53144
11.00	0.07396	0.12681	0.28368	0.44762	0.51016
12.00	0.09954	0.15236	0.29550	0.43755	0.49172
13.00	0.12682	0.17718	0.30551	0.42881	0.47575
14.00	0.15417	0.20050	0.31410	0.42120	0.46190
15.00	0.18033	0.22186	0.32154	0.41459	0.44990
16.00	0.20450	0.24109	0.32802	0.40886	0.43950
17.00	0.22630	0.25818	0.33370	0.40389	0.43049
18.00	0.24565	0.27325	0.33869	0.39961	0.42269
19.00	0.26266	0.28647	0.34309	0.39594	0.41596
20.00	0.27753	0.29804	0.34698	0.39280	0.41018
21.00	0.29051	0.30817	0.35046	0.39017	0.40523
22.00	0.30186	0.31706	0.35359	0.38799	0.40105
23.00	0.31178	0.32489	0.35645	0.38625	0.39757
24.00	0.32028	0.33163	0.35904	0.38496	0.39481
25.00	0.32508	0.33549	0.36065	0.38447	0.39353

BULK CONCENTRATION AT REACTOR EXIT = 0.373588

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	756.50	755.45	749.03	714.50	448.86
1.00	786.20	782.70	761.50	663.96	327.11
2.00	790.79	784.77	751.60	619.78	316.14
3.00	785.86	776.65	731.88	584.13	313.74
4.00	777.16	764.50	708.95	555.15	312.28
5.00	765.92	749.96	685.31	531.15	311.10
6.00	752.64	733.75	662.10	510.89	310.12
7.00	737.71	716.34	639.88	493.50	309.28
8.00	721.48	698.14	618.89	478.35	308.55
9.00	704.26	679.49	599.21	465.00	307.90
10.00	686.34	660.69	580.82	453.10	307.33
11.00	668.00	642.01	563.63	442.42	306.81
12.00	649.53	623.68	547.56	432.74	306.35
13.00	631.20	605.86	532.51	423.92	305.93
14.00	613.23	588.66	518.40	415.83	305.54
15.00	595.78	572.16	505.15	408.37	305.18
16.00	578.95	556.38	492.69	401.47	304.85
17.00	562.81	541.33	480.95	395.04	304.54
18.00	547.35	526.99	469.88	389.04	304.25
19.00	532.59	513.32	459.41	383.42	303.99
20.00	518.49	500.31	449.50	378.12	303.73
21.00	505.03	487.91	440.11	373.14	303.49
22.00	492.21	476.10	431.20	368.42	303.27
23.00	480.04	464.91	422.78	363.99	303.06
24.00	468.89	454.67	415.10	359.95	302.86
25.00	462.35	448.66	410.60	357.59	302.75

BULK TEMPERATURE AT REACTOR EXIT = 371.01

ITERATION NO. 449 TIME = 8.9798 SEC.

FINAL STEADY STATE CONDITIONS

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.66029	0.66853	0.71453	0.87162	0.97695
1.00	0.16547	0.18344	0.30050	0.73876	0.91808
2.00	0.03109	0.04365	0.15435	0.67281	0.85625
3.00	0.00736	0.01725	0.12415	0.62580	0.79792
4.00	0.00372	0.01474	0.13259	0.58768	0.74465
5.00	0.00436	0.01917	0.15507	0.55589	0.69679
6.00	0.00712	0.02784	0.18199	0.52934	0.65432
7.00	0.01233	0.04059	0.20853	0.50714	0.61697
8.00	0.02094	0.05746	0.23232	0.48851	0.58436
9.00	0.03390	0.07809	0.25263	0.47272	0.55602
10.00	0.05168	0.10162	0.26958	0.45924	0.53144
11.00	0.07394	0.12680	0.28367	0.44762	0.51015
12.00	0.09951	0.15233	0.29548	0.43755	0.49172
13.00	0.12676	0.17713	0.30549	0.42879	0.47574
14.00	0.15407	0.20041	0.31406	0.42118	0.46188
15.00	0.18017	0.22173	0.32147	0.41455	0.44986
16.00	0.20427	0.24090	0.32791	0.40878	0.43943
17.00	0.22598	0.25791	0.33352	0.40377	0.43038
18.00	0.24522	0.27289	0.33843	0.39942	0.42252
19.00	0.26210	0.28598	0.34272	0.39564	0.41569
20.00	0.27681	0.29739	0.34646	0.39237	0.40977
21.00	0.28957	0.30730	0.34973	0.38954	0.40464
22.00	0.30062	0.31590	0.35258	0.38709	0.40019
23.00	0.31016	0.32334	0.35507	0.38498	0.39634
24.00	0.31816	0.32959	0.35716	0.38321	0.39311
25.00	0.32248	0.33297	0.35830	0.38227	0.39138

BULK CONCENTRATION AT REACTOR EXIT = 0.371316

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	756.50	755.45	749.03	714.50	448.86
1.00	786.20	782.70	761.50	663.96	327.11
2.00	790.79	784.77	751.60	619.78	316.14
3.00	785.86	776.65	731.88	584.13	313.74
4.00	777.16	764.50	708.95	555.15	312.28
5.00	765.92	749.96	685.31	531.15	311.10
6.00	752.64	733.75	662.10	510.89	310.12
7.00	737.71	716.34	639.88	493.50	309.28
8.00	721.49	698.14	618.89	478.35	308.55
9.00	704.26	679.49	599.21	465.00	307.90
10.00	686.34	660.70	580.82	453.10	307.33
11.00	668.02	642.03	563.64	442.42	306.81
12.00	649.57	623.71	547.58	432.75	306.35
13.00	631.27	605.92	532.55	423.94	305.93
14.00	613.36	588.78	518.48	415.87	305.54
15.00	596.00	572.36	505.29	408.45	305.18
16.00	579.31	556.70	492.92	401.59	304.86
17.00	563.35	541.82	481.31	395.23	304.55
18.00	548.15	527.71	470.41	389.32	304.27
19.00	533.71	514.35	460.17	383.81	304.00
20.00	520.03	501.71	450.54	378.66	303.76
21.00	507.08	489.77	441.49	373.85	303.53
22.00	494.82	478.49	432.97	369.34	303.31
23.00	483.27	467.87	424.98	365.13	303.11
24.00	472.78	458.22	417.73	361.32	302.93
25.00	466.81	452.74	413.62	359.16	302.83

BULK TEMPERATURE AT REACTOR EXIT = 372.95

B-3

PROGRAM FOR HOMOGENEOUS REACTOR MODEL

SOURCE LISTING

```
C          ***** DEFINITION OF INPUT VARIABLES *****
C
C
C     RO        REACTOR RADIUS
C
C     SO        REACTOR LENGTH
C
C     CO        INLET CONCENTRATION
C
C     TO        INLET TEMPERATURE
C
C     RADIFF    AXIAL DIFFUSION COEFFICIENT
C
C     RRDIFF    RADIAL DIFFUSION COEFFICIENT
C
C     RACOND    AXIAL CONDUCTIVITY COEFFICIENT
C
C     RRCOND    RADIAL CONDUCTIVITY COEFFICIENT
C
C     BVEL      BULK FLUID LINEAR VELOCITY
C
C     DELH      HEAT OF REACTION
C
C     TW        COOLING FLUID TEMPERATURE
C
C     DTHETA    ITERATION TIME STEP
C
C     RHTCP     FLUID HEAT CAPACITY
C
C     RDEN      FLUID DENSITY
C
C     RPOR      REACTOR VOID FRACTION
C
C     WHTC      HEAT TRANSFER COEFFICIENT AT REACTOR WALL
C
C     DT        STEP CHANGE IN INLET TEMPERATURE
C
C     DC        STEP CHANGE IN INLET CONCENTRATION
C
C     CHTCP     CATALYST HEAT CAPACITY
C
C     CDEN      CATALYST DENSITY
C
C     CPOR      CATALYST POROSITY
C
C     EC        RELATIVE ERROR IN CONCENTRATION BETWEEN (N+1)
C               'TH AND N'TH ITERATIONS AT ASSUMED STEADY
C               -STATE
C
```

```
C       ET          ABSOLUTE ERROR IN TEMPERATURE BETWEEN (N+1)
C                   'TH AND N'TH ITERATIONS AT ASSUMED STEADY
C                   -STATE
C
C       ES          RELATIVE  ERROR IN CONCENTRATION BETWEEN SUC-
C                   CEEDING ITERATIONS AT NEWWTON-RAPHSON CONVER-
C                   GENCE
C
C       EX          ABSOLUTE ERROR IN TEMPERATURE BETWEEN SUC-
C                   CEEDING ITERATIONS AT NEWTON-RAPHSON CONVER-
C                   GENCE
C
C       M           NO. OF RADIAL GRID POINTS -1
C
C       N           NO. OF AXIAL GRID POINTS -1
C
C       NPI         FIRST TRANSIENT ITERATION TO BE PRINTED
C
C       NPK         THIS MANY ITERATIONS TO BE SKIPPED BETWEEN
C                   EACH TRANSIENT PRINTOUT
C
C       NO          NUMBER OF COPIES OF RESULTS REQUIRED
C
C       RRE(I)      STATEMENT OF REACTION RATE EXPRESSION  (NOT
C                   MORE THAN 72 CHARACTERS)
C
```

```
C      ***** PROGRAM FOR HOMOGENEOUS REACTOR MODEL *****
C
C                    ***** MAINLINE PROGRAM *****
C
C      THIS MAINLINE READS IN THE THERMODYNAMIC, PHYSICAL
C      AND KINETIC DATA FROM CARDS AND PRINTS OUT THIS DATA
C      ALONG WITH THE INITIAL STEADY STATE, THE INTERMEDIATE
C      TRANSIENT RESULTS AND THE FINAL STEADY STATE CONDITIONS.
C
       COMMON C1(300),C2(300),C3(300),C4(300),C5(300),C6(300)
      1,C7(300),C8(300),C9(300),T1(300),T2(300),T3(300),T4(300
      2),T5(300),T6(300),T7(300),T8(300),T9(300),C(330),T(300
      3),S(300),X(300),XN(300),SN(300),CN(300),TN(300),R(10),
      4RO,SO,CO,TO,RADIFF,RRDIFF,RACOND,RRCOND,BVEL,DELH,TW,
      5DTHETA,RHTCP,RDEN,RPOR,WHTC,DT,DC,EC,ET,ES,EX,DR,DX,
      6CPOR
       COMMON RL(100),CNORM(300)
       COMMON CHTCP,CDEN
       COMMON M,N,MP,NP,MN,L,JG,NI,NO
       DIMENSION RRE(20)
       DIMENSION QP(10)
C
C      READ IN PARAMETERS FROM PUNCHED CARDS
C
       READ (5,10) RO,SO,CO,TO,RADIFF,RRDIFF,RACOND,RRCOND,
      1BVEL,DELH,TW,DTHETA,RHTCP,RDEN,RPOR,WHTC,DT,DC,CHTCP,
      2CDEN,CPOR,EC,ET,ES,EX
       READ (5,11) M,N,NPK,NPI,NO
   10  FORMAT (1X,4E16.8)
   11  FORMAT (1X,5I6)
       READ (5,901) (RRE(I),I=1,20)
  901  FORMAT (20A4)
       CON=CO
       MP=M+1
       NP=N+1
       MN=MP*NP
C
C      WRITE OUT DATA ON TYPEWRITER
C
       DO 29 JW=1,NO
       WRITE (6,900) SO,RO,RRDIFF,RADIFF,RHTCP,RDEN,TW,BVEL,
      1CO,TO,RPOR
       WRITE (6,805) CHTCP,CDEN,CPOR
       WRITE (6,910) WHTC,DELH,DTHETA,MP,NP
       WRITE (6,902) (RRE(I),I=1,20)
  900  FORMAT (1H1////' ',12X,'PHYSICAL , THERMODYNAMIC AND '
      1,'KINETIC DATA'/'-',12X,'ALL UNITS ARE IN CM.,SEC.,CA'
      2,'L.,GM.-MOLES,DEGREES KELVIN '/'-',12X,'REACTOR LENG'
      3,'TH',26X,F16.6/'0',12X,'REACTOR RADIUS',26X,F16.6/'0'
      4,12X,'RADIAL DIFFUSION COEFFICIENT',12X,F16.6/'0',12X,
```

```
     5     'AXIAL DIFFUSION COEFFICIENT',13X,F16.6/'0',12X,
     6'FLUID HEAT CAPACITY',21X,F16.6/'0',12X,'FLUID DENSIT'
     7,'Y',27X,F16.6/'0',12X,'COOLING FLUID TEMPERATURE',15X
     8,F16.6/'0',12X,'BULK FLUID LINEAR VELOCITY',14X,F16.6/
     9'0',12X,'INLET REACTANT CONCENTRATION',12X,F16.6/'0',
     112X,'INLET FLUID TEMPERATURE',17X,F16.6/'0',12X,'REAC'
     2,'TOR VOID FRACTION',19X,F16.6)
  805 FORMAT ('0',12X,'CATALYST HEAT CAPACITY',18X,F16.6/'0'
     1,12X,'CATALYST DENSITY',24X,F16.6/'0',12X,'CATALYST V'
     2,'OID FRACTION',18X,F16.6)
  910 FORMAT ('0',12X,'HEAT TRANSFER COEFF AT REACTOR WALL',
     15X,F16.6/'0',12X,'HEAT OF REACTION',24X,F16.6/'0',12X,
     2'ITERATION TIME STEP',21X,F16.6/'0',12X,'NO. OF RADIA'
     3,'L POINTS',21X,I8/'0',12X,'NO. OF AXIAL POINTS',22X,
     4I8)
  902 FORMAT ('0',12X,'RATE OF REACTION = ',20A4)
   29 CONTINUE
      CALL COEFF
      QP(1)=3.14159*(DR/2.)**2.
      DO 613 I=2,M
      QP(I)=3.14159*((R(I)+DR/2.)**2.-(R(I)-DR/2.)**2.)
  613 CONTINUE
      QP(MP)=3.14159*(RO**2.-(RO-DR/2.)**2.)
C
C     INITIALIZE REACTOR AT INLET CONDITIONS
C
      DO 40 J=1,300
      C(J)=0.
      T(J)=0.
      S(J)=0.
      X(J)=0.
   40 CONTINUE
      DO 45 J=1,MN
      C(J)=CO
      CN(J)=CO
      T(J)=TO
      TN(J)=TO
   45 CONTINUE
      KT=0
   18 CONTINUE
      NI=0
      TIME=0.
      KZ=0
      JG=1
   51 CALL RETI
      JG=(-1)*JG
      NI=NI+1
      TIME=TIME+DTHETA
C
C     COMPARE (N+1)'TH ITERATION WITH N'TH ITERATION
```

```
C
      DO 81 I=1,MN
      IF (ABS((S(I)-CN(I))/S(I)).GT.EC) GO TO 31
      IF (ABS(X(I)-TN(I)).GT.ET) GO TO 31
   81 CONTINUE
      KZ=1
      GO TO 9
   31 DO 41 I=1,MN
      T(I)=X(I)
      TN(I)=X(I)
      C(I)=S(I)
      CN(I)=S(I)
   41 CONTINUE
      DO 211 I=1,MN
      CNORM(I)=C(I)/CON
  211 CONTINUE
      IF (NI.NE.NPO) GO TO 51
      NPO=NPO+NPT
    9 CONTINUE
      DO 39 JW=1,NO
      IF (KZ.NE.1) GO TO 61
      IF (KT.EQ.0) GO TO 17
      GO TO 19
C
C     PRINT OUT INTERMEDIATE TRANSIENT RESULTS
C
   61 WRITE (6,235) NI,TIME
  235 FORMAT (1H1////' ',18X,'ITERATION NO.',I6,5X,'TIME = '
     1,F10.4,' SEC.'/'-',26X,'NORMALIZED CONCENTRATION PROF'
     2,'ILE')
      GO TO 21
C
C     PRINT OUT INITIAL STEADY STATE CONDITIONS
C
   17 WRITE (6,240) DC,DT
  240 FORMAT (1H1////' ',18X                    /'0',12X,'IN'
     1,'ITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGE'
     2,'S OF'/'0',12X,F10.7,5X,'GM-MOLES/C.C. IN INLET CONC'
     3,'ENTRATION'/'0',12X, F8.2,7X,'DEGREES KELVIN  IN INL'
     4,'ET TEMPERATURE'/'-',26X,'NORMALIZED CONCENTRATION P'
     5,'ROFILE')
      GO TO 21
C
C     PRINT OUT FINAL STEADY STATE CONDITIONS
C
   19 WRITE (6,245) NI,TIME
  245 FORMAT (1H1////' ',18X,'ITERATION NO.',I6,5X,'TIME = '
     1,F10.4,' SEC.'/'0',26X,'FINAL STEADY STATE CONDITIONS'
     2/'-',26X,'NORMALIZED CONCENTRATION PROFILE')
   21 CONTINUE
```

```
      LMN=MN-MP
      BCE=0.
      BTE=0.
      DO 614 I=1,MP
      NML=I+LMN
      BCE=BCE+QP(I)*C(NML)
      BTE=BTE+QP(I)*T(NML)
  614 CONTINUE
      BCE=BCE/((3.14159*(RO**2))*CON)
      BTE=BTE/(3.14159*(RO**2.))
      WRITE (6,200) (R(I),I=1,MP)
  200 FORMAT ('-',12X,'DISTANCE FROM',5(F6.1,4X)/' ',12X,'C'
     1,'ENTER-LINE'/'0',12X,'DISTANCE FROM'/' ',12X,'ENTRAN'
     2,'CE'/' ',12X)
      K=1
      KK=MP
      DO 250 I=1,NP,2
      WRITE (6,204) RL(I),(CNORM(J),J=K,KK)
  204 FORMAT (' ', 9X,F10.2,3X,5F10.5)
      K=K+2*MP
      KK=KK+2*MP
  250 CONTINUE
      WRITE (6,615) BCE
  615 FORMAT ('-',12X,'BULK CONCENTRATION AT REACTOR EXIT = '
     1,F10.6)
      WRITE (6,230)
  230 FORMAT (1H1////' ',24X,'          TEMPERATURE PROFILE')
      WRITE (6,200) (R(I),I=1,MP)
      K=1
      KK=MP
      DO 260 I=1,NP,2
      WRITE (6,207) RL(I),(T(J),J=K,KK)
  207 FORMAT (' ', 9X,F10.2,5X,5(F8.2,2X))
      K=K+2*MP
      KK=KK+2*MP
  260 CONTINUE
      WRITE (6,616) BTE
  616 FORMAT ('-',12X,'BULK TEMPERATURE AT REACTOR EXIT = ',
     1F10.2)
   39 CONTINUE
      IF (KZ.NE.1) GO TO 51
      IF (KT.EQ.1) GO TO 99
C
C     INTRODUCE STEP CHANGE IN INLET CONDITIONS
C
      KT=1
      CO=CO+DC
      TO=TO+DT
      NPO=NPK
      NPT=NPI
```

```
      CALL COEFF
      GO TO 18
   99 STOP
      END
```

```
C                ***** SUBROUTINE COEFF *****
C
      SUBROUTINE COEFF
C     THIS SUBROUTINE CALCULATES THE COEFFICIENTS OF THE NON-
C     LINEAR ALGEBRAIC EQUATIONS DESCRIBING HEAT AND MASS
C     TRANSFER IN THE EXTERNAL REACTOR FIELD.
C
      COMMON C1(300),C2(300),C3(300),C4(300),C5(300),C6(300)
     1,C7(300),C8(300),C9(300),T1(300),T2(300),T3(300),T4(300
     2),T5(300),T6(300),T7(300),T8(300),T9(300),C(330),T(300
     3),S(300),X(300),XN(300),SN(300),CN(300),TN(300),R(10),
     4RO,SO,CO,TO,RADIFF,RRDIFF,RACOND,RRCOND,BVEL,DELH,TW,
     5DTHETA,RHTCP,RDEN,RPOR,WHTC,DT,DC,EC,ET,ES,EX,DR,DX,
     6CPOR
      COMMON RL(100),CNORM(300)
      COMMON CHTCP,CDEN
      COMMON M,N,MP,NP,MN,L,JG,NI,NO
      DR=RO/FLOAT(M)
      DX=SO/FLOAT(N)
      RL(1)=0.
      DO 707 I=2,NP
      RL(I)=RL(I-1)+DX
  707 CONTINUE
      R(1)=0.
      DO 7 I=2,MP
    7 R(I)=R(I-1)+DR
      DO 100 I=1,MN
      L=I+1-(((I-1)/(M+1))*(M+1)+1)
      IF (I.EQ.1) GO TO 10
      IF (I.EQ.MP) GO TO 20
      IF (I.LT.MP) GO TO 30
      IF (I.EQ.MN) GO TO 40
      IF (I.EQ.(MN-M)) GO TO 50
      IF (I.GT.(MN-M)) GO TO 60
      IF (L.EQ.1) GO TO 70
      IF (L.EQ.MP) GO TO 80
      SA=RPOR*3.14159*((R(L)+DR/2.)**2 -(R(L)-DR/2.)**2)
      AO=RPOR*2.*3.14159*DX*(R(L)+DR/2.)
      AI=RPOR*2.*3.14159*DX*(R(L)-DR/2.)
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/RPOR
      C8(I)=0.
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
```

```
      T3(I)=-T1(I)-T2(I)
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)
      T7(I)=DELH*C7(I)
      T8(I)=0.
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
      GO TO 100
   10 AO=RPOR*3.14159*DR*DX/2.
      SA=RPOR*3.14159*(DR**2)/4.
      C1(I)=0.
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)-BVEL*SA
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/(2.*RPOR)
      C8(I)=BVEL*SA*CO
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=0.
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)-BVEL*SA*RHTCP*RDEN
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)
      T7(I)=DELH*C7(I)
      T8(I)=BVEL*SA*RHTCP*RDEN*TO
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
      GO TO 100
   30 AI=RPOR*3.14159*(R(L)-DR/2.)*DX
      AO=RPOR*3.14159*(R(L)+DR/2.)*DX
      SA=RPOR*3.14159*((R(L)+DR/2.)**2-(R(L)-DR/2.)**2)
      C1(I)=0.
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-BVEL*SA
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/(2.*RPOR)
      C8(I)=BVEL*SA*CO
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=0.
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-BVEL*SA*RHTCP*RDEN
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)
      T7(I)=DELH*C7(I)
```

```
      T8(I)=BVEL*SA*RHTCP*RDEN*TO
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
      GO TO 100
   20 SA=RPOR*3.14159*(RO**2-(RO-DR/2.)**2)
      AO=RPOR*3.14159*DX*RO
      AI=RPOR*3.14159*DX*(RO-DR/2.)
      C1(I)=0.
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-BVEL*SA
      C5(I)=0.
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/(2.*RPOR)
      C8(I)=BVEL*SA*CO
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=0.
      T2(I)=RRCOND*AI/DR
      T3(I)=-T2(I)-BVEL*SA*RHTCP*RDEN
      T5(I)=0.
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-AO*WHTC
      T7(I)=DELH*C7(I)
      T8(I)=BVEL*SA*RHTCP*RDEN*TO    +AO*WHTC*TW
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
      GO TO 100
   70 SA=RPOR*3.14159*(DR**2)/4.
      AO=RPOR*3.14159*DR*DX
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/RPOR
      C8(I)=0.
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)
      T7(I)=DELH*C7(I)
      T8(I)=0.
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
      GO TO 100
   80 SA=RPOR*3.14159*(RO*DR-(DR**2)/4.)
```

```
      AO=RPOR*2.*3.14159*DX*RO
      AI=RPOR*2.*3.14159*(RO-DR/2.)*DX
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)
      C5(I)=0.
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/RPOR
      C8(I)=0.
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)
      T5(I)=0.
      T6(I)=RACOND*SA/DX
      T4(I)=-T6(I)                              -AO*WHTC
      T7(I)=DELH*C7(I)
      T8(I)=AO*WHTC*TW
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
      GO TO 100
   50 SA=RPOR*3.14159*(DR**2)/4.
      AO=RPOR*3.14159*DR*DX/2.
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)
      C5(I)=RRDIFF*AO/DR
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/(2.*RPOR)
      C8(I)=0.
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)
      T5(I)=RRCOND*AO/DR
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)
      T7(I)=DELH*C7(I)
      T8(I)=0.
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
      GO TO 100
   60 SA=RPOR*3.14159*((R(L)+DR/2.)**2-(R(L)-DR/2.)**2)
      AO=RPOR*3.14159*DX*(R(L)+DR/2.)
      AI=RPOR*3.14159*DX*(R(L)-DR/2.)
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)
```

```
      C5(I)=RRDIFF*AO/DR
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/(2.*RPOR)
      C8(I)=0.
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)
      T5(I)=RRCOND*AO/DR
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)
      T7(I)=DELH*C7(I)
      T8(I)=0.
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
      GO TO 100
   40 SA=RPOR*3.14159*(RO*DR-(DR**2)/4.)
      AO=RPOR*3.14159*DX*RO
      AI=RPOR*3.14159*DX*(RO-DR/2.)
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)
      C5(I)=0.
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)
      C7(I)=-SA*DX*(1.-RPOR)/(2.*RPOR)
      C8(I)=0.
      C9(I)=(SA*DX/RPOR)*(RPOR+(1.-RPOR)*CPOR)/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)
      T5(I)=0.
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)-AO*WHTC
      T7(I)=DELH*C7(I)
      T8(I)=AO*WHTC*TW
      T9(I)=SA*DX*(RHTCP*RDEN*RPOR+CHTCP*CDEN*(1.-RPOR))/(
     1DTHETA*RPOR)
  100 CONTINUE
      RETURN
      END
```

```
C                ***** SUBROUTINE RETI *****
C
      SUBROUTINE RETI
C
C     THIS SUBROUTINE CALCULATES THE TRANSIENT CONCENTRATION
C     AND TEMPERATURE PROFILES WITHIN THE REACTOR USING THE
C     ALTERNATING DIRECTION EXPLICIT PROCEDURE AS APPLIED TO
C     NONLINEAR EQUATIONS.
C
      COMMON C1(300),C2(300),C3(300),C4(300),C5(300),C6(300)
     1,C7(300),C8(300),C9(300),T1(300),T2(300),T3(300),T4(300
     2),T5(300),T6(300),T7(300),T8(300),T9(300),C(330),T(300
     3),S(300),X(300),XN(300),SN(300),CN(300),TN(300),R(10),
     4RO,SO,CO,TO,RADIFF,RRDIFF,RACOND,RRCOND,BVEL,DELH,TW,
     5DTHETA,RHTCP,RDEN,RPOR,WHTC,DT,DC,EC,ET,ES,EX,DR,DX,
     6CPOR
      COMMON RL(100),CNORM(300)
      COMMON CHTCP,CDEN
      COMMON M,N,MP,NP,MN,L,JG,NI,NO
C
C     THE FOLLOWING STATEMENTS DEFINE THE RATE OF REACTION
C     EXPRESSION AND ITS DERIVATIVE WITH RESPECT TO CONCEN-
C     TRATION WHERE Q AND Z ARE DUMMY VARIABLES REFERRING TO
C     CONCENTRATION AND TEMPERATURE.
C
      F(Q,Z)=(1.0E+08)*EXP(-12000./Z)*Q/(1.0+(1.0E+05)*Q)
      FD(Q,Z,W)=(1.0E+08)*EXP(-12000./Z)*(1.0/((1.0+(1.0E+05
     1)*Q)**2)+(Q/(1.0+(1.0E+05)*Q))*(12000./(Z**2))*W)
      IF (JG.EQ.(-1)) GO TO 401
C
C     FORWARD SWEEP OF THE ADEP
C
      DO 200 I=1,MN
      IMMP=I-MP
      IPMP=I+MP
      L=I+1-(((I-1)/(M+1))*(M+1)+1)
      S(I)=C(I)
      SN(I)=C(I)
      X(I)=T(I)
      XN(I)=T(I)
  280 IF (I.GT.MP) GO TO 230
      IF (I.GT.1) GO TO 220
      GO TO 210
  230 CONTINUE
      FUN=C1(I)*S(IMMP)+C2(I)*S(I-1)+(C3(I)-C9(I))*S(I)+(C4(
     1I)+C9(I))*C(I)+C5(I)*C(I+1)+C6(I)*C(IPMP)+C7(I)*F(S(I)
     2,X(I))+C8(I)
      GO TO 250
  210 FUN=(C3(I)-C9(I))*S(I)+(C4(I)+C9(I))*C(I)+C5(I)*C(I+1)
     1+C6(I)*C(IPMP)+C7(I)*F(S(I),X(I))+C8(I)
```

```
      GO TO 250
  220 FUN=C2(I)*S(I-1)+(C3(I)-C9(I))*S(I)+(C4(I)+C9(I))*C(I)
     1+C5(I)*C(I+1)+C6(I)*C(IPMP)+C7(I)*F(S(I),X(I))+C8(I)
  250 CONTINUE
      DER=-C3(I)+C9(I)-C7(I)*FD(S(I),X(I),((T7(I)/C7(I))*((
     1C3(I)-C9(I))/(T3(I)-T9(I)))))
C
C     NEWTON-RAPHSON ITERATION
C
      S(I)=S(I)+FUN/DER
      IF (S(I).GE.0.) GO TO 811
      S(I)=0.
  811 CONTINUE
      IF (I.EQ.1) GO TO 300
      IF (I.LT.MP) GO TO 310
      X(I)=-(T1(I)*X(IMMP)+T2(I)*X(I-1)+(T4(I)+T9(I))*T(I)+
     1T5(I)*T(I+1)+T6(I)*T(IPMP)+T8(I)-(T7(I)/C7(I))*(C1(I)*
     2S(IMMP)+C2(I)*S(I-1)+(C3(I)-C9(I))*S(I)+(C4(I)+C9(I))*
     3C(I)+C5(I)*C(I+1)+C6(I)*C(IPMP)+C8(I)))/(T3(I)-T9(I))
      GO TO 290
  300 X(I)=-((T4(I)+T9(I))*T(I)+T5(I)*T(I+1)+T6(I)*T(IPMP)+
     1T8(I)-(T7(I)/C7(I))*((C3(I)-C9(I))*S(I)+(C4(I)+C9(I))*
     2C(I)+C5(I)*C(I+1)+C6(I)*C(IPMP)+C8(I)))/(T3(I)-T9(I))
      GO TO 290
  310 X(I)=-(T2(I)*X(I-1)+(T4(I)+T9(I))*T(I)+T5(I)*T(I+1)+
     1T6(I)*T(IPMP)+T8(I)-(T7(I)/C7(I))*(C2(I)*S(I-1)+(C3(I)
     2-C9(I))*S(I)+(C4(I)+C9(I))*C(I)+C5(I)*C(I+1)+C6(I)*C(
     3IPMP)+C8(I)))/(T3(I)-T9(I))
  290 CONTINUE
      IF (S(I).LE.0.) GO TO 200
      IF (ABS((S(I)-SN(I))/S(I)).GT.ES) GO TO 260
      IF (ABS(X(I)-XN(I)).GT.EX) GO TO 260
      GO TO 200
  260 SN(I)=S(I)
      XN(I)=X(I)
      GO TO 280
  200 CONTINUE
      RETURN
C
C     REVERSE SWEEP OF THE ADEP
C
  401 CONTINUE
      DO 400 K=1,MN
      I=MN+1-K
      IMMP=I-MP
      IPMP=I+MP
      L=I+1-(((I-1)/(M+1))*(M+1)+1)
      S(I)=C(I)
      SN(I)=C(I)
      X(I)=T(I)
```

```
      XN(I)=T(I)
  480 IF (I.EQ.1) GO TO 410
      IF (I.LE.MP) GO TO 420
      FUN=C1(I)*C(IMMP)+C2(I)*C(I-1)+(C3(I)+C9(I))*C(I)+(C4(
     1I)-C9(I))*S(I)+C5(I)*S(I+1)+C6(I)*S(IPMP)+C7(I)*F(S(I)
     1,X(I))+C8(I)
      GO TO 450
  410 FUN=(C3(I)+C9(I))*C(I)+(C4(I)-C9(I))*S(I)+C5(I)*S(I+1)
     1+C6(I)*S(IPMP)+C7(I)*F(S(I),X(I))+C8(I)
      GO TO 450
  420 FUN=C2(I)*C(I-1)+(C3(I)+C9(I))*C(I)+(C4(I)-C9(I))*S(I)
     1+C5(I)*S(I+1)+C6(I)*S(IPMP)+C7(I)*F(S(I),X(I))+C8(I)
  450 CONTINUE
      DER=-C4(I)+C9(I)-C7(I)*FD(S(I),X(I),((T7(I)/C7(I))*((
     1C4(I)-C9(I))/(T4(I)-T9(I)))))
C
C     NEWTON-RAPHSON ITERATION
C
      S(I)=S(I)+FUN/DER
      IF (S(I).GE.0.) GO TO 511
      S(I)=0.
  511 CONTINUE
      IF (I.EQ.1) GO TO 500
      IF (I.LT.MP) GO TO 510
      X(I)=-(T1(I)*T(IMMP)+T2(I)*T(I-1)+(T3(I)+T9(I))*T(I)+
     1T5(I)*X(I+1)+T6(I)*X(IPMP)+T8(I)-(T7(I)/C7(I))*(C1(I)*
     2C(IMMP)+C2(I)*C(I-1)+(C3(I)+C9(I))*C(I)+(C4(I)-C9(I))*
     3S(I)+C5(I)*S(I+1)+C6(I)*S(IPMP)+C8(I)))/(T4(I)-T9(I))
      GO TO 490
  500 X(I)=-((T3(I)+T9(I))*T(I)+T5(I)*X(I+1)+T6(I)*X(IPMP)+
     1T8(I)-(T7(I)/C7(I))*((C3(I)+C9(I))*C(I)+(C4(I)-C9(I))*
     2S(I)+C5(I)*S(I+1)+C6(I)*S(IPMP)+C8(I)))/(T4(I)-T9(I))
      GO TO 490
  510 X(I)=-(T2(I)*T(I-1)+(T3(I)+T9(I))*T(I)+T5(I)*X(I+1)+T6
     1(I)*X(IPMP)+T8(I)-(T7(I)/C7(I))*(C2(I)*C(I-1)+(C3(I)+
     2C9(I))*C(I)+(C4(I)-C9(I))*S(I)+C5(I)*S(I+1)+C6(I)*S(
     3IPMP)+C8(I)))/(T4(I)-T9(I))
  490 CONTINUE
      IF (S(I).LE.0.) GO TO 400
      IF (ABS((S(I)-SN(I))/S(I)).GT.ES) GO TO 460
      IF (ABS(X(I)-XN(I)).GT.EX) GO TO 460
      GO TO 400
  460 SN(I)=S(I)
      XN(I)=X(I)
      GO TO 480
  400 CONTINUE
      RETURN
      END
```

APPENDIX C

COMPUTER PROGRAM FOR SURFACE RESISTANCE MODEL OF A PACKED BED REACTOR:

This section illustrates the use of the computer program which calculates the transient response of the surface resistance model to a step change in the inlet conditions. The program is coded in FORTRAN IV for an IBM 360/67 computer. Input data was entered on punched cards and the transient conditions were printed out at designated time intervals on an IBM high-speed printer.

The input variables are defined at the beginning of the program source listing. They must be punched on cards in the order given in this list. Table C-1 presents the input data used for the example in this section in the form in which it is to be punched on cards.

Also, a FORTRAN statement of the reaction rate expression and its derivative with respect to concentration must be included in the source program at the beginning of SUBROUTINE SURF. The correct place for these statements is indicated in the source listing of the program. For the second order reaction rate used in this section, the rate of reaction definition was given by:

```
F(Q,Z) = (1.0E+13)*EXP(-23844./(1.987*Z))*(ABS(Q)**2)
```

The derivative was given by:

```
FD(Q,Z,W) = (1.0E+13)*(EXP(-23844./(1.987*Z)))*(2.*Q +
            (ABS(Q)**2)*23844./(1.987*(Z**2))*W)
```

where Q, Z, and W are dummy variables referring to concentration, temperature, and the derivative of the temperature with respect to concentration. In the transient calculations, this derivative, W, is computed at each time step.

Table C-2 is a set of transient results given in computer output form, for the input parameters of Table C-1.

TABLE C-1

INPUT DATA FOR SURFACE RESISTANCE MODEL PROGRAM

INPUT CARD

	(RRDIFF)	(RADIFF)	(RRCOND)	(RACOND)
1	bbbb.57300000E+00	bbb.31500000E+01	bbb.32100000E-01	bbb.17640000E+00
	(RHTCP)	(RDEN)	(RPOR)	(RO)
2	bbbb.21860000E+02	bbb.25000000E-02	bbb.35000000E+00	bbb.20000000E+01
	(SO)	(TW)	(DTHETA)	(BVEL)
3	bbbb.25000000E+02	bbb.30000000E+03	bbb.20000000E-01	bbb.12600000E+02
	(SAPUV)	(SMTC)	(SHTC)	(CHTCP)
4	bbbb.31415900E+01	bbb.68600000E+00	bbb.55300000E-01	bbb.60000000E+01
	(CDEN)	(CPOR)	(RC)	(CO)
5	bbbb.11200000E-01	bbb.54300000E+00	bbb.25000000E+00	bbb.10000000E-04
	(TO)	(DC)	(DT)	(DELH)
6	bbbb.80000000E+03	bbb.00000000E+00	bbb.40000000E+02	bb-.35040000E-06
	(WHTC)	(EC)	(ET)	(ES)
7	bbbb.11300000E+01	bbb.10000000E-04	bbb.50000000E-01	bbb.10000000E-03
	(EX)			
8	bbbb.50000000E+00			
	(M) (N) (NPK) (NPI) (NO)			
9	bbbbbb4bbbb50bbbb25bbbb25bbbbb1			
	(RRE(I))			
10	b(1.0E+13)*EXP(-23844./(1.987*T))*(C**2)			

TABLE C-2

RESULTS FROM PROGRAM FOR SURFACE RESISTANCE MODEL

PHYSICAL , THERMODYNAMIC AND KINETIC DATA

ALL UNITS ARE IN CM.,SEC.,CAL.,GM.-MOLES,DEGREES KELVIN	
REACTOR LENGTH	25.000000
REACTOR RADIUS	2.000000
RADIAL DIFFUSION COEFFICIENT	0.573000
AXIAL DIFFUSION COEFFICIENT	3.150000
FLUID HEAT CAPACITY	21.859985
FLUID DENSITY	0.002500
COOLING FLUID TEMPERATURE	300.000000
BULK FLUID LINEAR VELOCITY	12.599999
INLET REACTANT CONCENTRATION	0.000010
INLET FLUID TEMPERATURE	800.000000
REACTOR VOID FRACTION	0.350000
MASS TRANSFER COEFF AT CATALYST SURFACE	0.686000
HEAT TRANSFER COEFF AT CATALYST SURFACE	0.055300
CATALYST HEAT CAPACITY	6.000000
CATALYST DENSITY	0.011200
CATALYST VOID FRACTION	0.543000
CATALYST PARTICLE RADIUS	0.250000
CATALYST SURFACE AREA PER UNIT VOLUME	3.141589
HEAT TRANSFER COEFF AT REACTOR WALL	1.129999
HEAT OF REACTION	-350400.000000
ITERATION TIME STEP	0.020000
NO. OF RADIAL POINTS	5
NO. OF AXIAL POINTS	51

RATE OF REACTION = (1.0E+13)*EXP(-23844./(1.987*T))*(C**2)

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

40.00 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.87346	0.87444	0.87998	0.90604	0.98260
1.00	0.66696	0.67152	0.69598	0.79656	0.93709
2.00	0.52021	0.53076	0.58255	0.75611	0.89144
3.00	0.41839	0.43641	0.51737	0.73536	0.85176
4.00	0.35016	0.37609	0.48361	0.71756	0.81762
5.00	0.30699	0.34056	0.46974	0.70013	0.78777
6.00	0.28263	0.32306	0.46782	0.68355	0.76131
7.00	0.27254	0.31867	0.47235	0.66838	0.73772
8.00	0.27337	0.32375	0.47971	0.65487	0.71670
9.00	0.28260	0.33547	0.48783	0.64297	0.69799
10.00	0.29810	0.35157	0.49573	0.63255	0.68138
11.00	0.31797	0.37016	0.50303	0.62344	0.66667
12.00	0.34043	0.38972	0.50966	0.61548	0.65368
13.00	0.36387	0.40907	0.51565	0.60853	0.64222
14.00	0.38697	0.42743	0.52106	0.60247	0.63213
15.00	0.40877	0.44434	0.52595	0.59719	0.62326
16.00	0.42870	0.45959	0.53035	0.59260	0.61547
17.00	0.44653	0.47313	0.53430	0.58861	0.60865
18.00	0.46224	0.48505	0.53783	0.58515	0.60268
19.00	0.47593	0.49546	0.54097	0.58214	0.59747
20.00	0.48781	0.50452	0.54375	0.57954	0.59291
21.00	0.49806	0.51237	0.54619	0.57729	0.58894
22.00	0.50690	0.51918	0.54834	0.57534	0.58548
23.00	0.51449	0.52504	0.55022	0.57365	0.58247
24.00	0.52084	0.52995	0.55180	0.57223	0.57994
25.00	0.52423	0.53259	0.55265	0.57145	0.57856

BULK CONCENTRATION AT REACTOR EXIT = 0.562823

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	807.67	807.01	802.72	773.06	470.98
1.00	818.77	815.80	798.59	712.45	330.89
2.00	823.66	817.04	783.95	659.83	318.20
3.00	822.85	811.92	763.50	617.35	315.37
4.00	817.06	801.78	740.23	583.15	313.64
5.00	807.09	787.87	715.99	555.20	312.27
6.00	793.77	771.24	691.85	531.94	311.14
7.00	777.88	752.75	668.46	512.20	310.18
8.00	760.09	733.10	646.16	495.19	309.36
9.00	740.99	712.82	625.09	480.30	308.64
10.00	721.09	692.35	605.29	467.13	308.00
11.00	700.81	672.02	586.72	455.34	307.43
12.00	680.50	652.09	569.32	444.71	306.92
13.00	660.46	632.75	553.01	435.06	306.46
14.00	640.90	614.11	537.72	426.22	306.04
15.00	621.99	596.27	523.39	418.11	305.65
16.00	603.83	579.26	509.94	410.62	305.29
17.00	586.49	563.10	497.32	403.69	304.96
18.00	569.99	547.77	485.47	397.25	304.65
19.00	554.33	533.28	474.35	391.26	304.36
20.00	539.51	519.59	463.91	385.67	304.09
21.00	525.50	506.67	454.11	380.46	303.84
22.00	512.28	494.50	444.91	375.58	303.61
23.00	499.87	483.08	436.31	371.05	303.39
24.00	488.65	472.76	428.56	366.96	303.20
25.00	482.34	466.97	424.21	364.68	303.09

BULK TEMPERATURE AT REACTOR EXIT = 379.75

NORMALIZED CATALYST CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.29378	0.29537	0.30588	0.38905	0.98249
1.00	0.24220	0.24818	0.28574	0.56134	0.93709
2.00	0.20773	0.21959	0.28966	0.67857	0.89144
3.00	0.18591	0.20442	0.30907	0.71236	0.85176
4.00	0.17393	0.19964	0.33830	0.71039	0.81762
5.00	0.17015	0.20355	0.37205	0.69769	0.78777
6.00	0.17366	0.21510	0.40521	0.68264	0.76131
7.00	0.18397	0.23334	0.43409	0.66802	0.73772
8.00	0.20069	0.25710	0.45724	0.65471	0.71670
9.00	0.22326	0.28478	0.47501	0.64290	0.69799
10.00	0.25067	0.31444	0.48854	0.63252	0.68138
11.00	0.28137	0.34411	0.49904	0.62342	0.66667
12.00	0.31342	0.37220	0.50746	0.61547	0.65368
13.00	0.34487	0.39775	0.51444	0.60853	0.64222
14.00	0.37420	0.42036	0.52039	0.60247	0.63213
15.00	0.40053	0.44004	0.52558	0.59719	0.62326
16.00	0.42357	0.45702	0.53015	0.59259	0.61547
17.00	0.44341	0.47163	0.53419	0.58861	0.60865
18.00	0.46038	0.48417	0.53776	0.58514	0.60268
19.00	0.47484	0.49496	0.54093	0.58214	0.59746
20.00	0.48717	0.50423	0.54372	0.57954	0.59291
21.00	0.49769	0.51220	0.54618	0.57729	0.58894
22.00	0.50668	0.51907	0.54833	0.57533	0.58548
23.00	0.51436	0.52498	0.55021	0.57364	0.58247
24.00	0.52075	0.52991	0.55179	0.57221	0.57993
25.00	0.52416	0.53255	0.55264	0.57144	0.57855

CATALYST TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	832.87	832.18	827.67	795.53	470.98
1.00	837.23	834.20	816.42	722.67	330.89
2.00	837.24	830.56	796.68	663.20	318.20
3.00	832.95	822.00	772.55	618.35	315.37
4.00	824.72	809.45	746.55	583.46	313.64
5.00	813.04	793.82	720.23	555.31	312.27
6.00	798.51	775.93	694.57	531.98	311.14
7.00	781.73	756.46	670.12	512.22	310.18
8.00	763.25	735.99	647.13	495.19	309.35
9.00	743.57	715.02	625.65	480.30	308.64
10.00	723.15	693.97	605.60	467.13	308.00
11.00	702.40	673.16	586.89	455.34	307.43
12.00	681.68	652.85	569.41	444.71	306.92
13.00	661.28	633.24	553.06	435.05	306.46
14.00	641.45	614.42	537.75	426.22	306.03
15.00	622.35	596.46	523.40	418.11	305.65
16.00	604.06	579.37	509.95	410.62	305.29
17.00	586.63	563.16	497.32	403.69	304.96
18.00	570.07	547.81	485.48	397.25	304.65
19.00	554.39	533.31	474.36	391.26	304.36
20.00	539.55	519.61	463.92	385.67	304.09
21.00	525.53	506.69	454.12	380.46	303.84
22.00	512.31	494.52	444.93	375.59	303.61
23.00	499.91	483.11	436.33	371.06	303.39
24.00	488.69	472.80	428.59	366.98	303.20
25.00	482.39	467.02	424.25	364.70	303.09

ITERATION NO. 25 TIME = 0.5000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.86226	0.86307	0.86775	0.89102	0.98016
1.00	0.64312	0.64698	0.66817	0.76076	0.92839
2.00	0.49432	0.50365	0.55062	0.71962	0.87902
3.00	0.39598	0.41260	0.48893	0.70831	0.83970
4.00	0.33333	0.35804	0.46222	0.70005	0.80824
5.00	0.29570	0.32841	0.45572	0.68973	0.78148
6.00	0.27577	0.31570	0.45968	0.67782	0.75756
7.00	0.26873	0.31462	0.46807	0.66544	0.73570
8.00	0.27143	0.32170	0.47765	0.65346	0.71569
9.00	0.28168	0.33452	0.48692	0.64234	0.69752
10.00	0.29769	0.35116	0.49535	0.63228	0.68118
11.00	0.31781	0.37000	0.50288	0.62334	0.66659
12.00	0.34037	0.38965	0.50960	0.61544	0.65365
13.00	0.36385	0.40905	0.51563	0.60852	0.64221
14.00	0.38696	0.42743	0.52106	0.60247	0.63213
15.00	0.40877	0.44434	0.52595	0.59719	0.62326
16.00	0.42871	0.45959	0.53035	0.59260	0.61547
17.00	0.44654	0.47314	0.53430	0.58861	0.60865
18.00	0.46224	0.48505	0.53783	0.58515	0.60268
19.00	0.47594	0.49547	0.54097	0.58215	0.59747
20.00	0.48782	0.50453	0.54375	0.57955	0.59292
21.00	0.49808	0.51239	0.54621	0.57730	0.58895
22.00	0.50692	0.51920	0.54836	0.57535	0.58550
23.00	0.51453	0.52507	0.55025	0.57367	0.58250
24.00	0.52088	0.53000	0.55184	0.57226	0.57997
25.00	0.52429	0.53265	0.55270	0.57150	0.57861

BULK CONCENTRATION AT REACTOR EXIT = 0.562872

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	846.97	846.30	841.84	810.42	484.63
1.00	854.67	851.62	833.80	743.13	333.27
2.00	853.37	846.62	812.58	682.85	319.42
3.00	845.20	834.10	784.61	633.19	316.19
4.00	832.40	816.96	754.45	593.25	314.18
5.00	816.74	797.39	724.77	561.20	312.60
6.00	799.37	776.73	696.85	535.26	311.33
7.00	780.88	755.69	671.10	513.93	310.28
8.00	761.59	734.56	647.46	496.03	309.41
9.00	741.69	713.50	625.69	480.69	308.66
10.00	721.40	692.65	605.55	467.29	308.01
11.00	700.94	672.15	586.83	455.41	307.44
12.00	680.55	652.14	569.36	444.74	306.92
13.00	660.48	632.76	553.03	435.06	306.46
14.00	640.91	614.12	537.73	426.23	306.04
15.00	621.99	596.27	523.39	418.11	305.65
16.00	603.83	579.26	509.94	410.62	305.29
17.00	586.49	563.09	497.32	403.69	304.96
18.00	569.98	547.77	485.47	397.25	304.65
19.00	554.32	533.27	474.34	391.25	304.36
20.00	539.48	519.56	463.89	385.66	304.09
21.00	525.46	506.63	454.08	380.44	303.84
22.00	512.22	494.44	444.87	375.56	303.61
23.00	499.78	483.00	436.25	371.01	303.39
24.00	488.52	472.65	428.47	366.92	303.20
25.00	482.18	466.82	424.10	364.62	303.09

BULK TEMPERATURE AT REACTOR EXIT = 379.68

NORMALIZED CATALYST CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.22152	0.22266	0.23033	0.29317	0.98030
1.00	0.19041	0.19496	0.22398	0.45892	0.92984
2.00	0.17215	0.18181	0.23999	0.61862	0.88168
3.00	0.16248	0.17861	0.27197	0.68464	0.84288
4.00	0.15919	0.18287	0.31372	0.69650	0.81116
5.00	0.16134	0.19333	0.35791	0.69049	0.78371
6.00	0.16870	0.20932	0.39809	0.67901	0.75903
7.00	0.18136	0.23034	0.43086	0.66628	0.73656
8.00	0.19941	0.25567	0.45588	0.65393	0.71615
9.00	0.22268	0.28416	0.47447	0.64256	0.69775
10.00	0.25043	0.31419	0.48834	0.63238	0.68128
11.00	0.28129	0.34402	0.49897	0.62337	0.66664
12.00	0.31339	0.37217	0.50743	0.61546	0.65367
13.00	0.34486	0.39774	0.51443	0.60852	0.64221
14.00	0.37420	0.42036	0.52039	0.60247	0.63213
15.00	0.40053	0.44004	0.52558	0.59719	0.62326
16.00	0.42357	0.45702	0.53015	0.59259	0.61547
17.00	0.44342	0.47163	0.53419	0.58861	0.60865
18.00	0.46039	0.48418	0.53777	0.58515	0.60268
19.00	0.47485	0.49496	0.54093	0.58215	0.59747
20.00	0.48719	0.50424	0.54373	0.57955	0.59292
21.00	0.49771	0.51222	0.54619	0.57730	0.58895
22.00	0.50671	0.51910	0.54835	0.57535	0.58549
23.00	0.51440	0.52502	0.55024	0.57367	0.58250
24.00	0.52081	0.52996	0.55184	0.57226	0.57997
25.00	0.52424	0.53262	0.55270	0.57150	0.57860

CATALYST TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	873.32	872.63	868.07	835.10	484.48
1.00	870.80	867.74	849.70	753.41	333.14
2.00	862.52	855.79	821.50	683.75	319.26
3.00	850.29	839.28	789.37	630.93	316.03
4.00	835.60	820.27	756.95	590.76	314.04
5.00	819.32	800.06	726.13	559.30	312.50
6.00	801.87	779.26	697.66	534.02	311.26
7.00	783.40	758.11	671.62	513.20	310.24
8.00	764.02	736.76	647.82	495.64	309.38
9.00	743.91	715.36	625.94	480.50	308.65
10.00	723.29	694.10	605.72	467.20	308.01
11.00	702.45	673.21	586.94	455.37	307.44
12.00	681.69	652.87	569.43	444.72	306.92
13.00	661.29	633.24	553.07	435.06	306.46
14.00	641.46	614.42	537.75	426.23	306.03
15.00	622.35	596.46	523.40	418.11	305.65
16.00	604.06	579.37	509.95	410.62	305.29
17.00	586.62	563.16	497.32	403.69	304.96
18.00	570.06	547.80	485.47	397.25	304.65
19.00	554.37	533.29	474.34	391.25	304.36
20.00	539.51	519.58	463.90	385.66	304.09
21.00	525.48	506.64	454.08	380.44	303.84
22.00	512.24	494.45	444.87	375.56	303.61
23.00	499.80	483.01	436.26	371.02	303.39
24.00	488.54	472.66	428.49	366.93	303.20
25.00	482.20	466.84	424.12	364.63	303.09

ITERATION NO. 50 TIME = 1.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.86059	0.86136	0.86585	0.88864	0.97912
1.00	0.63682	0.64043	0.66048	0.74993	0.92355
2.00	0.48174	0.49026	0.53389	0.69683	0.86747
3.00	0.37686	0.39180	0.46211	0.67728	0.82090
4.00	0.30878	0.33091	0.42702	0.66534	0.78403
5.00	0.26784	0.29737	0.41618	0.65478	0.75482
6.00	0.24716	0.28385	0.42066	0.64535	0.73139
7.00	0.24177	0.28486	0.43351	0.63738	0.71226
8.00	0.24792	0.29614	0.44960	0.63076	0.69626
9.00	0.26259	0.31416	0.46572	0.62507	0.68248
10.00	0.28322	0.33603	0.48026	0.61989	0.67022
11.00	0.30752	0.35945	0.49271	0.61490	0.65905
12.00	0.33350	0.38273	0.50308	0.60999	0.64873
13.00	0.35952	0.40474	0.51164	0.60515	0.63915
14.00	0.38438	0.42488	0.51872	0.60048	0.63031
15.00	0.40730	0.44290	0.52464	0.59607	0.62223
16.00	0.42791	0.45881	0.52965	0.59199	0.61492
17.00	0.44613	0.47273	0.53394	0.58829	0.60836
18.00	0.46204	0.48485	0.53765	0.58499	0.60254
19.00	0.47585	0.49537	0.54089	0.58207	0.59740
20.00	0.48777	0.50449	0.54371	0.57952	0.59289
21.00	0.49806	0.51237	0.54619	0.57729	0.58894
22.00	0.50692	0.51919	0.54836	0.57535	0.58549
23.00	0.51453	0.52508	0.55025	0.57368	0.58250
24.00	0.52089	0.53001	0.55185	0.57227	0.57998
25.00	0.52431	0.53266	0.55272	0.57151	0.57862

BULK CONCENTRATION AT REACTOR EXIT = 0.562883

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	848.29	847.61	843.08	811.42	484.68
1.00	859.69	856.59	838.49	746.83	333.42
2.00	863.35	856.45	821.75	689.74	319.70
3.00	859.81	848.46	797.82	642.43	316.58
4.00	849.99	834.19	770.07	603.54	314.62
5.00	835.10	815.30	740.77	571.28	313.05
6.00	816.48	793.37	711.47	544.18	311.73
7.00	795.40	769.76	683.26	521.19	310.61
8.00	772.98	745.55	656.80	501.52	309.66
9.00	750.03	721.52	632.40	484.59	308.84
10.00	727.14	698.14	610.09	469.91	308.14
11.00	704.68	675.71	589.74	457.08	307.52
12.00	682.87	654.34	571.14	445.76	306.97
13.00	661.84	634.06	554.07	435.66	306.49
14.00	641.68	614.85	538.31	426.56	306.05
15.00	622.41	596.66	523.70	418.29	305.66
16.00	604.05	579.46	510.10	410.71	305.29
17.00	586.59	563.19	497.40	403.73	304.96
18.00	570.03	547.81	485.50	397.27	304.65
19.00	554.34	533.29	474.36	391.26	304.36
20.00	539.49	519.57	463.90	385.66	304.09
21.00	525.45	506.63	454.08	380.44	303.84
22.00	512.21	494.43	444.86	375.56	303.61
23.00	499.76	482.98	436.23	371.00	303.39
24.00	488.48	472.61	428.45	366.91	303.20
25.00	482.13	466.78	424.07	364.61	303.09

BULK TEMPERATURE AT REACTOR EXIT = 379.66

NORMALIZED CATALYST CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.21696	0.21809	0.22564	0.28762	0.97898
1.00	0.17893	0.18320	0.21049	0.43304	0.92387
2.00	0.15457	0.16317	0.21516	0.57428	0.86834
3.00	0.14045	0.15423	0.23506	0.64127	0.82253
4.00	0.13453	0.15442	0.26761	0.65713	0.78649
5.00	0.13578	0.16290	0.30918	0.65507	0.75801
6.00	0.14382	0.17928	0.35388	0.64841	0.73504
7.00	0.15858	0.20297	0.39528	0.64126	0.71605
8.00	0.17987	0.23272	0.42952	0.63463	0.69987
9.00	0.20703	0.26641	0.45602	0.62851	0.68564
10.00	0.23876	0.30150	0.47601	0.62269	0.67280
11.00	0.27319	0.33555	0.49108	0.61702	0.66101
12.00	0.30815	0.36687	0.50259	0.61149	0.65012
13.00	0.34168	0.39459	0.51158	0.60616	0.64009
14.00	0.37237	0.41857	0.51879	0.60112	0.63091
15.00	0.39953	0.43907	0.52471	0.59645	0.62259
16.00	0.42305	0.45652	0.52969	0.59221	0.61512
17.00	0.44316	0.47138	0.53396	0.58841	0.60847
18.00	0.46026	0.48406	0.53766	0.58505	0.60260
19.00	0.47480	0.49491	0.54088	0.58210	0.59743
20.00	0.48716	0.50422	0.54371	0.57953	0.59290
21.00	0.49770	0.51222	0.54619	0.57729	0.58894
22.00	0.50671	0.51910	0.54835	0.57535	0.58550
23.00	0.51441	0.52502	0.55025	0.57368	0.58250
24.00	0.52082	0.52998	0.55185	0.57227	0.57998
25.00	0.52425	0.53264	0.55271	0.57151	0.57862

CATALYST TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	876.13	875.43	870.78	837.45	484.68
1.00	879.04	875.92	857.55	760.22	333.41
2.00	876.37	869.49	834.53	694.28	319.67
3.00	868.12	856.87	805.97	642.84	316.54
4.00	854.92	839.29	774.72	602.48	314.57
5.00	837.75	818.16	742.81	569.73	312.99
6.00	817.77	794.83	711.73	542.54	311.67
7.00	796.01	770.44	682.50	519.67	310.56
8.00	773.35	745.84	655.64	500.24	309.62
9.00	750.38	721.63	631.23	483.59	308.81
10.00	727.54	698.19	609.11	469.17	308.11
11.00	705.09	675.74	589.01	456.57	307.50
12.00	683.26	654.36	570.64	445.42	306.96
13.00	662.18	634.08	553.75	435.45	306.48
14.00	641.94	614.87	538.12	426.43	306.05
15.00	622.60	596.69	523.59	418.22	305.65
16.00	604.18	579.48	510.04	410.67	305.29
17.00	586.68	563.21	497.36	403.71	304.96
18.00	570.09	547.83	485.49	397.26	304.65
19.00	554.37	533.29	474.35	391.26	304.36
20.00	539.51	519.58	463.89	385.66	304.09
21.00	525.47	506.63	454.08	380.44	303.84
22.00	512.22	494.43	444.86	375.56	303.61
23.00	499.76	482.98	436.24	371.00	303.39
24.00	488.49	472.62	428.45	366.91	303.20
25.00	482.14	466.78	424.07	364.61	303.09

ITERATION NO. 100 TIME = 2.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.86038	0.86114	0.86561	0.88834	0.97895
1.00	0.63584	0.63941	0.65931	0.74829	0.92265
2.00	0.47920	0.48756	0.53052	0.69203	0.86471
3.00	0.37176	0.38623	0.45477	0.66826	0.81486
4.00	0.29996	0.32104	0.41367	0.65145	0.77339
5.00	0.25407	0.28170	0.39497	0.63523	0.73849
6.00	0.22725	0.26104	0.39063	0.61945	0.70866
7.00	0.21483	0.25416	0.39510	0.60496	0.68300
8.00	0.21364	0.25763	0.40439	0.59238	0.66099
9.00	0.22149	0.26895	0.41585	0.58197	0.64234
10.00	0.23670	0.28609	0.42797	0.57375	0.62679
11.00	0.25771	0.30725	0.44007	0.56759	0.61413
12.00	0.28288	0.33075	0.45193	0.56333	0.60410
13.00	0.31046	0.35515	0.46351	0.56073	0.59641
14.00	0.33877	0.37927	0.47477	0.55953	0.59071
15.00	0.36643	0.40229	0.48562	0.55945	0.58667
16.00	0.39246	0.42371	0.49594	0.56017	0.58391
17.00	0.41626	0.44323	0.50559	0.56140	0.58209
18.00	0.43758	0.46071	0.51443	0.56287	0.58089
19.00	0.45634	0.47612	0.52235	0.56436	0.58003
20.00	0.47262	0.48953	0.52930	0.56570	0.57932
21.00	0.48659	0.50105	0.53527	0.56679	0.57862
22.00	0.49846	0.51084	0.54029	0.56758	0.57785
23.00	0.50844	0.51907	0.54444	0.56807	0.57698
24.00	0.51660	0.52577	0.54775	0.56831	0.57608
25.00	0.52110	0.52949	0.54965	0.56855	0.57570

BULK CONCENTRATION AT REACTOR EXIT = 0.559877

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	848.47	847.78	843.24	811.54	484.68
1.00	860.54	857.42	839.23	747.38	333.45
2.00	865.64	858.68	823.75	691.18	319.77
3.00	864.48	852.99	801.85	645.15	316.71
4.00	857.85	841.79	776.76	607.76	314.83
5.00	846.59	826.39	750.40	577.07	313.32
6.00	831.54	807.87	723.89	551.40	312.07
7.00	813.48	787.10	697.87	529.48	311.01
8.00	793.11	764.78	672.73	510.43	310.09
9.00	771.06	741.52	648.69	493.61	309.27
10.00	747.91	717.81	625.86	478.58	308.55
11.00	724.20	694.10	604.30	465.04	307.90
12.00	700.41	670.79	584.03	452.76	307.31
13.00	676.98	648.19	565.05	441.60	306.77
14.00	654.26	626.55	547.35	431.44	306.28
15.00	632.51	606.04	530.91	422.16	305.84
16.00	611.91	586.75	515.68	413.70	305.44
17.00	592.53	568.69	501.59	405.98	305.07
18.00	574.39	551.84	488.57	398.91	304.73
19.00	557.46	536.16	476.54	392.43	304.42
20.00	541.66	521.57	465.42	386.47	304.13
21.00	526.93	507.99	455.11	380.99	303.87
22.00	513.18	495.32	445.54	375.92	303.63
23.00	500.38	483.55	436.67	371.24	303.40
24.00	488.87	472.97	428.72	367.05	303.20
25.00	482.39	467.02	424.25	364.70	303.09

BULK TEMPERATURE AT REACTOR EXIT = 379.78

NORMALIZED CATALYST CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.21640	0.21754	0.22514	0.28709	0.97875
1.00	0.17705	0.18131	0.20842	0.42929	0.92266
2.00	0.15054	0.15895	0.20974	0.56414	0.86473
3.00	0.13345	0.14655	0.22366	0.62649	0.81492
4.00	0.12370	0.14200	0.24724	0.63827	0.77352
5.00	0.12016	0.14425	0.27770	0.63102	0.73873
6.00	0.12236	0.15296	0.31160	0.61828	0.70906
7.00	0.13030	0.16805	0.34504	0.60502	0.68362
8.00	0.14423	0.18934	0.37489	0.59311	0.66190
9.00	0.16439	0.21619	0.39985	0.58320	0.64359
10.00	0.19065	0.24725	0.42026	0.57544	0.62844
11.00	0.22214	0.28053	0.43725	0.56972	0.61619
12.00	0.25714	0.31390	0.45193	0.56586	0.60655
13.00	0.29334	0.34567	0.46512	0.56359	0.59919
14.00	0.32855	0.37487	0.47729	0.56264	0.59374
15.00	0.36122	0.40114	0.48860	0.56267	0.58983
16.00	0.39057	0.42446	0.49908	0.56338	0.58707
17.00	0.41637	0.44497	0.50868	0.56449	0.58513
18.00	0.43875	0.46286	0.51732	0.56572	0.58370
19.00	0.45797	0.47832	0.52494	0.56690	0.58254
20.00	0.47433	0.49156	0.53153	0.56789	0.58148
21.00	0.48816	0.50281	0.53712	0.56861	0.58041
22.00	0.49980	0.51229	0.54178	0.56904	0.57929
23.00	0.50953	0.52021	0.54560	0.56921	0.57810
24.00	0.51744	0.52664	0.54863	0.56917	0.57693
25.00	0.52178	0.53019	0.55035	0.56924	0.57638

CATALYST TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	876.46	875.75	871.07	837.67	484.69
1.00	880.47	877.31	858.82	761.24	333.45
2.00	879.89	872.93	837.66	696.72	319.77
3.00	874.74	863.31	811.81	646.91	316.71
4.00	865.30	849.38	783.82	608.24	314.82
5.00	852.05	832.02	755.21	577.09	313.32
6.00	835.53	812.02	726.87	551.20	312.06
7.00	816.34	790.06	699.41	529.15	311.00
8.00	795.04	766.73	673.19	509.97	310.07
9.00	772.21	742.56	648.40	493.05	309.26
10.00	748.39	718.07	625.09	477.94	308.53
11.00	724.09	693.72	603.24	464.35	307.88
12.00	699.84	669.95	582.84	452.07	307.29
13.00	676.08	647.09	563.85	440.93	306.75
14.00	653.18	625.35	546.21	430.81	306.26
15.00	631.40	604.86	529.88	421.61	305.82
16.00	610.86	585.67	514.79	413.23	305.42
17.00	591.60	567.77	500.85	405.58	305.05
18.00	573.62	551.09	487.98	398.59	304.72
19.00	556.84	535.57	476.08	392.18	304.41
20.00	541.19	521.13	465.07	386.29	304.13
21.00	526.58	507.66	454.86	380.85	303.86
22.00	512.93	495.09	445.36	375.82	303.62
23.00	500.21	483.39	436.55	371.17	303.40
24.00	488.75	472.86	428.64	367.01	303.20
25.00	482.31	466.94	424.19	364.67	303.09

ITERATION NO. 150 TIME = 2.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.86037	0.86114	0.86561	0.88834	0.97895
1.00	0.63581	0.63938	0.65928	0.74825	0.92263
2.00	0.47911	0.48748	0.53042	0.69189	0.86463
3.00	0.37156	0.38601	0.45449	0.66794	0.81465
4.00	0.29952	0.32055	0.41303	0.65085	0.77295
5.00	0.25319	0.28070	0.39364	0.63419	0.73765
6.00	0.22560	0.25916	0.38819	0.61770	0.70718
7.00	0.21193	0.25086	0.39105	0.60213	0.68054
8.00	0.20883	0.25224	0.39827	0.58800	0.65711
9.00	0.21398	0.26072	0.40724	0.57552	0.63650
10.00	0.22563	0.27430	0.41646	0.56467	0.61843
11.00	0.24233	0.29134	0.42525	0.55533	0.60266
12.00	0.26270	0.31042	0.43342	0.54738	0.58899
13.00	0.28536	0.33033	0.44101	0.54074	0.57726
14.00	0.30897	0.35011	0.44816	0.53531	0.56731
15.00	0.33240	0.36912	0.45498	0.53103	0.55904
16.00	0.35483	0.38700	0.46160	0.52786	0.55234
17.00	0.37579	0.40363	0.46811	0.52575	0.54711
18.00	0.39510	0.41901	0.47458	0.52464	0.54326
19.00	0.41279	0.43325	0.48106	0.52448	0.54069
20.00	0.42899	0.44647	0.48757	0.52519	0.53928
21.00	0.44384	0.45877	0.49410	0.52668	0.53890
22.00	0.45748	0.47025	0.50064	0.52881	0.53942
23.00	0.47001	0.48095	0.50709	0.53147	0.54066
24.00	0.48120	0.49063	0.51325	0.53442	0.54242
25.00	0.48816	0.49678	0.51749	0.53693	0.54429

BULK CONCENTRATION AT REACTOR EXIT = 0.528015

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	848.48	847.79	843.24	811.54	484.68
1.00	860.56	857.44	839.25	747.39	333.45
2.00	865.72	858.76	823.82	691.22	319.77
3.00	864.68	853.18	802.01	645.25	316.72
4.00	858.29	842.21	777.11	607.97	314.84
5.00	847.46	827.22	751.10	577.46	313.34
6.00	833.08	809.33	725.10	552.06	312.10
7.00	815.95	789.44	699.80	530.52	311.06
8.00	796.80	768.28	675.55	511.93	310.16
9.00	776.20	746.37	652.53	495.65	309.37
10.00	754.65	724.13	630.79	481.19	308.67
11.00	732.54	701.90	610.30	468.21	308.05
12.00	710.24	679.93	591.00	456.44	307.48
13.00	688.01	658.41	572.79	445.69	306.97
14.00	666.12	637.51	555.62	435.79	306.49
15.00	644.78	617.34	539.41	426.64	306.05
16.00	624.14	597.99	524.12	418.14	305.65
17.00	604.32	579.51	509.71	410.24	305.27
18.00	585.41	561.96	496.16	402.89	304.92
19.00	567.46	545.35	483.43	396.04	304.59
20.00	550.51	529.69	471.50	389.66	304.28
21.00	534.55	514.98	460.34	383.73	304.00
22.00	519.59	501.20	449.94	378.22	303.74
23.00	505.65	488.38	440.28	373.13	303.49
24.00	493.13	476.87	431.64	368.58	303.28
25.00	486.02	470.35	426.74	366.01	303.15

BULK TEMPERATURE AT REACTOR EXIT = 381.38

NORMALIZED CATALYST CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.21639	0.21753	0.22513	0.28708	0.97874
1.00	0.17700	0.18126	0.20837	0.42920	0.92263
2.00	0.15040	0.15880	0.20956	0.56383	0.86463
3.00	0.13314	0.14622	0.22319	0.62592	0.81465
4.00	0.12309	0.14130	0.24613	0.63738	0.77295
5.00	0.11899	0.14287	0.27541	0.62962	0.73766
6.00	0.12025	0.15039	0.30750	0.61604	0.70720
7.00	0.12667	0.16356	0.33863	0.60151	0.68057
8.00	0.13825	0.18202	0.36592	0.58779	0.65716
9.00	0.15504	0.20509	0.38819	0.57551	0.63659
10.00	0.17686	0.23165	0.40569	0.56477	0.61858
11.00	0.20309	0.26013	0.41943	0.55555	0.60288
12.00	0.23255	0.28884	0.43049	0.54773	0.58932
13.00	0.26354	0.31633	0.43977	0.54122	0.57772
14.00	0.29427	0.34168	0.44794	0.53597	0.56794
15.00	0.32329	0.36455	0.45542	0.53189	0.55987
16.00	0.34980	0.38500	0.46252	0.52895	0.55340
17.00	0.37356	0.40330	0.46942	0.52710	0.54843
18.00	0.39473	0.41977	0.47622	0.52626	0.54485
19.00	0.41364	0.43474	0.48300	0.52638	0.54255
20.00	0.43062	0.44845	0.48977	0.52734	0.54140
21.00	0.44599	0.46111	0.49653	0.52905	0.54125
22.00	0.45997	0.47283	0.50324	0.53136	0.54195
23.00	0.47269	0.48368	0.50981	0.53414	0.54331
24.00	0.48398	0.49342	0.51602	0.53715	0.54513
25.00	0.49095	0.49958	0.52027	0.53967	0.54701

CATALYST TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	876.46	875.76	871.08	837.67	484.69
1.00	880.50	877.35	858.85	761.26	333.45
2.00	880.00	873.04	837.76	696.79	319.77
3.00	875.04	863.59	812.06	647.07	316.72
4.00	865.95	849.99	784.36	608.55	314.84
5.00	853.27	833.19	756.22	577.65	313.34
6.00	837.61	814.01	728.58	552.12	312.10
7.00	819.58	793.17	702.02	530.52	311.06
8.00	799.74	771.21	676.87	511.90	310.16
9.00	778.57	748.61	653.22	495.58	309.37
10.00	756.49	725.73	631.07	481.09	308.67
11.00	733.87	702.91	610.29	468.07	308.04
12.00	711.05	680.41	590.78	456.26	307.48
13.00	688.35	658.45	572.43	445.46	306.96
14.00	666.04	637.21	555.14	435.52	306.48
15.00	644.35	616.79	538.84	426.33	306.04
16.00	623.46	597.26	523.49	417.81	305.64
17.00	603.48	578.68	509.04	409.89	305.26
18.00	584.48	561.07	495.46	402.52	304.90
19.00	566.50	544.44	482.73	395.68	304.58
20.00	549.56	528.81	470.83	389.31	304.27
21.00	533.65	514.15	459.72	383.41	303.99
22.00	518.77	500.45	449.37	377.93	303.73
23.00	504.92	487.71	439.78	372.87	303.48
24.00	492.49	476.29	431.20	368.35	303.27
25.00	485.45	469.82	426.35	365.80	303.15

ITERATION NO. 200 TIME = 3.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.86037	0.86114	0.86561	0.88834	0.97895
1.00	0.63581	0.63938	0.65928	0.74825	0.92263
2.00	0.47911	0.48747	0.53041	0.69189	0.86463
3.00	0.37155	0.38600	0.45448	0.66793	0.81465
4.00	0.29951	0.32053	0.41300	0.65083	0.77293
5.00	0.25314	0.28065	0.39358	0.63414	0.73762
6.00	0.22550	0.25905	0.38805	0.61761	0.70712
7.00	0.21173	0.25064	0.39079	0.60198	0.68041
8.00	0.20846	0.25182	0.39782	0.58774	0.65689
9.00	0.21329	0.25997	0.40652	0.57508	0.63613
10.00	0.22444	0.27306	0.41538	0.56396	0.61782
11.00	0.24041	0.28941	0.42368	0.55423	0.60169
12.00	0.25980	0.30760	0.43120	0.54575	0.58752
13.00	0.28122	0.32641	0.43796	0.53836	0.57508
14.00	0.30339	0.34490	0.44404	0.53195	0.56420
15.00	0.32520	0.36243	0.44953	0.52642	0.55470
16.00	0.34583	0.37861	0.45453	0.52168	0.54645
17.00	0.36480	0.39329	0.45911	0.51767	0.53934
18.00	0.38192	0.40647	0.46333	0.51432	0.53325
19.00	0.39718	0.41823	0.46727	0.51160	0.52812
20.00	0.41072	0.42874	0.47097	0.50948	0.52387
21.00	0.42274	0.43816	0.47452	0.50792	0.52044
22.00	0.43348	0.44667	0.47798	0.50693	0.51781
23.00	0.44312	0.45443	0.48139	0.50647	0.51592
24.00	0.45162	0.46137	0.48472	0.50653	0.51477
25.00	0.45666	0.46558	0.48697	0.50702	0.51460

BULK CONCENTRATION AT REACTOR EXIT = 0.497817

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	848.48	847.79	843.24	811.54	484.68
1.00	860.56	857.44	839.25	747.39	333.45
2.00	865.72	858.76	823.82	691.22	319.77
3.00	864.69	853.18	802.02	645.25	316.72
4.00	858.31	842.23	777.13	607.98	314.84
5.00	847.50	827.26	751.13	577.48	313.34
6.00	833.17	809.41	725.17	552.10	312.11
7.00	816.13	789.61	699.94	530.59	311.06
8.00	797.11	768.57	675.79	512.06	310.16
9.00	776.73	746.87	652.92	495.85	309.38
10.00	755.49	724.92	631.39	481.50	308.69
11.00	733.80	703.07	611.18	468.67	308.07
12.00	712.02	681.58	592.23	457.08	307.51
13.00	690.43	660.63	574.44	446.54	307.01
14.00	669.25	640.37	557.74	436.89	306.55
15.00	648.66	620.89	542.04	428.00	306.12
16.00	628.78	602.23	527.26	419.78	305.72
17.00	609.68	584.41	513.34	412.13	305.36
18.00	591.41	567.44	500.22	405.00	305.02
19.00	573.98	551.31	487.85	398.34	304.70
20.00	557.39	535.99	476.17	392.09	304.40
21.00	541.63	521.46	465.15	386.23	304.12
22.00	526.69	507.71	454.77	380.74	303.86
23.00	512.61	494.76	445.02	375.59	303.61
24.00	499.82	483.00	436.19	370.95	303.39
25.00	492.51	476.29	431.16	368.30	303.26

BULK TEMPERATURE AT REACTOR EXIT = 384.21

NORMALIZED CATALYST CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.21639	0.21753	0.22513	0.28708	0.97874
1.00	0.17700	0.18126	0.20836	0.42920	0.92263
2.00	0.15040	0.15880	0.20956	0.56382	0.86463
3.00	0.13313	0.14621	0.22318	0.62590	0.81465
4.00	0.12306	0.14127	0.24608	0.63735	0.77293
5.00	0.11893	0.14280	0.27529	0.62956	0.73762
6.00	0.12012	0.15023	0.30724	0.61594	0.70712
7.00	0.12640	0.16324	0.33816	0.60132	0.68042
8.00	0.13774	0.18140	0.36519	0.58747	0.65689
9.00	0.15409	0.20397	0.38711	0.57496	0.63613
10.00	0.17520	0.22980	0.40418	0.56391	0.61783
11.00	0.20041	0.25732	0.41737	0.55422	0.60171
12.00	0.22852	0.28488	0.42771	0.54576	0.58754
13.00	0.25792	0.31108	0.43606	0.53840	0.57512
14.00	0.28695	0.33502	0.44304	0.53201	0.56425
15.00	0.31421	0.35635	0.44906	0.52651	0.55478
16.00	0.33888	0.37504	0.45437	0.52181	0.54658
17.00	0.36065	0.39133	0.45915	0.51785	0.53951
18.00	0.37961	0.40551	0.46352	0.51457	0.53349
19.00	0.39606	0.41792	0.46758	0.51194	0.52844
20.00	0.41037	0.42885	0.47141	0.50991	0.52429
21.00	0.42290	0.43857	0.47510	0.50848	0.52099
22.00	0.43400	0.44733	0.47871	0.50763	0.51850
23.00	0.44393	0.45530	0.48229	0.50734	0.51678
24.00	0.45267	0.46245	0.48580	0.50758	0.51581
25.00	0.45786	0.46680	0.48818	0.50820	0.51576

CATALYST TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	876.46	875.76	871.08	837.67	484.69
1.00	880.50	877.35	858.85	761.26	333.45
2.00	880.01	873.04	837.76	696.79	319.77
3.00	875.05	863.60	812.07	647.08	316.72
4.00	865.98	850.02	784.38	608.57	314.84
5.00	853.33	833.25	756.27	577.68	313.34
6.00	837.74	814.14	728.68	552.17	312.10
7.00	819.83	793.40	702.22	530.62	311.06
8.00	800.18	771.63	677.20	512.06	310.16
9.00	779.28	749.29	653.75	495.85	309.38
10.00	757.60	726.78	631.86	481.50	308.69
11.00	735.50	704.43	611.43	468.65	308.07
12.00	713.32	682.50	592.34	457.06	307.51
13.00	691.35	661.21	574.46	446.51	307.01
14.00	669.83	640.68	557.69	436.84	306.54
15.00	648.96	620.99	541.94	427.94	306.12
16.00	628.85	602.18	527.12	419.69	305.72
17.00	609.58	584.24	513.15	412.03	305.36
18.00	591.17	567.18	499.99	404.88	305.01
19.00	573.63	550.96	487.57	398.19	304.69
20.00	556.96	535.58	475.86	391.93	304.39
21.00	541.14	521.00	464.81	386.05	304.11
22.00	526.15	507.21	454.39	380.54	303.85
23.00	512.04	494.23	444.63	375.39	303.60
24.00	499.23	482.46	435.79	370.74	303.38
25.00	491.91	475.74	430.75	368.09	303.25

ITERATION NO. 250 TIME = 4.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.86037	0.86114	0.86561	0.88834	0.97895
1.00	0.63581	0.63938	0.65928	0.74825	0.92263
2.00	0.47911	0.48747	0.53041	0.69189	0.86463
3.00	0.37155	0.38600	0.45448	0.66793	0.81465
4.00	0.29951	0.32053	0.41300	0.65083	0.77293
5.00	0.25314	0.28065	0.39358	0.63414	0.73762
6.00	0.22550	0.25905	0.38805	0.61761	0.70712
7.00	0.21172	0.25063	0.39078	0.60197	0.68041
8.00	0.20844	0.25180	0.39780	0.58773	0.65688
9.00	0.21325	0.25992	0.40648	0.57506	0.63611
10.00	0.22435	0.27297	0.41530	0.56392	0.61779
11.00	0.24025	0.28925	0.42356	0.55416	0.60164
12.00	0.25952	0.30734	0.43102	0.54563	0.58742
13.00	0.28079	0.32601	0.43769	0.53818	0.57492
14.00	0.30275	0.34433	0.44364	0.53167	0.56395
15.00	0.32431	0.36164	0.44897	0.52600	0.55432
16.00	0.34465	0.37756	0.45375	0.52107	0.54589
17.00	0.36327	0.39191	0.45804	0.51679	0.53851
18.00	0.37996	0.40468	0.46187	0.51308	0.53208
19.00	0.39469	0.41593	0.46531	0.50989	0.52648
20.00	0.40759	0.42579	0.46839	0.50715	0.52162
21.00	0.41883	0.43442	0.47114	0.50481	0.51742
22.00	0.42859	0.44196	0.47362	0.50284	0.51382
23.00	0.43707	0.44854	0.47585	0.50121	0.51076
24.00	0.44424	0.45414	0.47782	0.49992	0.50826
25.00	0.44818	0.45724	0.47897	0.49931	0.50699

BULK CONCENTRATION AT REACTOR EXIT = 0.489967

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	848.48	847.79	843.24	811.54	484.68
1.00	860.56	857.44	839.25	747.39	333.45
2.00	865.72	858.76	823.82	691.22	319.77
3.00	864.69	853.18	802.02	645.25	316.72
4.00	858.31	842.23	777.13	607.98	314.84
5.00	847.50	827.26	751.13	577.48	313.34
6.00	833.17	809.41	725.18	552.10	312.11
7.00	816.14	789.62	699.94	530.59	311.06
8.00	797.13	768.59	675.80	512.06	310.16
9.00	776.76	746.90	652.95	495.86	309.38
10.00	755.55	724.98	631.44	481.53	308.69
11.00	733.92	703.18	611.26	468.71	308.07
12.00	712.21	681.75	592.35	457.15	307.52
13.00	690.72	660.90	574.64	446.64	307.01
14.00	669.68	640.76	558.02	437.04	306.55
15.00	649.27	621.44	542.44	428.21	306.13
16.00	629.61	602.99	527.82	420.06	305.74
17.00	610.78	585.42	514.08	412.51	305.38
18.00	592.83	568.74	501.17	405.49	305.04
19.00	575.74	552.92	489.04	398.95	304.73
20.00	559.53	537.94	477.61	392.84	304.44
21.00	544.16	523.77	466.86	387.12	304.16
22.00	529.60	510.37	456.74	381.76	303.91
23.00	515.88	497.74	447.23	376.74	303.67
24.00	503.41	486.28	438.62	372.21	303.45
25.00	496.33	479.78	433.75	369.65	303.33

BULK TEMPERATURE AT REACTOR EXIT = 385.87

NORMALIZED CATALYST CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.21639	0.21753	0.22513	0.28708	0.97874
1.00	0.17700	0.18126	0.20836	0.42920	0.92263
2.00	0.15040	0.15880	0.20956	0.56382	0.86463
3.00	0.13313	0.14621	0.22318	0.62590	0.81465
4.00	0.12306	0.14127	0.24608	0.63735	0.77293
5.00	0.11893	0.14279	0.27529	0.62956	0.73762
6.00	0.12011	0.15023	0.30723	0.61593	0.70712
7.00	0.12639	0.16322	0.33814	0.60131	0.68041
8.00	0.13770	0.18136	0.36515	0.58745	0.65688
9.00	0.15402	0.20389	0.38704	0.57494	0.63611
10.00	0.17507	0.22965	0.40407	0.56386	0.61779
11.00	0.20016	0.25706	0.41720	0.55413	0.60164
12.00	0.22810	0.28447	0.42747	0.54562	0.58742
13.00	0.25729	0.31050	0.43572	0.53817	0.57492
14.00	0.28604	0.33424	0.44256	0.53167	0.56395
15.00	0.31299	0.35531	0.44838	0.52601	0.55432
16.00	0.33732	0.37371	0.45343	0.52108	0.54590
17.00	0.35870	0.38963	0.45787	0.51680	0.53853
18.00	0.37720	0.40336	0.46180	0.51310	0.53210
19.00	0.39309	0.41520	0.46529	0.50992	0.52651
20.00	0.40669	0.42541	0.46841	0.50719	0.52167
21.00	0.41836	0.43425	0.47120	0.50488	0.51749
22.00	0.42839	0.44192	0.47371	0.50293	0.51391
23.00	0.43704	0.44860	0.47598	0.50133	0.51088
24.00	0.44432	0.45428	0.47799	0.50008	0.50842
25.00	0.44832	0.45742	0.47918	0.49950	0.50718

CATALYST TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	876.46	875.76	871.08	837.67	484.69
1.00	880.50	877.35	858.85	761.26	333.45
2.00	880.01	873.04	837.76	696.79	319.77
3.00	875.05	863.60	812.07	647.08	316.72
4.00	865.98	850.02	784.38	608.57	314.84
5.00	853.33	833.25	756.27	577.68	313.34
6.00	837.75	814.14	728.69	552.17	312.10
7.00	819.84	793.41	702.23	530.62	311.06
8.00	800.20	771.65	677.22	512.07	310.16
9.00	779.34	749.33	653.79	495.87	309.38
10.00	757.69	726.86	631.93	481.53	308.69
11.00	735.66	704.57	611.54	468.71	308.07
12.00	713.57	682.74	592.50	457.15	307.52
13.00	691.73	661.56	574.71	446.64	307.01
14.00	670.39	641.19	558.06	437.03	306.55
15.00	649.74	621.70	542.45	428.20	306.13
16.00	629.90	603.13	527.81	420.05	305.74
17.00	610.94	585.48	514.06	412.50	305.38
18.00	592.88	568.74	501.14	405.47	305.04
19.00	575.73	552.88	488.98	398.92	304.73
20.00	559.47	537.86	477.54	392.80	304.43
21.00	544.05	523.66	466.77	387.07	304.16
22.00	529.45	510.22	456.63	381.70	303.90
23.00	515.70	497.57	447.10	376.67	303.66
24.00	503.19	486.08	438.47	372.13	303.45
25.00	496.09	479.56	433.58	369.56	303.32

ITERATION NO. 311 TIME = 6.2199 SEC.

FINAL STEADY STATE CONDITIONS

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.86037	0.86114	0.86561	0.88834	0.97895
1.00	0.63581	0.63938	0.65928	0.74825	0.92263
2.00	0.47911	0.48747	0.53041	0.69189	0.86463
3.00	0.37155	0.38600	0.45448	0.66793	0.81465
4.00	0.29951	0.32053	0.41300	0.65083	0.77293
5.00	0.25314	0.28065	0.39358	0.63414	0.73762
6.00	0.22550	0.25905	0.38805	0.61761	0.70712
7.00	0.21172	0.25063	0.39078	0.60197	0.68041
8.00	0.20844	0.25180	0.39780	0.58773	0.65688
9.00	0.21325	0.25992	0.40648	0.57506	0.63611
10.00	0.22435	0.27296	0.41530	0.56392	0.61779
11.00	0.24024	0.28925	0.42355	0.55416	0.60164
12.00	0.25950	0.30732	0.43101	0.54563	0.58742
13.00	0.28076	0.32599	0.43767	0.53817	0.57492
14.00	0.30270	0.34429	0.44362	0.53166	0.56393
15.00	0.32423	0.36158	0.44893	0.52597	0.55430
16.00	0.34453	0.37746	0.45369	0.52102	0.54585
17.00	0.36311	0.39178	0.45794	0.51672	0.53845
18.00	0.37974	0.40449	0.46174	0.51297	0.53198
19.00	0.39441	0.41568	0.46512	0.50973	0.52633
20.00	0.40723	0.42546	0.46811	0.50692	0.52140
21.00	0.41835	0.43397	0.47076	0.50448	0.51711
22.00	0.42797	0.44137	0.47310	0.50238	0.51337
23.00	0.43625	0.44776	0.47515	0.50057	0.51014
24.00	0.44319	0.45313	0.47689	0.49905	0.50741
25.00	0.44692	0.45603	0.47784	0.49824	0.50595

BULK CONCENTRATION AT REACTOR EXIT = 0.488870

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	848.48	847.79	843.24	811.54	484.68
1.00	860.56	857.44	839.25	747.39	333.45
2.00	865.72	858.76	823.82	691.22	319.77
3.00	864.69	853.18	802.02	645.25	316.72
4.00	858.31	842.23	777.13	607.98	314.84
5.00	847.50	827.26	751.13	577.48	313.34
6.00	833.17	809.41	725.18	552.10	312.11
7.00	816.14	789.62	699.94	530.59	311.06
8.00	797.13	768.59	675.80	512.06	310.16
9.00	776.76	746.90	652.95	495.86	309.38
10.00	755.55	724.98	631.44	481.53	308.69
11.00	733.92	703.18	611.27	468.71	308.07
12.00	712.22	681.76	592.36	457.15	307.52
13.00	690.74	660.91	574.65	446.65	307.01
14.00	669.72	640.80	558.05	437.05	306.55
15.00	649.33	621.50	542.48	428.23	306.13
16.00	629.71	603.08	527.88	420.10	305.74
17.00	610.93	585.55	514.18	412.56	305.38
18.00	593.04	568.93	501.32	405.57	305.04
19.00	576.04	553.19	489.23	399.05	304.73
20.00	559.93	538.31	477.88	392.98	304.44
21.00	544.69	524.25	467.22	387.30	304.17
22.00	530.29	510.99	457.20	381.99	303.92
23.00	516.74	498.53	447.81	377.04	303.68
24.00	504.46	487.24	439.33	372.58	303.47
25.00	497.53	480.88	434.56	370.07	303.35

BULK TEMPERATURE AT REACTOR EXIT = 386.40

NORMALIZED CATALYST CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.21639	0.21753	0.22513	0.28708	0.97874
1.00	0.17700	0.18126	0.20836	0.42920	0.92263
2.00	0.15040	0.15880	0.20956	0.56382	0.86463
3.00	0.13313	0.14621	0.22318	0.62590	0.81465
4.00	0.12306	0.14127	0.24608	0.63735	0.77293
5.00	0.11893	0.14279	0.27529	0.62956	0.73762
6.00	0.12011	0.15023	0.30723	0.61593	0.70712
7.00	0.12639	0.16322	0.33814	0.60131	0.68041
8.00	0.13770	0.18136	0.36515	0.58745	0.65688
9.00	0.15402	0.20389	0.38704	0.57494	0.63611
10.00	0.17506	0.22964	0.40407	0.56386	0.61779
11.00	0.20015	0.25705	0.41720	0.55413	0.60163
12.00	0.22807	0.28445	0.42746	0.54561	0.58742
13.00	0.25724	0.31045	0.43570	0.53816	0.57492
14.00	0.28596	0.33417	0.44252	0.53165	0.56393
15.00	0.31287	0.35521	0.44833	0.52597	0.55430
16.00	0.33715	0.37357	0.45335	0.52102	0.54585
17.00	0.35848	0.38945	0.45776	0.51672	0.53845
18.00	0.37692	0.40313	0.46163	0.51297	0.53198
19.00	0.39273	0.41489	0.46506	0.50973	0.52633
20.00	0.40624	0.42501	0.46808	0.50692	0.52141
21.00	0.41778	0.43372	0.47075	0.50448	0.51711
22.00	0.42764	0.44122	0.47309	0.50238	0.51338
23.00	0.43607	0.44768	0.47515	0.50057	0.51014
24.00	0.44309	0.45309	0.47690	0.49906	0.50742
25.00	0.44686	0.45601	0.47785	0.49825	0.50596

CATALYST TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	876.46	875.76	871.08	837.67	484.69
1.00	880.50	877.35	858.85	761.26	333.45
2.00	880.00	873.04	837.76	696.79	319.77
3.00	875.05	863.60	812.07	647.08	316.72
4.00	865.98	850.02	784.38	608.57	314.84
5.00	853.33	833.25	756.27	577.68	313.34
6.00	837.75	814.14	728.69	552.17	312.10
7.00	819.84	793.41	702.23	530.62	311.06
8.00	800.20	771.65	677.22	512.07	310.16
9.00	779.34	749.33	653.79	495.87	309.38
10.00	757.69	726.86	631.93	481.53	308.69
11.00	735.66	704.58	611.54	468.71	308.07
12.00	713.58	682.75	592.51	457.15	307.52
13.00	691.76	661.59	574.73	446.65	307.01
14.00	670.44	641.23	558.10	437.05	306.55
15.00	649.82	621.77	542.51	428.23	306.13
16.00	630.03	603.24	527.90	420.10	305.74
17.00	611.13	585.65	514.19	412.56	305.38
18.00	593.16	568.98	501.32	405.56	305.04
19.00	576.11	553.22	489.23	399.05	304.73
20.00	559.96	538.32	477.88	392.98	304.44
21.00	544.70	524.25	467.21	387.30	304.17
22.00	530.28	510.98	457.19	381.99	303.92
23.00	516.73	498.51	447.80	377.03	303.68
24.00	504.43	487.22	439.31	372.57	303.47
25.00	497.50	480.85	434.54	370.06	303.35

C-3

PROGRAM FOR SURFACE RESISTANCE MODEL

SOURCE LISTING

```
C          ***** DEFINITION OF INPUT VARIABLES *****
C
C
C     RRDIFF   RADIAL DIFFUSION COEFFICIENT
C
C     RADIFF   AXIAL DIFFUSION COEFFICIENT
C
C     RRCOND   RADIAL CONDUCTIVITY COEFFICIENT
C
C     RACOND   AXIAL CONDUCTIVITY COEFFICIENT
C
C     RHTCP    FLUID HEAT CAPACITY
C
C     RDEN     FLUID DENSITY
C
C     RPOR     REACTOR VOID FRACTION
C
C     RO       REACTOR RADIUS
C
C     SO       REACTOR LENGTH
C
C     TW       COOLING FLUID TEMPERATURE
C
C     DTHETA   ITERATION TIME STEP
C
C     BVEL     BULK FLUID LINEAR VELOCITY
C
C     SAPUV    SURFACE AREA OF CATALYST PER UNIT VOLUME
C
C     SMTC     MASS TRANSFER COEFFICIENT ACROSS CATALYST SUR-
C              FACE
C
C     SHTC     HEAT TRANSFER COEFFICIENT ACROSS CATALYST SUR-
C              FACE
C
C     CHTCP    CATALYST HEAT CAPACITY
C
C     CDEN     CATALYST DENSITY
C
C     CPOR     CATALYST POROSITY
C
C     RC       CATALYST RADIUS
C
C     CO       INLET CONCENTRATION
C
C     TO       INLET TEMPERATURE
C
C     DC       STEP CHANGE IN INLET CONCENTRATION
C
C     DT       STEP CHANGE IN INLET TEMPERATURE
```

```
C
C       DELH        HEAT OF REACTION
C
C       WHTC        HEAT TRANSFER COEFFICIENT AT REACTOR WALL
C
C       EC          RELATIVE ERROR IN CONCENTRATION BETWEEN (N+1)
C                   'TH AND N'TH ITERATIONS AT ASSUMED STEADY
C                   -STATE
C
C       ET          ABSOLUTE ERROR IN TEMPERATURE BETWEEN (N+1)
C                   'TH AND N'TH ITERATIONS AT ASSUMED STEADY
C                   -STATE
C
C       ES          RELATIVE  ERROR IN CONCENTRATION BETWEEN SUC-
C                   CEEDING ITERATIONS AT NEWWTON-RAPHSON CONVER-
C                   GENCE
C
C       EX          ABSOLUTE ERROR IN TEMPERATURE BETWEEN SUC-
C                   CEEDING ITERATIONS AT NEWTON-RAPHSON CONVER-
C                   GENCE
C
C       M           NO. OF RADIAL GRID POINTS -1
C
C       N           NO. OF AXIAL GRID POINTS -1
C
C       NPK         FIRST TRANSIENT ITERATION TO BE PRINTED
C
C       NPI         THIS MANY ITERATIONS TO BE SKIPPED BETWEEN
C                   EACH TRANSIENT PRINTOUT
C
C       NO          NUMBER OF COPIES OF RESULTS REQUIRED
C
C       RRE(I)      STATEMENT OF REACTION RATE EXPRESSION  (NOT
C                   MORE THAN 72 CHARACTERS)
```

```
C      ***** PROGRAM FOR SURFACE RESISTANCE MODEL *****
C
C                  ***** MAINLINE PROGRAM *****
C
C      THIS MAINLINE READS IN THE INPUT PARAMETERS AND WRITES
C      OUT THE REACTOR PARAMETERS AND THE TRANSIENT RESULTS .
C      IT ALSO SUPERVISES THE COMPUTATIONAL PROCEDURE .
C
       COMMON TS(300),CS(300),XS,XSP,SS,SSP,CONC(300),TEMP(300)
      1,CZNC(300),TZMP(300),TZ(300),CZ(300),RR(10),C1(300),C2
      2(300),C3(300),C4(300),C5(300),C6(300),C7(300),C8(300),
      3C9(300),T1(300),T2(300),T3(300),T4(300),T5(300),T6(300)
      4,T7(300),T8(300),T9(300),RRDIFF,RADIFF,RRCOND,RACOND,
      5RHTCP,RDEN,RPOR,SAPUV,BVEL,SO,RO,CO,TO,TW,DTHETA,SMTC,
      6SHTC,CDEN,CPOR,CHTCP,RC,DELH,EC,ES,ET,EX,ALPHA,BETA,
      7GAMMA,SIGMA,PHI,ZETA,SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,
      8ST3,ST4,ST5,ST6,WHTC,DR,DX
       COMMON RL(100),CNORM(300),CSNORM(300)
       COMMON M,N,MP,NP,MN,IN,NI,ISS,NC,JG,LR,NO
       DIMENSION RRE(20)
       DIMENSION QP(10)
C
C      READ THE INPUT DATA
C
       READ (5,310) RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,RDEN,
      1RPOR,RO,SO,TW,DTHETA,BVEL,SAPUV,SMTC,SHTC,CHTCP,CDEN,
      2CPOR,RC,CO,TO,DC,DT,DELH,WHTC,EC,ET,ES,EX
  310  FORMAT (1X,4E16.8)
       READ (5,350) M,N,NPK,NPI,NO
  350  FORMAT (1X,5I6)
       READ (5,901) (RRE(I),I=1,20)
  901  FORMAT (20A4)
       CON=CO
       MP=M+1
       NP=N+1
       MN=MP*NP
C
C      WRITE THE REACTOR PARAMETERS
C
       DO 29 JW=1,NO
       WRITE (6,899)
  899  FORMAT (1H1/'0',10X)
       WRITE (6,900) SO,RO,RRDIFF,RADIFF,RHTCP,RDEN,TW,BVEL,
      1CO,TO,RPOR
       WRITE (6,905) SMTC,SHTC,CHTCP,CDEN,CPOR,RC,SAPUV
       WRITE (6,910) WHTC,DELH,DTHETA,MP,NP
       WRITE (6,902) (RRE(I),I=1,20)
  900  FORMAT (/12X,'PHYSICAL , THERMODYNAMIC AND KINETIC '
      1,'DATA'/'-',12X,'ALL UNITS ARE IN CM.,SEC.,CAL.,GM.-M'
      2,'OLES,DEGREES KELVIN  '/'-',12X,'REACTOR LENGTH',26X,
```

```
     3F16.6/'0',12X,'REACTOR RADIUS',26X,F16.6/'0',12X,'RAD'
     4,'IAL DIFFUSION COEFFICIENT',13X,F16.6/'0',12X,'AXIAL'
     5,' DIFFUSION COEFFICIENT',14X,F16.6/'0',12X,'FLUID HE'
     6,'AT CAPACITY',21X,F16.6/'0',12X,'FLUID DENSITY',27X,
     7F16.6/'0',12X,'COOLING FLUID TEMPERATURE',15X,F16.6/
     8'0',12X,'BULK FLUID LINEAR VELOCITY',14X,F16.6/'0',12X
     9,'INLET REACTANT CONCENTRATION',12X,F16.6/'0',12X,'IN'
     1,'LET FLUID TEMPERATURE',17X,F16.6/'0',12X,'REACTOR V'
     2,'OID FRACTION',19X,F16.6)
 905 FORMAT ('0',12X,'MASS TRANSFER COEFF AT CATALYST SURF'
     1,'ACE',1X,F16.6/'0',12X,'HEAT TRANSFER COEFF AT CATAL'
     2,'YST SURFACE',1X,F16.6/'0',12X,'CATALYST HEAT CAPACI'
     3,'TY',18X,F16.6/'0',12X,'CATALYST DENSITY',24X,F16.6/
     4'0',12X,'CATALYST VOID FRACTION',18X,F16.6/'0',12X,'C'
     5,'ATALYST PARTICLE RADIUS',16X,F16.6/'0',12X,'CATALYS'
     6,'T SURFACE AREA PER UNIT VOLUME',3X,F16.6)
 910 FORMAT ('0',12X,'HEAT TRANSFER COEFF AT REACTOR WALL',
     15X,F16.6/'0',12X,'HEAT OF REACTION',24X,F16.6/'0',12X,
     2'ITERATION TIME STEP',21X,F16.6/'0',12X,'NO. OF RADIA'
     3,'L POINTS',21X,I8/'0',12X,'NO. OF AXIAL POINTS',22X,
     4I8)
 902 FORMAT ('0',12X,'RATE OF REACTION = ',20A4)
  29 CONTINUE
C
C      INITIALIZE THE DEPENDENT VARIABLES
C
      DO 333 I=1,300
      CZNC(I)=0.
      CONC(I)=0.
      CS(I)=0.
      TZMP(I)=0.
      TEMP(I)=0.
      TS(I)=0.
 333 CONTINUE
      DO 330 I=1,MN
      CONC(I)=CO
      CS(I)=CO
      TEMP(I)=TO
      TS(I)=TO
 330 CONTINUE
      ISS=0
      IN=0
  70 CALL COEFF
C
C      COMPUTE THE CROSS-SECTIONAL AREA REPRSENTED BY EACH
C      RADIAL GRID
C
      QP(1)=3.14159*(DR/2.)**2.
      DO 613 I=2,M
      QP(I)=3.14159*((RR(I)+DR/2.)**2.-(RR(I)-DR/2.)**2.)
```

```
  613 CONTINUE
      QP(MP)=3.14159*(RO**2.-(RO-DR/2.)**2.)
      KFSS=0
      NI=0
      TIME=0.
      JG=1
   10 CALL RETI
      JG=JG*(-1)
      NI=NI+1
      TIME=TIME+DTHETA
C
C     COMPARE THE SOLUTION AT THE (N+1)'TH ITERATION WITH
C     THE SOLUTION AT THE N'TH ITERATION
C
      DO 40 I=1,MN
      IF (ABS((CZNC(I)-CONC(I))/CZNC(I)).GT.EC) GO TO 20
      IF (ABS(TZMP(I)-TEMP(I)).GT.ET) GO TO 20
      IF (ABS((CS(I)-CZ(I))/CS(I)).GT.EC) GO TO 20
      IF (ABS(TS(I)-TZ(I)).GT.ET) GO TO 20
   40 CONTINUE
      KFSS=1
      GO TO 9
   20 DO 50 I=1,MN
      CZ(I)=CS(I)
      TZ(I)=TS(I)
      CONC(I)=CZNC(I)
   50 TEMP(I)=TZMP(I)
      DO 211 I=1,MN
      CNORM(I)=CONC(I)/CON
      CSNORM(I)=CS(I)/CON
  211 CONTINUE
      IF (NI.NE.NPO) GO TO 10
      NPO=NPO+NPT
    9 CONTINUE
      DO 39 JW=1,NO
      IF (KFSS.NE.1) GO TO 61
      IF (IN.EQ.0) GO TO 17
      GO TO 19
C
C     WRITE OUT THE TRANSIENT RESULTS
C
   61 WRITE (6,235) NI,TIME
  235 FORMAT (1H1////' ',18X,'ITERATION NO.',I6,5X,'TIME = '
     1,F10.4,' SEC.'/'-',26X,'NORMALIZED CONCENTRATION PROF'
     2,'ILE')
      GO TO 21
C
C     WRITE OUT THE INITIAL OPERATING CONDITIONS
C
   17 WRITE (6,240) DC,DT
```

```
  240 FORMAT (1H1////' ',18X                          /'0',12X,'IN'
     1,'ITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGE'
     2,'S OF'/'0',12X,F10.7,5X,'GM-MOLES/C.C. IN INLET CONC'
     3,'ENTRATION'/'0',12X, F8.2,7X,'DEGREES KELVIN  IN INL'
     4,'ET TEMPERATURE'/'-',26X,'NORMALIZED CONCENTRATION P'
     5,'ROFILE')
      GO TO 21
C
C     WRITE OUT THE FINAL OPERATING CONDITIONS
C
   19 WRITE (6,245) NI,TIME
  245 FORMAT (1H1////' ',18X,'ITERATION NO.',I6,5X,'TIME = '
     1,F10.4,' SEC.'/'0',26X,'FINAL STEADY STATE CONDITIONS'
     2/'-',26X,'NORMALIZED CONCENTRATION PROFILE')
   21 CONTINUE
C
C     COMPUTE THE BULK CONCENTRATION AND TEMPERATURE AT THE
C     REACTOR EXIT
C
      LMN=MN-MP
      BCE=0.
      BTE=0.
      DO 614 I=1,MP
      NML=I+LMN
      BCE=BCE+QP(I)*CONC(NML)
      BTE=BTE+QP(I)*TEMP(NML)
  614 CONTINUE
      BCE=BCE/((3.14159*(RO**2.))*CON)
      BTE=BTE/(3.14159*(RO**2.))
      WRITE (6,200) (RR(I),I=1,MP)
  200 FORMAT ('-',12X,'DISTANCE FROM',5(F6.1,4X)/' ',12X,'C'
     1,'ENTER-LINE'/'0',12X,'DISTANCE FROM'/' ',12X,'ENTRAN'
     2,'CE'/' ',12X)
      K=1
      KK=MP
      DO 250 I=1,NP,2
      WRITE (6,204) RL(I),(CNORM(J),J=K,KK)
  204 FORMAT (' ', 9X,F10.2,3X,5F10.5)
      K=K+2*MP
      KK=KK+2*MP
  250 CONTINUE
      WRITE (6,615) BCE
  615 FORMAT ('-',12X,'BULK CONCENTRATION AT REACTOR EXIT = '
     1,F10.6)
      WRITE (6,230)
  230 FORMAT (1H1////' ',26X,'          TEMPERATURE PROFILE')
      WRITE (6,200) (RR(I),I=1,MP)
      K=1
      KK=MP
      DO 260 I=1,NP,2
```

```
      WRITE (6,207) RL(I),(TEMP(J),J=K,KK)
  207 FORMAT (' ', 9X,F10.2,5X,5(F8.2,2X))
      K=K+2*MP
      KK=KK+2*MP
  260 CONTINUE
      WRITE (6,616) BTE
  616 FORMAT ('-',12X,'BULK TEMPERATURE AT REACTOR EXIT = ',
     1F10.2)
      WRITE (6,444)
  444 FORMAT (1H1////' ',24X,'NORMALIZED CATALYST CONCENTRA'
     1,'TION PROFILE')
      WRITE (6,200) (RR(I),I=1,MP)
      K=1
      KK=MP
      DO 445 I=1,NP,2
      WRITE (6,204) RL(I),(CSNORM(J),J=K,KK)
      K=K+2*MP
      KK=KK+2*MP
  445 CONTINUE
      WRITE (6,464)
  464 FORMAT (1H1////' ',28X,'CATALYST TEMPERATURE PROFILE')
      WRITE (6,200) (RR(I),I=1,MP)
      K=1
      KK=MP
      DO 465 I=1,NP,2
      WRITE (6,207) RL(I),(TS(J),J=K,KK)
      K=K+2*MP
      KK=KK+2*MP
  465 CONTINUE
   39 CONTINUE
      IF (KFSS.EQ.1) GO TO 30
      GO TO 10
   30 IF (IN.EQ.1) GO TO 60
C
C     IMPLEMENT THE STEP CHANGE AT THE INLET CONDITION
C
      IN=1
      CO=CO+DC
      TO=TO+DT
      NPO=NPK
      NPT=NPI
      GO TO 70
   60 CONTINUE
      STOP
      END
```

```
C                ***** SUBROUTINE COEFF *****
C
      SUBROUTINE COEFF
C
C     THIS SUBROUTINE CALCULATES THE COEFFICIENTS OF THE EQ-
C     UATIONS DESCRIBING HEAT AND MASS TRANSFER IN THE EX-
C     TERNAL FIELD OF THE REACTOR
C
      COMMON TS(300),CS(300),XS,XSP,SS,SSP,CONC(300),TEMP(300)
     1,CZNC(300),TZMP(300),TZ(300),CZ(300),RR(10),C1(300),C2
     2(300),C3(300),C4(300),C5(300),C6(300),C7(300),C8(300),
     3C9(300),T1(300),T2(300),T3(300),T4(300),T5(300),T6(300)
     4,T7(300),T8(300),T9(300),RRDIFF,RADIFF,RRCOND,RACOND,
     5RHTCP,RDEN,RPOR,SAPUV,BVEL,SO,RO,CO,TO,TW,DTHETA,SMTC,
     6SHTC,CDEN,CPOR,CHTCP,RC,DELH,EC,ES,ET,EX,ALPHA,BETA,
     7GAMMA,SIGMA,PHI,ZETA,SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,
     8ST3,ST4,ST5,ST6,WHTC,DR,DX
      COMMON RL(100),CNORM(300),CSNORM(300)
      COMMON M,N,MP,NP,MN,IN,NI,ISS,NC,JG,LR,NO
      DR=RO/M
      DX=SO/N
      RR(1)=0.
      DO 7 I=2,MP
    7 RR(I)=RR(I-1)+DR
      RL(1)=0.
      DO 707 I=2,NP
      RL(I)=RL(I-1)+DX
  707 CONTINUE
      DO 100 I=1,MN
      LR=I+1-(((I-1)/(M+1))*(M+1)+1)
      IF (I.EQ.1) GO TO 10
      IF (I.EQ.MP) GO TO 20
      IF (I.LT.MP) GO TO 30
      IF (I.EQ.MN) GO TO 40
      IF (I.EQ.(MN-M)) GO TO 50
      IF (I.GT.(MN-M)) GO TO 60
      IF (LR.EQ.1) GO TO 70
      IF (LR.EQ.MP) GO TO 80
      SA=3.14159*((RR(LR)+DR/2.)**2-(RR(LR)-DR/2.)**2)*RPOR
      AO=2.*3.14159*DX*(RR(LR)+DR/2.)*RPOR
      AI=2.*3.14159*DX*(RR(LR)-DR/2.)*RPOR
      CDEP=SA*DX*SAPUV*SMTC/(2.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
```

```
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(2.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=0.
      GO TO 100
   10 AO=RPOR*3.14159*DR*DX/2.
      SA=3.14159*RPOR*(DR**2)/4.
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=0.
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)-CDEP-BVEL*SA
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=BVEL*SA*CO
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
      T1(I)=0.
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)-TDEP-BVEL*SA*RHTCP*RDEN
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=BVEL*SA*RHTCP*RDEN*TO
      GO TO 100
   30 AI=RPOR*3.14159*(RR(LR)-DR/2.)*DX
      AO=RPOR*3.14159*(RR(LR)+DR/2.)*DX
      SA=RPOR*3.14159*((RR(LR)+DR/2.)**2-(RR(LR)-DR/2.)**2)
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=0.
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP-BVEL*SA
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=BVEL*SA*CO
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
```

```
      T1(I)=0.
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP-BVEL*SA*RHTCP*RDEN
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=BVEL*SA*RHTCP*RDEN*TO
      GO TO 100
   20 SA=RPOR*3.14159*(RO**2-(RO-DR/2.)**2)
      AO=RPOR*3.14159*DX*RO
      AI=RPOR*3.14159*DX*(RO-DR/2.)
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=0.
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP-BVEL*SA
      C5(I)=0.
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=BVEL*SA*CO
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
      T1(I)=0.
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP-BVEL*SA*RHTCP*RDEN
      T5(I)=0.
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP-AO*WHTC
      T7(I)=TDEP
      T8(I)=BVEL*SA*RHTCP*RDEN*TO    +AO*WHTC*TW
      GO TO 100
   70 SA=RPOR*3.14159*(DR**2)/4.
      AO=RPOR*3.14159*DR*DX
      CDEP=SA*DX*SAPUV*SMTC/(2.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(2.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)-TDEP
```

```
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=0.
      GO TO 100
   80 SA=RPOR*3.14159*(RO*DR-(DR**2)/4.)
      AO=RPOR*2.*3.14159*DX*RO
      AI=RPOR*2.*3.14159*(RO-DR/2.)*DX
      CDEP=SA*DX*SAPUV*SMTC/(2.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=0.
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(2.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=0.
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP-AO*WHTC
      T7(I)=TDEP
      T8(I)=AO*WHTC*TW
      GO TO 100
   50 SA=RPOR*3.14159*(DR**2)/4.
      AO=RPOR*3.14159*DR*DX/2.
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=RRDIFF*AO/DR
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=RRCOND*AO/DR
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)-TDEP
```

```
      T7(I)=TDEP
      T8(I)=0.
      GO TO 100
   60 SA=RPOR*3.14159*((RR(LR)+DR/2.)**2-(RR(LR)-DR/2.)**2)
      AO=RPOR*3.14159*DX*(RR(LR)+DR/2.)
      AI=RPOR*3.14159*DX*(RR(LR)-DR/2.)
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=RRDIFF*AO/DR
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=RRCOND*AO/DR
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=0.
      GO TO 100
   40 SA=RPOR*3.14159*(RO*DR-(DR**2)/4.)
      AO=RPOR*3.14159*DX*RO
      AI=RPOR*3.14159*DX*(RO-DR/2.)
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/DTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=0.
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/DTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=0.
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)-TDEP-AO*WHTC
      T7(I)=TDEP
      T8(I)=AO*WHTC*TW
```

```
  100 CONTINUE
      RETURN
      END
```

```
C                ***** SUBROUTINE SURF *****
C
      SUBROUTINE SURF
C
C     THIS SUBROUTINE CALCULATES THE COEFFICIENTS OF THE EQ-
C     UATIONS DESCRIBING HEAT AND MASS TRANSFER ACROSS THE
C     CATALYST SURFACE . IT ALSO COMPUTES THE CONCENTRATION
C     AND TEMPERATURE ON THE SURFACE OF THE CATALYST AT THE
C     (N+1)'TH ITERATION OR TIME STEP
C
      COMMON TS(300),CS(300),XS,XSP,SS,SSP,CONC(300),TEMP(300)
     1,CZNC(300),TZMP(300),TZ(300),CZ(300),RR(10),C1(300),C2
     2(300),C3(300),C4(300),C5(300),C6(300),C7(300),C8(300),
     3C9(300),T1(300),T2(300),T3(300),T4(300),T5(300),T6(300)
     4,T7(300),T8(300),T9(300),RRDIFF,RADIFF,RRCOND,RACOND,
     5RHTCP,RDEN,RPOR,SAPUV,BVEL,SO,RO,CO,TO,TW,DTHETA,SMTC,
     6SHTC,CDEN,CPOR,CHTCP,RC,DELH,EC,ES,ET,EX,ALPHA,BETA,
     7GAMMA,SIGMA,PHI,ZETA,SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,
     8ST3,ST4,ST5,ST6,WHTC,DR,DX
      COMMON RL(100),CNORM(300),CSNORM(300)
      COMMON M,N,MP,NP,MN,IN,NI,ISS,NC,JG,LR,NO
C
C     THE FOLLOWING STATEMENTS DEFINE THE RATE OF REACTION
C     EXPRESSION AND IT'S DERIVATIVE WITH RESPECT TO CONCEN-
C     TRATION
C
      F(Q,Z)=(1.0E+13)*EXP(-23844./(1.987*Z))*(ABS(Q)**2)
      FD(Q,Z,W)=(1.0E+13)*(EXP(-23844./(1.987*Z)))*(2.*Q+(
     1ABS(Q)**2)*23844./(1.987*(Z**2))*W)
      IF (JG.EQ.(-1)) GO TO 300
      IF (ISS.EQ.1) GO TO 13
C
C     COMPUTATION OF THE SURFACE EQUATIONS' COEFFICIENTS
C
      ISS=1
      SC1=SMTC*RC**2
      SC2=-SC1
      SC5=-(RC**3)/3.
      SC6=((RC**3)/3.)*CPOR/DTHETA
      ST1=SHTC*RC**2
      ST2=-ST1
      ST5=SC5*DELH
      ST6=((RC**3)/3.)*CDEN*CHTCP/DTHETA
C
C     NEWTON RAPHSON ITERATION ON FORWARD SWEEP OF THE ADEP
C
   13 CONTINUE
      PHI=-SC1*C7(NC)/(C3(NC)-C9(NC))+SC2-SC6
      GAMMA=-SC1*ALPHA/(C3(NC)-C9(NC))+SC6*CS(NC)
      ZETA=-ST1*T7(NC)/(T3(NC)-T9(NC))+ST2-ST6
```

```
      SIGMA=-ST1*BETA/(T3(NC)-T9(NC))+ST6*TS(NC)
   15 FUN=PHI*SS+GAMMA+SC5*F(SS,XS)
      DER=-PHI-SC5*FD(SS,XS,((ST5/SC5)*(PHI/ZETA)))
   29 CONTINUE
      SSP=SS
      XSP=XS
      SS=SSP+FUN/DER
      IF (SS.GE.0.) GO TO 811
      SS=0.
  811 CONTINUE
      XS=(-SIGMA+(ST5/SC5)*(PHI*SS+GAMMA))/ZETA
      IF (SS.LE.0.) GO TO 19
      IF (ABS(XS-XSP).GT.EX) GO TO 15
      IF (ABS((SS-SSP)/SS).GT.ES) GO TO 15
   19 RETURN
C
C     NEWTON RAPHSON ITERATION ON THE REVERSE SWEEP OF THE ADEP
C
  300 CONTINUE
      SS=CS(NC)
      XS=TS(NC)
  315 FUN=SC1*CONC(NC)+(SC2+SC6)*CS(NC)-SC6*SS+SC5*F(SS,XS)
      DER=SC6-SC5*FD(SS,XS,((ST5/SC5)*(SC6/ST6)))
      XSP=XS
      SSP=SS
      SS=SSP+FUN/DER
      IF (SS.GE.0.) GO TO 511
      SS=0.
  511 CONTINUE
      XS=-(ST1*TEMP(NC)+(ST2+ST6)*TS(NC)-(ST5/SC5)*(SC1*CONC
     1(NC)+(SC2+SC6)*CS(NC)-SC6*SS))/(-ST6)
      IF (SS.LE.0.) GO TO 567
      IF (ABS((SS-SSP)/SS).GT.ES) GO TO 315
      IF (ABS(XS-XSP).GT.EX) GO TO 315
  567 CONTINUE
      RETURN
      END
```

```
C                ***** SUBROUTINE RETI *****
C
      SUBROUTINE RETI
C
C     THIS SUBROUTINE CALCULATES THE EXTERNAL FIELD CONCEN-
C     TRATION AND TEMPERATURE AT EACH GRID POINT IN TERMS
C     OF THE CONCENTRATION AND TEMPERATURE ON THE SURFACE
C     OF THE CATALYST AT THESE GRID POINTS
C
      COMMON TS(300),CS(300),XS,XSP,SS,SSP,CONC(300),TEMP(300)
     1,CZNC(300),TZMP(300),TZ(300),CZ(300),RR(10),C1(300),C2
     2(300),C3(300),C4(300),C5(300),C6(300),C7(300),C8(300),
     3C9(300),T1(300),T2(300),T3(300),T4(300),T5(300),T6(300)
     4,T7(300),T8(300),T9(300),RRDIFF,RADIFF,RRCOND,RACOND,
     5RHTCP,RDEN,RPOR,SAPUV,BVEL,SO,RO,CO,TO,TW,DTHETA,SMTC,
     6SHTC,CDEN,CPOR,CHTCP,RC,DELH,EC,ES,ET,EX,ALPHA,BETA,
     7GAMMA,SIGMA,PHI,ZETA,SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,
     8ST3,ST4,ST5,ST6,WHTC,DR,DX
      COMMON RL(100),CNORM(300),CSNORM(300)
      COMMON M,N,MP,NP,MN,IN,NI,ISS,NC,JG,LR,NO
      IF (JG.EQ.(-1)) GO TO 300
C
C     FORWARD SWEEP OF THE ADEP
C
      DO 100 I=1,MN
      NC=I
      IMMP=I-MP
      IPMP=I+MP
      LR=I+1-(((I-1)/(M+1))*(M+1)+1)
      SS=CS(I)
      XS=TS(I)
   28 IF (I.EQ.1) GO TO 10
      IF (I.LE.MP) GO TO 20
      ALPHA=C4(I)*CONC(I)+C5(I)*CONC(I+1)+C6(I)*CONC(IPMP)+
     1C7(I)*CS(I)+C8(I)+C2(I)*CZNC(I-1)+C1(I)*CZNC(IMMP)+C9(
     21)*CONC(I)
      BETA=T4(I)*TEMP(I)+T5(I)*TEMP(I+1)+T6(I)*TEMP(IPMP)+T7
     1(I)*TS(I)+T8(I)+T2(I)*TZMP(I-1)+T1(I)*TZMP(IMMP)+T9(I)
     2*TEMP(I)
      CALL SURF
      GO TO 38
   10 ALPHA=C4(I)*CONC(I)+C5(I)*CONC(I+1)+C6(I)*CONC(IPMP)+
     1C7(I)*CS(I)+C8(I)+C9(I)*CONC(I)
      BETA=T4(I)*TEMP(I)+T5(I)*TEMP(I+1)+T6(I)*TEMP(IPMP)+T7
     1(I)*TS(I)+T8(I)+T9(I)*TEMP(I)
      CALL SURF
      GO TO 38
   20 ALPHA=C4(I)*CONC(I)+C5(I)*CONC(I+1)+C6(I)*CONC(IPMP)+
     1C7(I)*CS(I)+C8(I)+C9(I)*CONC(I)+C2(I)*CZNC(I-1)
      BETA=T4(I)*TEMP(I)+T5(I)*TEMP(I+1)+T6(I)*TEMP(IPMP)+T7
```

```
     1(I)*TS(I)+T8(I)+T9(I)*TEMP(I)+T2(I)*TZMP(I-1)
      CALL SURF
   38 CZNC(I)=(-ALPHA-C7(I)*SS)/(C3(I)-C9(I))
      TZMP(I)=(-BETA-T7(I)*XS)/(T3(I)-T9(I))
   18 CS(NC)=SS
      TS(NC)=XS
  100 CONTINUE
      RETURN
C
C     REVERSE SWEEP OF THE ADEP
C
  300 CONTINUE
      DO 200 K=1,MN
      I=MN+1-K
      NC=I
      CALL SURF
      IMMP=I-MP
      IPMP=I+MP
      IF (I.EQ.1) GO TO 110
      IF (I.LE.MP) GO TO 120
      CZNC(I)=-(C1(I)*CONC(IMMP)+C2(I)*CONC(I-1)+C3(I)*CONC(
     1I)+C5(I)*CZNC(I+1)+C6(I)*CZNC(IPMP)+C7(I)*(CS(I)+SS)+
     2C8(I)+C9(I)*CONC(I))/(C4(I)-C9(I))
      TZMP(I)=-(T1(I)*TEMP(IMMP)+T2(I)*TEMP(I-1)+T3(I)*TEMP(
     1I)+T5(I)*TZMP(I+1)+T6(I)*TZMP(IPMP)+T7(I)*(TS(I)+XS)+
     2T8(I)+T9(I)*TEMP(I))/(T4(I)-T9(I))
      GO TO 138
  110 CZNC(I)=-(C3(I)*CONC(I)+C5(I)*CZNC(I+1)+C6(I)*CZNC(IPMP
     1)+C7(I)*(CS(I)+SS)+C8(I)+C9(I)*CONC(I))/(C4(I)-C9(I))
      TZMP(I)=-(T3(I)*TEMP(I)+T5(I)*TZMP(I+1)+T6(I)*TZMP(IPMP
     1)+T7(I)*(TS(I)+XS)+T8(I)+T9(I)*TEMP(I))/(T4(I)-T9(I))
      GO TO 138
  120 CZNC(I)=-(C2(I)*CONC(I-1)+C3(I)*CONC(I)+C5(I)*CZNC(I+1
     1)+C6(I)*CZNC(IPMP)+C7(I)*(CS(I)+SS)+C8(I)+C9(I)*CONC(
     2I))/(C4(I)-C9(I))
      TZMP(I)=-(T2(I)*TEMP(I-1)+T3(I)*TEMP(I)+T5(I)*TZMP(I+1
     1)+T6(I)*TZMP(IPMP)+T7(I)*(TS(I)+XS)+T8(I)+T9(I)*TEMP(
     2I))/(T4(I)-T9(I))
  138 CONTINUE
      CS(NC)=SS
      TS(NC)=XS
  200 CONTINUE
      RETURN
      END
```

APPENDIX D

COMPUTER PROGRAM FOR INTERNAL RESISTANCE MODEL OF A PACKED BED REACTOR:

This section illustrates the use of the computer program which calculates the transient response of the internal resistance model to a step change in the inlet conditions. The program is coded in FORTRAN IV for an IBM 360/67 computer. Input data was entered on punched cards and the transient results were printed out at designated time intervals on an IBM high-speed printer. If the time allotted to run the program is not sufficient to complete the transient run, then the intermediate results may be stored on magnetic tape, and the calculations may be continued from this point on a subsequent run.

the input variables are defined at the beginning of the program source listing. They must be punched on cards in the order given in this list. Table D-1 presents the input data used for the example in this section in the form in which it is to be punched on cards.

The first card of input data contains some variables which are related to the use of magnetic tapes for the storage of intermediate transient results. Some background information is in order at this point. The computer

execution time is directly proportional to the number of grid points in the reactor and in the catalyst. As a guide, there were 255 reactor grid points and 25 catalyst grid points in the example used in this section. Thus the total number of grid points is: N = (255 x 25) + 255 = 6630. With this grid system, the IBM 360/67 was able to compute 12 time steps per minute of computer time. If a catalyst time step to reactor time step ratio of 3 was used then 35 time steps may be computed in an allotted amount of computer time.

As an illustration suppose that the following conditions are present:

i) Maximum computing time allowed per run = 10 minutes

ii) Expected number of iterations per minute = 20
(This should be a conservative figure)

iii) The initial steady state is reached after 353 iterations.

iv) The final steady state resulting from the given step change in the inlet conditions is reached after 479 time steps.

v) The time step used in arriving at both steady-states os .02 sec.

vi) Every fiftieth time step is to be printed out.

The execution of the program would proceed as follows:

RUN #1

The first data card should appear as follows:

bbbbb50bbbb50bbb200bbbbb0bbbbb0bbbbb1bbbb0.0

The program will execute 200 time steps, printing out every fiftieth iteration on the typewriter. The results of the two-hundredth iteration which corresponds to 4.0 seconds of reactor time will be stored on tape.

RUN #2

The first data card should now appear as follows:

bbbb250bbbb50bbb400bbb200bbbbb1bbbbb1bbbb4.0

The program will continue the computations beginning with the results of iteration number 200. It will print out iterations 250, 300 and 350. Upon computing the conditions at iteration number 353 and determining that a steady-state exists, these results will be stored on tape and the program execution terminated.

RUN #3

The first data card should now appear as follows:

bbbbb50bbbb50bbb200bbbbb0bbbbb1bbbbb1bbbb0.0

Essentially, the program now begins the computation of a realistic transient process beginning with the steady-state conditions stored on tape by RUN #2. Time steps 50, 100, 150, and 200 will be printed out. The results of time step 200 will be stored on tape.

RUN #4

The first data card will appear as follows:

bbbb250bbbb50bbb400bbb200bbbbb1bbbbb1bbbb4.0

Time steps 250, 300, 350 and 400 will be printed out, and the results of time step 400 will be stored on tape.

RUN #5

The first data card will appear as follows:

bbbb450bbbb50bbb600bbb400bbbbb1bbbbb1bbbb8.0

Beginning with the results stored on tape by RUN #4 the transient computations continue. Time step 450 will be printed out. After computing the conditions at time step 479 and determining that this is at steady-state, this time step will be printed out and the execution of the program terminated.

The above program always refers to the tape from which previous results are being read as 1; i.e.) READ (1). The tape on which results are to be stored is referred to as 2; i.e.) WRITE (2). An explanation of the program control cards required to facilitate the interfacing of the magnetic tapes with the computing system must be obtained from the particular computing centre, as all control cards are peculiar to each centre.

As in the previous described programs, a FORTRAN statement of the reaction rate expression and its

derivative with respect to concentration must be included in the source program. The reaction rate expression appears at the beginning of

i) SUBROUTINE SSCAT

ii) SUBROUTINE SURF

iii) SUBROUTINE CATPRO

The expression for the derivative also appears in these subroutines. The correct place for these statements is indicated in the source program listing. For the first order reaction rate used in this section, the rate of reaction definition was given by:

```
F(Q,Z) = (1.0E+07)*EXP(-12000./Z)*Q
```

The derivative was given by:

```
FD(Q,Z,W) = (1.0E+07)*EXP(-12000./Z)*(1.0+Q*12000./(Z**2)
            *W)
```

where Q, Z, and W are dummy variables referring to concentration, temperature, and the derivative of the temperature with respect to concentration. In the transient calculations, this derivative, W, is computed at each time step.

Table D-2 is a set of transient results given in computer output form, for the input parameters of TABLE D-1.

TABLE D-1

INPUT DATA FOR INTERNAL RESISTANCE MODEL

INPUT CARD

	(NPI)	(NPO)	(NICO)	(NI)	(KM)	(NO)	TIME
1	bbbbb50	bbbb50	bbb200	bbbbb0	bbbbb0	bbbbb1	bbbb0.0

	(RRDIFF)	(RADIFF)	(RRCOND)	(RACOND)
2	bbbb.77000000E+00	bbb.31500000E+01	bbb.43100000E-01	bbb.17640000E+00

	(RHTCP)	(RDEN)	(RPOR)	(RO)
3	bbbb.21860000E+02	bbb.25000000E-02	bbb.35000000E+00	bbb.20000000E+01

	(SO)	(TW)	(BVEL)	(SAPUV)
4	bbbb.25000000E+02	bbb.30000000E+03	bbb.12600000E+02	bbb.31415900E+01

	(SMTC)	(SHTC)	(CDIFF)	(CCOND)
5	bbbb.68600000E+00	bbb.55300000E-01	bbb.51500000E-02	bbb.50000000E-03

	(CHTCP)	(CDEN)	(CPOR)	(RC)
6	bbbb.50000000E+01	bbb.11200000E-01	bbb.54300000E+00	bbb.25000000E+00

	(CO)	(TO)	(DC)	(DT)
7	bbbb.10000000E-04	bbb.60000000E+03	bbb.00000000E+00	bbb.30000000E+02

TABLE D-1 (Continued)

INPUT CARD

```
                (DELH)                  (WHTC)                  (EC)                    (ET)
 8      bbb-.35040000E+07bbb.11300000E+01bbb.50000000E-05bbb.10000000E-02

                (ES)                    (EX)                    (TM1)                   (TM2)
 9      bbbb.10000000E-04bbb.50000000E-01bbb.20000000E-01bbb.20000000E-01

                (TM3)                   (TM4)                   (RAT1)                  (RAT2)
10      bbbb.20000000E-01bbb.20000000E-01bbb.10000000E+01bbb.30000000E+01

                (RAT3)                  (RAT4)
11      bbbb.30000000E+01bbb.30000000E+01

                (M)     (N)     (L)
12      bbbbbb4bbbb50bbbb25

                        (RRE(I))
13      b(1.0E+07)*EXP(-23844./(1.987*T))*C
```

TABLE D-2

RESULTS FROM PROGRAM FOR INTERNAL RESISTANCE MODEL

PHYSICAL,THERMODYNAMIC AND KINETIC DATA

ALL UNITS ARE IN CM.,SEC.,CAL.,GM.-MOLES,DEGREES KELVIN

REACTOR LENGTH	25.000000
REACTOR RADIUS	2.000000
RADIAL DIFFUSION COEFFICIENT	0.770000
AXIAL DIFFUSION COEFFICIENT	3.150000
FLUID HEAT CAPACITY	21.859985
FLUID DENSITY	0.002500
REACTOR VOID FRACTION	0.350000
COOLING FLUID TEMPERATURE	300.000000
BULK FLUID LINEAR VELOCITY	12.599999
INLET REACTANT CONCENTRATION	0.000010
INLET FLUID TEMPERATURE	600.000000
CATALYST SURFACE AREA PER UNIT VOLUME	3.141589
MASS TRANSFER COEFF AT CATALYST SURFACE	0.686000
HEAT TRANSFER COEFF AT CATALYST SURFACE	0.055300
HEAT TRANSFER COEFF AT REACTOR WALL	1.129999
CATALYST PARTICLE RADIUS	0.250000
DIFFUSION COEFF IN CATALYST	0.005150
CATALYST THERMAL CONDUCTIVITY	0.000500
CATALYST HEAT CAPACITY	5.000000
CATALYST DENSITY	0.011200
CATALYST VOID FRACTION	0.543000
HEAT OF REACTION	-3504000.000000
NO. OF RADIAL POINTS	5
NO. OF AXIAL POINTS	51

RATE OF REACTION = (1.0E+07)*EXP(-23844./(1.987*T))*C

INITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGES OF

0.0 GM-MOLES/C.C. IN INLET CONCENTRATION

30.0 DEGREES KELVIN IN INLET TEMPERATURE

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.99923	0.99928	0.99946	0.99979	0.99996
1.00	0.99790	0.99813	0.99879	0.99960	0.99985
2.00	0.99706	0.99748	0.99851	0.99948	0.99974
3.00	0.99668	0.99722	0.99842	0.99936	0.99963
4.00	0.99665	0.99721	0.99840	0.99927	0.99952
5.00	0.99681	0.99734	0.99841	0.99918	0.99942
6.00	0.99706	0.99752	0.99845	0.99912	0.99933
7.00	0.99733	0.99771	0.99849	0.99906	0.99925
8.00	0.99758	0.99789	0.99853	0.99902	0.99919
9.00	0.99781	0.99805	0.99857	0.99899	0.99913
10.00	0.99799	0.99819	0.99861	0.99896	0.99908
11.00	0.99815	0.99831	0.99865	0.99894	0.99904
12.00	0.99828	0.99841	0.99868	0.99892	0.99901
13.00	0.99839	0.99849	0.99872	0.99891	0.99898
14.00	0.99848	0.99857	0.99874	0.99891	0.99897
15.00	0.99856	0.99863	0.99877	0.99891	0.99895
16.00	0.99863	0.99868	0.99880	0.99891	0.99895
17.00	0.99868	0.99873	0.99882	0.99891	0.99894
18.00	0.99873	0.99877	0.99884	0.99891	0.99894
19.00	0.99878	0.99881	0.99886	0.99892	0.99894
20.00	0.99882	0.99884	0.99889	0.99893	0.99895
21.00	0.99885	0.99887	0.99891	0.99894	0.99896
22.00	0.99889	0.99890	0.99893	0.99896	0.99897
23.00	0.99892	0.99893	0.99895	0.99897	0.99898
24.00	0.99895	0.99896	0.99897	0.99899	0.99899
25.00	0.99897	0.99898	0.99899	0.99900	0.99900

BULK CONCENTRATION AT REACTOR EXIT = 0.998994

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	599.85	599.24	595.77	575.64	404.27
1.00	598.11	595.46	582.20	527.43	320.91
2.00	593.42	587.94	564.16	490.50	312.69
3.00	585.67	577.30	544.85	462.82	310.46
4.00	575.29	564.48	525.84	441.53	309.04
5.00	562.94	550.31	507.84	424.66	307.95
6.00	549.31	535.50	491.11	410.96	307.06
7.00	534.97	520.54	475.70	399.55	306.33
8.00	520.41	505.80	461.56	389.88	305.71
9.00	505.98	491.52	448.62	381.54	305.17
10.00	491.92	477.85	436.76	374.25	304.71
11.00	478.40	464.90	425.89	367.80	304.30
12.00	465.54	452.69	415.92	362.05	303.93
13.00	453.38	441.25	406.77	356.88	303.60
14.00	441.96	430.56	398.36	352.21	303.31
15.00	431.27	420.61	390.62	347.97	303.04
16.00	421.30	411.37	383.50	344.11	302.79
17.00	412.02	402.79	376.95	340.58	302.57
18.00	403.41	394.84	370.91	337.34	302.36
19.00	395.42	387.48	365.34	334.38	302.18
20.00	388.02	380.67	360.21	331.66	302.00
21.00	381.16	374.38	355.48	329.15	301.84
22.00	374.83	368.56	351.12	326.85	301.70
23.00	368.99	363.20	347.11	324.73	301.57
24.00	363.79	358.44	343.54	322.85	301.45
25.00	360.90	355.78	341.56	321.81	301.38

BULK TEMPERATURE AT REACTOR EXIT = 326.81

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.99572	0.99588	0.99661	0.99860	0.99997
1.00	0.99471	0.99533	0.99723	0.99946	0.99987
2.00	0.99451	0.99549	0.99777	0.99946	0.99976
3.00	0.99488	0.99595	0.99810	0.99937	0.99965
4.00	0.99548	0.99647	0.99827	0.99929	0.99954
5.00	0.99611	0.99694	0.99837	0.99921	0.99944
6.00	0.99667	0.99731	0.99843	0.99914	0.99935
7.00	0.99713	0.99762	0.99849	0.99908	0.99927
8.00	0.99749	0.99786	0.99854	0.99904	0.99921
9.00	0.99777	0.99805	0.99859	0.99901	0.99915
10.00	0.99798	0.99820	0.99863	0.99898	0.99910
11.00	0.99816	0.99833	0.99867	0.99896	0.99906
12.00	0.99830	0.99843	0.99870	0.99895	0.99903
13.00	0.99841	0.99852	0.99874	0.99894	0.99900
14.00	0.99851	0.99859	0.99876	0.99893	0.99899
15.00	0.99858	0.99865	0.99879	0.99893	0.99898
16.00	0.99865	0.99871	0.99882	0.99893	0.99897
17.00	0.99871	0.99875	0.99884	0.99893	0.99896
18.00	0.99876	0.99880	0.99887	0.99894	0.99897
19.00	0.99880	0.99884	0.99889	0.99895	0.99896
20.00	0.99884	0.99887	0.99891	0.99896	0.99897
21.00	0.99888	0.99891	0.99894	0.99897	0.99898
22.00	0.99892	0.99894	0.99896	0.99898	0.99900
23.00	0.99895	0.99897	0.99898	0.99901	0.99901
24.00	0.99898	0.99900	0.99901	0.99902	0.99903
25.00	0.99900	0.99902	0.99902	0.99903	0.99904

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	601.39	600.73	597.02	576.17	404.27
1.00	599.51	596.69	582.89	527.51	320.91
2.00	594.54	588.82	564.49	490.51	312.70
3.00	586.46	577.87	545.00	462.82	310.46
4.00	575.81	564.81	525.91	441.53	309.04
5.00	563.26	550.50	507.87	424.66	307.95
6.00	549.48	535.60	491.12	410.95	307.06
7.00	535.07	520.59	475.70	399.55	306.33
8.00	520.46	505.82	461.56	389.88	305.71
9.00	506.00	491.53	448.61	381.54	305.17
10.00	491.93	477.85	436.76	374.24	304.71
11.00	478.40	464.89	425.88	367.80	304.30
12.00	465.53	452.68	415.91	362.04	303.93
13.00	453.37	441.24	406.76	356.87	303.61
14.00	441.94	430.55	398.34	352.20	303.31
15.00	431.25	420.59	390.61	347.96	303.04
16.00	421.28	411.34	383.48	344.10	302.80
17.00	411.99	402.76	376.93	340.57	302.57
18.00	403.38	394.81	370.88	337.33	302.37
19.00	395.38	387.45	365.32	334.36	302.18
20.00	387.97	380.63	360.18	331.64	302.01
21.00	381.12	374.33	355.45	329.13	301.85
22.00	374.77	368.51	351.08	326.82	301.70
23.00	368.93	363.14	347.07	324.71	301.57
24.00	363.73	358.37	343.50	322.83	301.45
25.00	360.83	355.72	341.51	321.78	301.38

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.92184	0.92488	0.93907	0.97686	1.00003
1.00	0.92881	0.93893	0.96810	0.99675	0.99992
2.00	0.94420	0.95737	0.98456	0.99903	0.99982
3.00	0.96075	0.97264	0.99229	0.99933	0.99971
4.00	0.97417	0.98311	0.99576	0.99932	0.99960
5.00	0.98360	0.98964	0.99729	0.99926	0.99950
6.00	0.98968	0.99347	0.99800	0.99920	0.99942
7.00	0.99337	0.99568	0.99833	0.99915	0.99934
8.00	0.99556	0.99690	0.99850	0.99911	0.99927
9.00	0.99680	0.99761	0.99860	0.99908	0.99922
10.00	0.99754	0.99803	0.99869	0.99905	0.99918
11.00	0.99797	0.99829	0.99874	0.99904	0.99914
12.00	0.99825	0.99845	0.99878	0.99903	0.99912
13.00	0.99842	0.99858	0.99882	0.99902	0.99909
14.00	0.99857	0.99868	0.99886	0.99902	0.99908
15.00	0.99867	0.99876	0.99889	0.99903	0.99908
16.00	0.99875	0.99882	0.99893	0.99904	0.99907
17.00	0.99882	0.99887	0.99896	0.99905	0.99908
18.00	0.99888	0.99892	0.99899	0.99906	0.99909
19.00	0.99893	0.99897	0.99902	0.99907	0.99910
20.00	0.99898	0.99902	0.99905	0.99910	0.99911
21.00	0.99903	0.99906	0.99908	0.99912	0.99913
22.00	0.99907	0.99910	0.99911	0.99914	0.99915
23.00	0.99912	0.99914	0.99915	0.99916	0.99917
24.00	0.99916	0.99918	0.99918	0.99919	0.99920
25.00	0.99917	0.99920	0.99919	0.99921	0.99921

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	628.04	626.35	617.78	584.01	404.27
1.00	623.28	617.03	593.39	528.48	320.92
2.00	612.68	602.56	569.25	490.65	312.70
3.00	598.76	586.27	547.08	462.84	310.47
4.00	583.47	569.62	526.80	441.52	309.05
5.00	567.75	553.12	508.24	424.65	307.95
6.00	551.98	536.96	491.24	410.94	307.07
7.00	536.40	521.26	475.73	399.53	306.33
8.00	521.12	506.12	461.55	389.86	305.71
9.00	506.28	491.64	448.58	381.51	305.18
10.00	492.01	477.86	436.70	374.21	304.71
11.00	478.39	464.83	425.81	367.76	304.30
12.00	465.45	452.59	415.82	361.99	303.94
13.00	453.25	441.11	406.65	356.82	303.61
14.00	441.78	430.40	398.22	352.13	303.31
15.00	431.06	420.42	390.46	347.88	303.04
16.00	421.06	411.14	383.32	344.01	302.80
17.00	411.75	402.53	376.75	340.46	302.57
18.00	403.09	394.55	370.68	337.22	302.37
19.00	395.06	387.15	365.09	334.24	302.18
20.00	387.62	380.31	359.93	331.50	302.01
21.00	380.73	373.97	355.17	328.98	301.84
22.00	374.36	368.12	350.78	326.66	301.70
23.00	368.47	362.72	346.74	324.53	301.56
24.00	363.24	357.92	343.15	322.64	301.44
25.00	360.32	355.24	341.15	321.59	301.37

ITERATION NO. 50 TIME = 1.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.99876	0.99884	0.99913	0.99966	0.99993
1.00	0.99673	0.99708	0.99810	0.99937	0.99977
2.00	0.99558	0.99619	0.99774	0.99920	0.99960
3.00	0.99518	0.99594	0.99768	0.99906	0.99945
4.00	0.99528	0.99607	0.99773	0.99896	0.99932
5.00	0.99565	0.99636	0.99782	0.99888	0.99920
6.00	0.99611	0.99671	0.99793	0.99883	0.99911
7.00	0.99656	0.99705	0.99804	0.99879	0.99904
8.00	0.99697	0.99735	0.99815	0.99877	0.99899
9.00	0.99732	0.99762	0.99826	0.99877	0.99895
10.00	0.99761	0.99785	0.99835	0.99877	0.99892
11.00	0.99785	0.99804	0.99844	0.99879	0.99891
12.00	0.99806	0.99820	0.99852	0.99881	0.99891
13.00	0.99823	0.99834	0.99860	0.99883	0.99891
14.00	0.99837	0.99846	0.99867	0.99885	0.99892
15.00	0.99849	0.99857	0.99873	0.99888	0.99894
16.00	0.99860	0.99866	0.99879	0.99891	0.99896
17.00	0.99869	0.99874	0.99884	0.99894	0.99898
18.00	0.99877	0.99881	0.99889	0.99897	0.99900
19.00	0.99883	0.99887	0.99894	0.99900	0.99902
20.00	0.99889	0.99892	0.99897	0.99902	0.99904
21.00	0.99894	0.99896	0.99900	0.99905	0.99906
22.00	0.99897	0.99899	0.99903	0.99906	0.99907
23.00	0.99900	0.99902	0.99904	0.99907	0.99908
24.00	0.99902	0.99903	0.99905	0.99907	0.99908
25.00	0.99903	0.99904	0.99906	0.99907	0.99908

BULK CONCENTRATION AT REACTOR EXIT = 0.999066

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	629.70	629.03	625.18	603.01	414.67
1.00	627.36	624.42	609.76	549.58	322.96
2.00	621.52	615.46	589.31	508.60	313.91
3.00	612.15	602.96	567.44	477.85	311.43
4.00	599.80	588.00	545.91	454.14	309.85
5.00	585.26	571.56	525.51	435.32	308.63
6.00	569.29	554.39	506.51	419.97	307.64
7.00	552.53	537.05	488.95	407.15	306.81
8.00	535.50	519.94	472.77	396.21	306.11
9.00	518.62	503.33	457.90	386.73	305.51
10.00	502.21	487.44	444.25	378.41	304.98
11.00	486.52	472.45	431.77	371.06	304.51
12.00	471.74	458.46	420.41	364.54	304.09
13.00	458.00	445.55	410.12	358.75	303.73
14.00	445.34	433.72	400.82	353.60	303.40
15.00	433.74	422.92	392.44	349.01	303.11
16.00	423.15	413.11	384.89	344.91	302.85
17.00	413.49	404.17	378.06	341.23	302.62
18.00	404.67	396.03	371.87	337.91	302.41
19.00	396.59	388.59	366.24	334.91	302.22
20.00	389.19	381.78	361.11	332.19	302.04
21.00	382.39	375.53	356.42	329.70	301.88
22.00	376.15	369.80	352.12	327.43	301.74
23.00	370.44	364.56	348.19	325.36	301.61
24.00	365.38	359.91	344.72	323.53	301.49
25.00	362.56	357.33	342.79	322.52	301.43

BULK TEMPERATURE AT REACTOR EXIT = 327.62

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.99243	0.99271	0.99398	0.99752	0.99995
1.00	0.99131	0.99231	0.99545	0.99911	0.99978
2.00	0.99149	0.99299	0.99656	0.99918	0.99962
3.00	0.99243	0.99401	0.99719	0.99908	0.99947
4.00	0.99359	0.99500	0.99755	0.99899	0.99934
5.00	0.99469	0.99581	0.99777	0.99891	0.99923
6.00	0.99560	0.99644	0.99793	0.99886	0.99914
7.00	0.99631	0.99694	0.99806	0.99882	0.99907
8.00	0.99686	0.99732	0.99818	0.99881	0.99901
9.00	0.99728	0.99762	0.99829	0.99880	0.99897
10.00	0.99761	0.99787	0.99839	0.99881	0.99895
11.00	0.99787	0.99807	0.99847	0.99881	0.99894
12.00	0.99807	0.99823	0.99855	0.99883	0.99893
13.00	0.99825	0.99837	0.99863	0.99885	0.99893
14.00	0.99839	0.99849	0.99869	0.99887	0.99894
15.00	0.99851	0.99859	0.99875	0.99890	0.99896
16.00	0.99861	0.99867	0.99881	0.99893	0.99897
17.00	0.99870	0.99875	0.99886	0.99895	0.99899
18.00	0.99877	0.99882	0.99890	0.99898	0.99901
19.00	0.99883	0.99887	0.99894	0.99900	0.99903
20.00	0.99889	0.99892	0.99897	0.99902	0.99904
21.00	0.99893	0.99896	0.99900	0.99904	0.99906
22.00	0.99896	0.99898	0.99901	0.99905	0.99906
23.00	0.99898	0.99900	0.99903	0.99905	0.99906
24.00	0.99899	0.99901	0.99902	0.99905	0.99905
25.00	0.99899	0.99901	0.99902	0.99904	0.99905

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	631.56	630.80	626.56	603.20	414.44
1.00	628.77	625.57	610.06	549.05	322.95
2.00	622.32	615.92	589.00	508.05	313.91
3.00	612.36	602.87	566.86	477.34	311.44
4.00	599.56	587.55	545.22	453.69	309.87
5.00	584.72	570.89	524.80	434.91	308.65
6.00	568.56	553.63	505.81	419.59	307.66
7.00	551.72	536.25	488.28	406.80	306.84
8.00	534.67	519.14	472.14	395.89	306.14
9.00	517.82	502.57	457.32	386.44	305.54
10.00	501.47	486.76	443.74	378.16	305.01
11.00	485.88	471.86	431.34	370.86	304.55
12.00	471.22	457.99	420.07	364.39	304.14
13.00	457.61	445.19	409.87	358.64	303.77
14.00	445.07	433.47	400.66	353.54	303.44
15.00	433.58	422.78	392.35	348.99	303.15
16.00	423.08	413.05	384.86	344.92	302.89
17.00	413.50	404.18	378.08	341.27	302.66
18.00	404.73	396.09	371.93	337.98	302.45
19.00	396.70	388.69	366.34	334.99	302.26
20.00	389.33	381.91	361.23	332.28	302.09
21.00	382.56	375.70	356.56	329.80	301.93
22.00	376.35	369.99	352.27	327.54	301.79
23.00	370.66	364.77	348.36	325.48	301.66
24.00	365.62	360.15	344.91	323.66	301.54
25.00	362.82	357.57	342.99	322.65	301.48

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.89000	0.89440	0.91498	0.96845	0.99991
1.00	0.90680	0.92023	0.95879	0.99572	0.99980
2.00	0.93100	0.94745	0.98102	0.99871	0.99969
3.00	0.95354	0.96766	0.99083	0.99912	0.99958
4.00	0.97036	0.98059	0.99506	0.99914	0.99948
5.00	0.98154	0.98829	0.99689	0.99911	0.99939
6.00	0.98849	0.99268	0.99772	0.99907	0.99931
7.00	0.99262	0.99516	0.99812	0.99903	0.99925
8.00	0.99504	0.99654	0.99834	0.99900	0.99919
9.00	0.99643	0.99733	0.99845	0.99898	0.99914
10.00	0.99724	0.99779	0.99855	0.99896	0.99910
11.00	0.99772	0.99809	0.99861	0.99894	0.99906
12.00	0.99802	0.99826	0.99865	0.99892	0.99902
13.00	0.99821	0.99838	0.99868	0.99890	0.99899
14.00	0.99832	0.99847	0.99869	0.99887	0.99895
15.00	0.99841	0.99851	0.99869	0.99884	0.99891
16.00	0.99845	0.99853	0.99868	0.99880	0.99886
17.00	0.99846	0.99853	0.99864	0.99875	0.99880
18.00	0.99845	0.99850	0.99860	0.99868	0.99872
19.00	0.99840	0.99845	0.99853	0.99860	0.99864
20.00	0.99834	0.99839	0.99845	0.99851	0.99854
21.00	0.99825	0.99829	0.99834	0.99839	0.99842
22.00	0.99813	0.99818	0.99822	0.99826	0.99828
23.00	0.99800	0.99803	0.99807	0.99811	0.99813
24.00	0.99784	0.99788	0.99791	0.99794	0.99796
25.00	0.99773	0.99776	0.99779	0.99782	0.99784

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	652.23	650.06	639.20	599.35	409.70
1.00	642.11	634.68	607.45	537.94	322.40
2.00	626.58	615.22	579.17	497.44	313.73
3.00	608.81	595.40	554.39	467.84	311.36
4.00	590.74	576.29	532.25	445.24	309.86
5.00	573.04	558.01	512.31	427.45	308.70
6.00	555.83	540.57	494.30	413.07	307.77
7.00	539.23	523.94	478.03	401.20	307.00
8.00	523.24	508.14	463.32	391.21	306.36
9.00	507.95	493.23	450.01	382.67	305.81
10.00	493.42	479.21	437.94	375.25	305.34
11.00	479.67	466.08	426.98	368.75	304.92
12.00	466.73	453.84	417.00	362.99	304.56
13.00	454.63	442.46	407.90	357.85	304.23
14.00	443.34	431.90	399.59	353.23	303.93
15.00	432.84	422.14	391.99	349.07	303.67
16.00	423.12	413.12	385.05	345.30	303.43
17.00	414.14	404.81	378.70	341.87	303.21
18.00	405.85	397.17	372.89	338.77	303.01
19.00	398.24	390.15	367.58	335.93	302.84
20.00	391.24	383.72	362.73	333.36	302.67
21.00	384.84	377.83	358.30	331.01	302.52
22.00	378.98	372.45	354.27	328.88	302.39
23.00	373.66	367.57	350.61	326.95	302.27
24.00	369.00	363.29	347.41	325.27	302.16
25.00	366.44	360.94	345.65	324.34	302.11

ITERATION NO. 100 TIME = 2.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.99794	0.99812	0.99868	0.99953	0.99990
1.00	0.99478	0.99544	0.99720	0.99911	0.99967
2.00	0.99316	0.99422	0.99670	0.99886	0.99943
3.00	0.99272	0.99394	0.99661	0.99865	0.99921
4.00	0.99298	0.99419	0.99669	0.99849	0.99902
5.00	0.99359	0.99466	0.99682	0.99838	0.99885
6.00	0.99430	0.99519	0.99699	0.99830	0.99871
7.00	0.99499	0.99570	0.99715	0.99825	0.99861
8.00	0.99560	0.99616	0.99732	0.99822	0.99853
9.00	0.99613	0.99656	0.99748	0.99822	0.99847
10.00	0.99656	0.99690	0.99762	0.99823	0.99844
11.00	0.99693	0.99719	0.99776	0.99825	0.99842
12.00	0.99723	0.99743	0.99788	0.99828	0.99842
13.00	0.99748	0.99764	0.99799	0.99831	0.99843
14.00	0.99769	0.99782	0.99810	0.99835	0.99845
15.00	0.99787	0.99797	0.99819	0.99839	0.99847
16.00	0.99802	0.99810	0.99828	0.99844	0.99850
17.00	0.99815	0.99821	0.99835	0.99848	0.99853
18.00	0.99826	0.99831	0.99842	0.99853	0.99857
19.00	0.99836	0.99840	0.99849	0.99857	0.99860
20.00	0.99844	0.99848	0.99854	0.99861	0.99863
21.00	0.99852	0.99854	0.99860	0.99865	0.99867
22.00	0.99858	0.99860	0.99864	0.99868	0.99870
23.00	0.99864	0.99865	0.99869	0.99872	0.99873
24.00	0.99868	0.99870	0.99872	0.99875	0.99875
25.00	0.99871	0.99873	0.99875	0.99877	0.99877

BULK CONCENTRATION AT REACTOR EXIT = 0.998757

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	630.43	629.69	625.66	603.25	414.69
1.00	629.23	626.09	610.91	550.15	323.00
2.00	624.12	617.77	590.91	509.42	313.95
3.00	615.23	605.70	569.37	478.86	311.49
4.00	603.24	591.08	548.12	455.31	309.92
5.00	589.01	574.94	527.98	436.63	308.71
6.00	573.37	558.10	509.25	421.42	307.73
7.00	557.02	541.15	491.99	408.75	306.91
8.00	540.48	524.48	476.16	397.99	306.22
9.00	524.14	508.38	461.67	388.70	305.63
10.00	508.28	493.01	448.40	380.58	305.11
11.00	493.08	478.46	436.26	373.40	304.65
12.00	478.65	464.79	425.13	367.00	304.25
13.00	465.06	452.01	414.93	361.25	303.88
14.00	452.32	440.11	405.57	356.07	303.55
15.00	440.43	429.04	396.99	351.37	303.25
16.00	429.37	418.79	389.10	347.09	302.98
17.00	419.11	409.31	381.86	343.19	302.74
18.00	409.62	400.55	375.21	339.64	302.51
19.00	400.84	392.47	369.10	336.38	302.30
20.00	392.75	385.03	363.49	333.41	302.12
21.00	385.30	378.18	358.35	330.69	301.94
22.00	378.45	371.89	353.64	328.20	301.79
23.00	372.19	366.15	349.34	325.93	301.64
24.00	366.66	361.07	345.54	323.93	301.52
25.00	363.56	358.23	343.42	322.81	301.45

BULK TEMPERATURE AT REACTOR EXIT = 328.02

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.98682	0.98764	0.99073	0.99672	0.99992
1.00	0.98595	0.98809	0.99356	0.99880	0.99969
2.00	0.98702	0.98963	0.99514	0.99883	0.99946
3.00	0.98880	0.99129	0.99599	0.99868	0.99925
4.00	0.99066	0.99275	0.99646	0.99853	0.99905
5.00	0.99230	0.99394	0.99677	0.99842	0.99889
6.00	0.99364	0.99487	0.99700	0.99835	0.99876
7.00	0.99469	0.99558	0.99720	0.99830	0.99865
8.00	0.99549	0.99614	0.99737	0.99827	0.99857
9.00	0.99611	0.99659	0.99753	0.99827	0.99851
10.00	0.99659	0.99695	0.99768	0.99828	0.99849
11.00	0.99697	0.99724	0.99781	0.99829	0.99847
12.00	0.99728	0.99749	0.99793	0.99832	0.99846
13.00	0.99753	0.99769	0.99805	0.99836	0.99847
14.00	0.99774	0.99788	0.99815	0.99840	0.99849
15.00	0.99791	0.99802	0.99824	0.99844	0.99851
16.00	0.99807	0.99815	0.99832	0.99848	0.99854
17.00	0.99819	0.99826	0.99839	0.99852	0.99857
18.00	0.99830	0.99835	0.99846	0.99856	0.99860
19.00	0.99840	0.99844	0.99852	0.99860	0.99863
20.00	0.99847	0.99851	0.99858	0.99864	0.99866
21.00	0.99854	0.99858	0.99862	0.99867	0.99870
22.00	0.99861	0.99863	0.99867	0.99871	0.99872
23.00	0.99866	0.99868	0.99871	0.99874	0.99875
24.00	0.99870	0.99872	0.99874	0.99876	0.99877
25.00	0.99872	0.99875	0.99876	0.99879	0.99879

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	634.72	633.73	628.70	604.19	414.61
1.00	632.54	628.81	612.13	550.04	322.99
2.00	626.29	619.31	591.23	509.20	313.96
3.00	616.45	606.41	569.28	478.63	311.50
4.00	603.76	591.26	547.86	455.09	309.93
5.00	589.08	574.81	527.65	436.42	308.71
6.00	573.18	557.80	508.90	421.22	307.73
7.00	556.67	540.76	491.64	408.56	306.92
8.00	540.06	524.07	475.82	397.81	306.23
9.00	523.70	507.96	461.34	388.53	305.64
10.00	507.84	492.59	448.09	380.42	305.12
11.00	492.65	478.06	435.96	373.25	304.66
12.00	478.24	464.42	424.85	366.86	304.26
13.00	464.68	451.66	414.67	361.13	303.89
14.00	451.96	439.78	405.34	355.95	303.56
15.00	440.10	428.75	396.77	351.26	303.27
16.00	429.08	418.52	388.91	347.00	302.99
17.00	418.85	409.07	381.69	343.12	302.75
18.00	409.39	400.34	375.06	339.57	302.52
19.00	400.65	392.29	368.98	336.33	302.32
20.00	392.59	384.88	363.39	333.37	302.13
21.00	385.17	378.06	358.27	330.66	301.96
22.00	378.36	371.81	353.58	328.18	301.80
23.00	372.13	366.09	349.30	325.92	301.66
24.00	366.64	361.05	345.53	323.94	301.53
25.00	363.56	358.23	343.43	322.83	301.46

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.68624	0.71805	0.81670	0.94892	0.99994
1.00	0.78846	0.83666	0.93069	0.99386	0.99978
2.00	0.87051	0.90858	0.97084	0.99828	0.99962
3.00	0.92286	0.94881	0.98666	0.99887	0.99948
4.00	0.95462	0.97120	0.99316	0.99890	0.99934
5.00	0.97342	0.98353	0.99589	0.99888	0.99922
6.00	0.98430	0.99021	0.99708	0.99883	0.99913
7.00	0.99042	0.99380	0.99765	0.99880	0.99905
8.00	0.99383	0.99574	0.99796	0.99877	0.99900
9.00	0.99572	0.99681	0.99814	0.99877	0.99895
10.00	0.99678	0.99743	0.99829	0.99877	0.99892
11.00	0.99741	0.99781	0.99839	0.99877	0.99890
12.00	0.99779	0.99806	0.99848	0.99878	0.99889
13.00	0.99805	0.99823	0.99855	0.99879	0.99888
14.00	0.99823	0.99838	0.99861	0.99881	0.99888
15.00	0.99838	0.99848	0.99866	0.99882	0.99888
16.00	0.99848	0.99855	0.99871	0.99883	0.99888
17.00	0.99856	0.99862	0.99873	0.99883	0.99888
18.00	0.99862	0.99867	0.99875	0.99884	0.99888
19.00	0.99865	0.99870	0.99877	0.99884	0.99887
20.00	0.99868	0.99872	0.99877	0.99883	0.99886
21.00	0.99869	0.99873	0.99877	0.99881	0.99883
22.00	0.99869	0.99872	0.99875	0.99879	0.99880
23.00	0.99867	0.99870	0.99873	0.99876	0.99877
24.00	0.99864	0.99867	0.99869	0.99871	0.99872
25.00	0.99862	0.99864	0.99866	0.99868	0.99869

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	734.99	723.24	684.94	616.50	413.10
1.00	695.79	676.05	628.70	547.47	322.78
2.00	660.38	641.16	593.85	505.34	313.85
3.00	632.20	614.22	566.46	474.73	311.40
4.00	608.62	591.40	542.87	451.33	309.85
5.00	587.68	570.89	521.85	432.82	308.65
6.00	568.34	551.83	502.86	417.77	307.67
7.00	550.09	533.86	485.62	405.28	306.87
8.00	532.70	516.84	469.96	394.70	306.19
9.00	516.12	500.75	455.72	385.59	305.61
10.00	500.36	485.60	442.75	377.66	305.10
11.00	485.45	471.39	430.94	370.68	304.66
12.00	471.43	458.15	420.17	364.48	304.26
13.00	458.33	445.85	410.35	358.95	303.91
14.00	446.14	434.45	401.40	353.98	303.59
15.00	434.83	423.93	393.23	349.51	303.31
16.00	424.39	414.24	385.78	345.46	303.05
17.00	414.76	405.34	378.98	341.80	302.82
18.00	405.91	397.18	372.77	338.48	302.61
19.00	397.78	389.69	367.11	335.46	302.42
20.00	390.33	382.84	361.94	332.72	302.24
21.00	383.51	376.56	357.23	330.22	302.09
22.00	377.26	370.83	352.93	327.95	301.94
23.00	371.57	365.61	349.02	325.89	301.81
24.00	366.56	361.01	345.58	324.08	301.70
25.00	363.78	358.46	343.68	323.08	301.64

ITERATION NO. 150 TIME = 2.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.94814	0.95656	0.98558	0.99858	0.99973
1.00	0.88613	0.92824	0.98215	0.99684	0.99902
2.00	0.91156	0.94514	0.98275	0.99588	0.99832
3.00	0.94146	0.95989	0.98477	0.99544	0.99776
4.00	0.96047	0.97092	0.98721	0.99540	0.99741
5.00	0.97273	0.97892	0.98955	0.99560	0.99723
6.00	0.98080	0.98458	0.99154	0.99591	0.99718
7.00	0.98614	0.98851	0.99311	0.99625	0.99722
8.00	0.98969	0.99122	0.99431	0.99656	0.99729
9.00	0.99207	0.99308	0.99520	0.99683	0.99738
10.00	0.99368	0.99437	0.99585	0.99705	0.99747
11.00	0.99479	0.99528	0.99634	0.99724	0.99755
12.00	0.99558	0.99593	0.99671	0.99739	0.99763
13.00	0.99616	0.99642	0.99700	0.99751	0.99770
14.00	0.99659	0.99679	0.99723	0.99762	0.99777
15.00	0.99693	0.99708	0.99741	0.99772	0.99784
16.00	0.99720	0.99731	0.99757	0.99781	0.99790
17.00	0.99741	0.99750	0.99770	0.99789	0.99796
18.00	0.99759	0.99767	0.99782	0.99797	0.99803
19.00	0.99775	0.99781	0.99793	0.99804	0.99809
20.00	0.99788	0.99793	0.99802	0.99811	0.99815
21.00	0.99800	0.99804	0.99811	0.99818	0.99821
22.00	0.99811	0.99814	0.99819	0.99825	0.99827
23.00	0.99820	0.99823	0.99827	0.99831	0.99833
24.00	0.99829	0.99831	0.99834	0.99837	0.99838
25.00	0.99834	0.99836	0.99838	0.99841	0.99842

BULK CONCENTRATION AT REACTOR EXIT = 0.998397

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	659.79	653.95	632.70	603.86	414.73
1.00	690.03	663.02	619.19	551.57	323.08
2.00	667.44	643.89	598.62	511.23	314.06
3.00	641.82	623.55	575.98	480.78	311.61
4.00	620.07	603.36	553.56	457.17	310.04
5.00	600.15	583.60	532.41	438.35	308.82
6.00	581.16	564.46	512.90	422.98	307.82
7.00	562.82	546.08	495.09	410.18	307.00
8.00	545.11	528.54	478.88	399.30	306.30
9.00	528.08	511.90	464.13	389.93	305.71
10.00	511.80	496.19	450.69	381.74	305.18
11.00	496.34	481.42	438.41	374.51	304.72
12.00	481.73	467.59	427.19	368.06	304.31
13.00	467.99	454.69	416.90	362.27	303.95
14.00	455.13	442.68	407.47	357.05	303.61
15.00	443.14	431.52	398.81	352.31	303.31
16.00	431.97	421.17	390.86	348.00	303.04
17.00	421.61	411.59	383.55	344.07	302.79
18.00	412.01	402.74	376.83	340.47	302.56
19.00	403.13	394.56	370.64	337.18	302.35
20.00	394.92	387.01	364.95	334.16	302.16
21.00	387.34	380.04	359.72	331.39	301.99
22.00	380.36	373.63	354.91	328.85	301.83
23.00	373.94	367.74	350.51	326.53	301.68
24.00	368.25	362.52	346.61	324.47	301.55
25.00	365.07	359.61	344.43	323.32	301.48

BULK TEMPERATURE AT REACTOR EXIT = 328.67

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.64288	0.66270	0.82799	0.99497	0.99981
1.00	0.59574	0.85362	0.98118	0.99718	0.99925
2.00	0.91063	0.94736	0.98453	0.99674	0.99868
3.00	0.94729	0.96451	0.98733	0.99643	0.99823
4.00	0.96584	0.97544	0.98975	0.99638	0.99793
5.00	0.97701	0.98265	0.99172	0.99650	0.99775
6.00	0.98398	0.98741	0.99325	0.99668	0.99768
7.00	0.98841	0.99055	0.99439	0.99689	0.99765
8.00	0.99128	0.99265	0.99524	0.99707	0.99766
9.00	0.99316	0.99408	0.99588	0.99723	0.99769
10.00	0.99444	0.99507	0.99635	0.99737	0.99772
11.00	0.99533	0.99578	0.99671	0.99749	0.99777
12.00	0.99597	0.99630	0.99700	0.99759	0.99781
13.00	0.99645	0.99670	0.99722	0.99769	0.99786
14.00	0.99682	0.99701	0.99741	0.99777	0.99791
15.00	0.99711	0.99726	0.99757	0.99785	0.99796
16.00	0.99735	0.99746	0.99770	0.99793	0.99802
17.00	0.99755	0.99764	0.99782	0.99800	0.99807
18.00	0.99771	0.99779	0.99793	0.99807	0.99812
19.00	0.99786	0.99792	0.99803	0.99813	0.99818
20.00	0.99799	0.99803	0.99812	0.99820	0.99824
21.00	0.99810	0.99814	0.99820	0.99827	0.99829
22.00	0.99820	0.99823	0.99828	0.99833	0.99835
23.00	0.99829	0.99832	0.99835	0.99839	0.99840
24.00	0.99837	0.99839	0.99842	0.99844	0.99846
25.00	0.99841	0.99844	0.99846	0.99848	0.99849

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	782.11	770.75	685.87	605.39	414.73
1.00	794.96	684.12	618.88	551.36	323.06
2.00	663.02	640.50	597.30	510.79	314.04
3.00	637.14	620.23	574.47	480.30	311.59
4.00	616.69	600.69	552.20	456.72	310.02
5.00	597.76	581.59	531.30	437.95	308.80
6.00	579.48	563.00	512.04	422.66	307.81
7.00	561.63	545.02	494.44	409.91	306.99
8.00	544.24	527.76	478.37	399.08	306.30
9.00	527.42	511.30	463.73	389.75	305.70
10.00	511.27	495.71	450.35	381.58	305.18
11.00	495.89	481.01	438.12	374.36	304.72
12.00	481.33	467.23	426.93	367.93	304.31
13.00	467.63	454.36	416.66	362.15	303.94
14.00	454.79	442.37	407.25	356.94	303.61
15.00	442.82	431.23	398.60	352.20	303.31
16.00	431.67	420.89	390.66	347.90	303.04
17.00	421.32	411.33	383.35	343.97	302.79
18.00	411.73	402.48	376.64	340.37	302.56
19.00	402.86	394.31	370.46	337.09	302.35
20.00	394.66	386.77	364.78	334.07	302.16
21.00	387.10	379.82	359.56	331.31	301.99
22.00	380.12	373.42	354.76	328.77	301.83
23.00	373.72	367.54	350.36	326.45	301.68
24.00	368.05	362.34	346.47	324.40	301.55
25.00	364.88	359.43	344.30	323.26	301.48

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.0	0.0	0.03361	0.93359	0.99993
1.00	0.00011	0.08033	0.89977	0.99235	0.99967
2.00	0.68972	0.84377	0.96040	0.99756	0.99941
3.00	0.87276	0.92343	0.98164	0.99822	0.99918
4.00	0.93230	0.95869	0.99026	0.99827	0.99899
5.00	0.96191	0.97667	0.99400	0.99827	0.99883
6.00	0.97787	0.98618	0.99572	0.99825	0.99872
7.00	0.98662	0.99127	0.99659	0.99824	0.99863
8.00	0.99144	0.99403	0.99708	0.99825	0.99858
9.00	0.99410	0.99557	0.99740	0.99827	0.99853
10.00	0.99561	0.99646	0.99762	0.99829	0.99851
11.00	0.99650	0.99702	0.99780	0.99832	0.99850
12.00	0.99706	0.99739	0.99794	0.99835	0.99850
13.00	0.99743	0.99765	0.99806	0.99839	0.99851
14.00	0.99769	0.99787	0.99817	0.99842	0.99852
15.00	0.99790	0.99803	0.99825	0.99846	0.99854
16.00	0.99806	0.99815	0.99834	0.99850	0.99856
17.00	0.99819	0.99827	0.99841	0.99853	0.99859
18.00	0.99830	0.99836	0.99846	0.99857	0.99862
19.00	0.99838	0.99844	0.99852	0.99860	0.99863
20.00	0.99846	0.99850	0.99857	0.99863	0.99866
21.00	0.99852	0.99856	0.99861	0.99866	0.99868
22.00	0.99857	0.99860	0.99864	0.99868	0.99869
23.00	0.99861	0.99864	0.99866	0.99870	0.99871
24.00	0.99864	0.99866	0.99868	0.99870	0.99871
25.00	0.99865	0.99868	0.99869	0.99872	0.99872

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	986.75	984.33	964.76	625.26	414.10
1.00	978.66	943.04	643.93	550.99	322.92
2.00	729.84	669.46	601.88	508.40	313.92
3.00	655.74	628.60	572.60	477.62	311.47
4.00	622.34	601.25	548.25	454.08	309.90
5.00	597.58	578.75	526.83	435.44	308.69
6.00	576.43	558.67	507.57	420.27	307.72
7.00	557.19	540.10	490.13	407.65	306.90
8.00	539.20	522.68	474.26	396.95	306.22
9.00	522.18	506.25	459.81	387.72	305.63
10.00	506.04	490.79	446.63	379.66	305.11
11.00	490.79	476.28	434.58	372.54	304.66
12.00	476.41	462.71	423.56	366.20	304.26
13.00	462.95	450.07	413.48	360.52	303.89
14.00	450.38	438.32	404.25	355.41	303.57
15.00	438.67	427.44	395.80	350.78	303.28
16.00	427.82	417.37	388.07	346.58	303.01
17.00	417.77	408.09	380.98	342.77	302.77
18.00	408.50	399.54	374.48	339.30	302.55
19.00	399.97	391.67	368.54	336.13	302.35
20.00	392.11	384.45	363.09	333.24	302.16
21.00	384.90	377.82	358.11	330.60	302.00
22.00	378.28	371.74	353.55	328.19	301.84
23.00	372.22	366.19	349.39	326.00	301.70
24.00	366.88	361.29	345.73	324.07	301.58
25.00	363.91	358.56	343.69	323.00	301.51

ITERATION NO. 200 TIME = 4.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.92117	0.92764	0.95562	0.99576	0.99900
1.00	0.77736	0.80465	0.93371	0.98802	0.99599
2.00	0.68300	0.73754	0.92506	0.98184	0.99228
3.00	0.66716	0.76769	0.92226	0.97697	0.98850
4.00	0.74800	0.82017	0.92665	0.97396	0.98526
5.00	0.81705	0.86171	0.93437	0.97279	0.98295
6.00	0.86555	0.89348	0.94308	0.97308	0.98170
7.00	0.89981	0.91758	0.95160	0.97443	0.98142
8.00	0.92439	0.93594	0.95939	0.97645	0.98193
9.00	0.94237	0.95002	0.96626	0.97882	0.98301
10.00	0.95574	0.96088	0.97216	0.98131	0.98446
11.00	0.96580	0.96930	0.97715	0.98377	0.98610
12.00	0.97346	0.97586	0.98133	0.98608	0.98777
13.00	0.97932	0.98097	0.98479	0.98816	0.98939
14.00	0.98381	0.98495	0.98761	0.99000	0.99088
15.00	0.98726	0.98804	0.98989	0.99158	0.99221
16.00	0.98989	0.99044	0.99172	0.99291	0.99335
17.00	0.99190	0.99228	0.99317	0.99400	0.99431
18.00	0.99343	0.99369	0.99431	0.99489	0.99511
19.00	0.99458	0.99477	0.99520	0.99560	0.99576
20.00	0.99546	0.99559	0.99589	0.99617	0.99628
21.00	0.99612	0.99621	0.99642	0.99662	0.99670
22.00	0.99662	0.99669	0.99684	0.99698	0.99703
23.00	0.99701	0.99706	0.99716	0.99726	0.99730
24.00	0.99730	0.99734	0.99741	0.99748	0.99751
25.00	0.99748	0.99751	0.99756	0.99762	0.99764

BULK CONCENTRATION AT REACTOR EXIT = 0.997593

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	678.77	673.84	651.82	605.55	414.81
1.00	762.86	742.36	647.85	556.49	323.35
2.00	808.78	767.99	632.06	518.62	314.49
3.00	800.27	731.82	610.75	489.81	312.14
4.00	736.27	684.85	585.69	466.80	310.62
5.00	681.43	644.27	560.20	447.73	309.39
6.00	638.62	609.52	535.99	431.54	308.35
7.00	603.95	579.56	513.77	417.63	307.46
8.00	574.88	553.46	493.71	405.58	306.69
9.00	549.83	530.49	475.76	395.08	306.03
10.00	527.83	510.11	459.75	385.90	305.44
11.00	508.26	491.91	445.45	377.84	304.93
12.00	490.69	475.56	432.66	370.71	304.48
13.00	474.83	460.81	421.19	364.39	304.08
14.00	460.44	447.45	410.87	358.75	303.72
15.00	447.34	435.32	401.56	353.70	303.40
16.00	435.39	424.28	393.12	349.15	303.11
17.00	424.47	414.19	385.45	345.04	302.85
18.00	414.45	404.96	378.46	341.32	302.62
19.00	405.27	396.51	372.08	337.92	302.40
20.00	396.83	388.75	366.24	334.83	302.20
21.00	389.07	381.62	360.89	331.99	302.03
22.00	381.93	375.07	355.98	329.40	301.86
23.00	375.38	369.06	351.48	327.03	301.71
24.00	369.58	363.74	347.50	324.93	301.58
25.00	366.33	360.76	345.28	323.76	301.50

BULK TEMPERATURE AT REACTOR EXIT = 329.21

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.56497	0.57943	0.64316	0.99140	0.99907
1.00	0.39911	0.42252	0.92023	0.98812	0.99622
2.00	0.32880	0.35526	0.92277	0.98267	0.99268
3.00	0.30136	0.70317	0.92388	0.97815	0.98911
4.00	0.69704	0.81568	0.92977	0.97539	0.98608
5.00	0.81511	0.86522	0.93785	0.97437	0.98396
6.00	0.86976	0.89834	0.94643	0.97473	0.98283
7.00	0.90469	0.92219	0.95463	0.97608	0.98262
8.00	0.92878	0.93991	0.96206	0.97803	0.98315
9.00	0.94603	0.95332	0.96856	0.98029	0.98421
10.00	0.95872	0.96357	0.97412	0.98265	0.98558
11.00	0.96820	0.97148	0.97881	0.98496	0.98712
12.00	0.97537	0.97762	0.98271	0.98711	0.98869
13.00	0.98084	0.98237	0.98591	0.98905	0.99019
14.00	0.98501	0.98607	0.98853	0.99075	0.99156
15.00	0.98819	0.98893	0.99064	0.99220	0.99278
16.00	0.99062	0.99113	0.99231	0.99341	0.99382
17.00	0.99246	0.99282	0.99364	0.99441	0.99470
18.00	0.99386	0.99411	0.99468	0.99522	0.99542
19.00	0.99492	0.99510	0.99549	0.99587	0.99601
20.00	0.99571	0.99584	0.99611	0.99638	0.99648
21.00	0.99632	0.99641	0.99660	0.99679	0.99686
22.00	0.99678	0.99685	0.99698	0.99712	0.99716
23.00	0.99714	0.99718	0.99728	0.99737	0.99740
24.00	0.99740	0.99744	0.99751	0.99757	0.99760
25.00	0.99757	0.99760	0.99765	0.99770	0.99772

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	831.10	822.55	783.48	607.41	414.82
1.00	922.15	901.14	651.81	556.31	323.34
2.00	953.38	914.91	631.48	518.04	314.47
3.00	937.30	749.24	608.53	489.03	312.12
4.00	748.62	682.43	583.02	465.93	310.59
5.00	678.13	640.03	557.64	446.85	309.36
6.00	634.35	605.63	533.76	430.72	308.32
7.00	600.32	576.40	511.91	416.90	307.44
8.00	572.04	551.00	492.22	404.96	306.67
9.00	547.67	528.61	474.58	394.57	306.01
10.00	526.21	508.69	458.83	385.49	305.43
11.00	507.05	490.84	444.74	377.51	304.92
12.00	489.80	474.76	432.12	370.46	304.47
13.00	474.16	460.21	420.79	364.19	304.07
14.00	459.95	447.01	410.57	358.60	303.72
15.00	446.98	434.99	401.32	353.59	303.40
16.00	435.12	424.02	392.94	349.06	303.11
17.00	424.25	414.00	385.31	344.97	302.85
18.00	414.28	404.81	378.35	341.26	302.62
19.00	405.12	396.38	371.98	337.87	302.40
20.00	396.70	388.64	366.16	334.78	302.21
21.00	388.95	381.52	360.81	331.96	302.03
22.00	381.82	374.97	355.91	329.36	301.86
23.00	375.28	368.97	351.41	326.99	301.71
24.00	369.48	363.65	347.44	324.90	301.58
25.00	366.24	360.68	345.22	323.73	301.51

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.0	0.91887	0.99961
1.00	0.00000	0.00000	0.79113	0.98738	0.99835
2.00	0.00000	0.00000	0.91622	0.99132	0.99690
3.00	0.00009	0.67111	0.95036	0.99082	0.99558
4.00	0.72226	0.86995	0.96558	0.99036	0.99459
5.00	0.87991	0.92553	0.97401	0.99041	0.99400
6.00	0.93081	0.95238	0.97953	0.99086	0.99379
7.00	0.95607	0.96753	0.98356	0.99156	0.99386
8.00	0.97042	0.97685	0.98668	0.99239	0.99415
9.00	0.97918	0.98293	0.98915	0.99323	0.99456
10.00	0.98481	0.98708	0.99112	0.99405	0.99503
11.00	0.98860	0.99001	0.99271	0.99479	0.99551
12.00	0.99121	0.99213	0.99395	0.99544	0.99597
13.00	0.99308	0.99367	0.99493	0.99600	0.99639
14.00	0.99442	0.99484	0.99571	0.99647	0.99675
15.00	0.99541	0.99570	0.99631	0.99687	0.99707
16.00	0.99615	0.99635	0.99678	0.99718	0.99733
17.00	0.99669	0.99685	0.99715	0.99744	0.99756
18.00	0.99711	0.99722	0.99744	0.99766	0.99774
19.00	0.99743	0.99751	0.99767	0.99783	0.99789
20.00	0.99767	0.99773	0.99785	0.99797	0.99801
21.00	0.99786	0.99791	0.99800	0.99809	0.99812
22.00	0.99801	0.99806	0.99812	0.99818	0.99821
23.00	0.99814	0.99817	0.99822	0.99826	0.99829
24.00	0.99824	0.99827	0.99830	0.99833	0.99835
25.00	0.99830	0.99832	0.99834	0.99838	0.99839

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	1017.31	1014.00	996.35	632.13	414.52
1.00	1024.53	1010.35	687.87	554.53	323.09
2.00	1008.87	983.11	623.08	512.44	314.12
3.00	978.42	728.00	588.66	481.94	311.69
4.00	706.64	640.75	561.24	458.34	310.13
5.00	634.06	602.95	537.48	439.43	308.90
6.00	598.69	575.41	516.33	423.88	307.90
7.00	572.50	552.46	497.37	410.84	307.06
8.00	550.50	532.21	480.30	399.73	306.35
9.00	530.96	513.88	464.91	390.15	305.74
10.00	513.15	497.09	450.99	381.79	305.20
11.00	496.74	481.62	438.36	374.42	304.73
12.00	481.55	467.34	426.90	367.88	304.32
13.00	467.45	454.16	416.46	362.03	303.95
14.00	454.40	441.98	406.93	356.77	303.61
15.00	442.30	430.75	398.23	352.01	303.31
16.00	431.11	420.37	390.27	347.70	303.04
17.00	420.76	410.82	382.98	343.78	302.79
18.00	411.22	402.01	376.29	340.20	302.56
19.00	402.41	393.90	370.16	336.94	302.35
20.00	394.29	386.43	364.54	333.95	302.16
21.00	386.81	379.56	359.37	331.23	301.99
22.00	379.93	373.25	354.64	328.72	301.83
23.00	373.63	367.46	350.31	326.44	301.69
24.00	368.05	362.34	346.48	324.42	301.56
25.00	364.93	359.49	344.35	323.30	301.49

ITERATION NO. 250 TIME = 5.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.91539	0.91927	0.93694	0.99253	0.99795
1.00	0.75411	0.76900	0.84426	0.97399	0.99112
2.00	0.63117	0.66624	0.84265	0.95919	0.98213
3.00	0.54689	0.60239	0.83905	0.94783	0.97288
4.00	0.49669	0.56851	0.83230	0.93823	0.96405
5.00	0.48543	0.57367	0.82903	0.93048	0.95609
6.00	0.53557	0.64947	0.83573	0.92546	0.94955
7.00	0.64002	0.71707	0.84858	0.92338	0.94487
8.00	0.72044	0.77051	0.86367	0.92384	0.94219
9.00	0.77928	0.81253	0.87904	0.92631	0.94144
10.00	0.82329	0.84594	0.89372	0.93022	0.94238
11.00	0.85704	0.87278	0.90727	0.93509	0.94465
12.00	0.88347	0.89455	0.91953	0.94052	0.94792
13.00	0.90447	0.91235	0.93048	0.94619	0.95182
14.00	0.92136	0.92700	0.94015	0.95183	0.95608
15.00	0.93505	0.93911	0.94865	0.95728	0.96045
16.00	0.94624	0.94916	0.95608	0.96241	0.96477
17.00	0.95542	0.95752	0.96253	0.96716	0.96889
18.00	0.96298	0.96450	0.96811	0.97149	0.97275
19.00	0.96924	0.97033	0.97294	0.97538	0.97631
20.00	0.97443	0.97521	0.97709	0.97885	0.97953
21.00	0.97874	0.97931	0.98065	0.98192	0.98241
22.00	0.98233	0.98273	0.98369	0.98460	0.98495
23.00	0.98530	0.98559	0.98627	0.98693	0.98718
24.00	0.98772	0.98793	0.98842	0.98889	0.98907
25.00	0.98925	0.98942	0.98981	0.99018	0.99032

BULK CONCENTRATION AT REACTOR EXIT = 0.990009

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	683.49	680.17	664.54	607.56	414.92
1.00	781.78	768.70	703.61	564.73	323.81
2.00	850.93	821.72	682.43	531.03	315.23
3.00	890.21	845.23	661.66	504.88	313.06
4.00	902.30	844.67	642.23	484.24	311.68
5.00	884.67	814.94	620.72	467.07	310.57
6.00	828.35	747.98	594.64	451.70	309.59
7.00	746.54	688.44	566.95	437.41	308.69
8.00	681.63	638.97	540.09	424.08	307.85
9.00	630.91	597.78	515.18	411.74	307.07
10.00	590.13	563.14	492.63	400.46	306.36
11.00	556.49	533.71	472.50	390.26	305.71
12.00	528.19	508.49	454.67	381.12	305.14
13.00	504.05	486.72	438.95	372.98	304.62
14.00	483.23	467.82	425.09	365.75	304.16
15.00	465.13	451.31	412.88	359.36	303.76
16.00	449.28	436.81	402.10	353.69	303.40
17.00	435.32	424.02	392.55	348.66	303.08
18.00	422.95	412.68	384.08	344.19	302.80
19.00	411.94	402.58	376.52	340.21	302.55
20.00	402.09	393.54	369.76	336.65	302.32
21.00	393.25	385.43	363.70	333.46	302.12
22.00	385.28	378.13	358.24	330.58	301.94
23.00	378.10	371.54	353.32	327.99	301.77
24.00	371.82	365.79	349.02	325.73	301.63
25.00	368.31	362.57	346.62	324.47	301.55

BULK TEMPERATURE AT REACTOR EXIT = 330.08

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.56058	0.57208	0.62078	0.98788	0.99810
1.00	0.38827	0.39833	0.51931	0.97509	0.99178
2.00	0.30789	0.32987	0.83042	0.96223	0.98359
3.00	0.25885	0.29545	0.84065	0.95191	0.97519
4.00	0.23780	0.28045	0.83946	0.94317	0.96716
5.00	0.24382	0.25181	0.84119	0.93637	0.96000
6.00	0.26384	0.66260	0.85036	0.93227	0.95424
7.00	0.66082	0.74274	0.86365	0.93090	0.95029
8.00	0.74893	0.79526	0.87834	0.93186	0.94826
9.00	0.80492	0.83449	0.89293	0.93460	0.94801
10.00	0.84524	0.86504	0.90665	0.93859	0.94927
11.00	0.87569	0.88933	0.91916	0.94334	0.95167
12.00	0.89933	0.90887	0.93035	0.94848	0.95488
13.00	0.91799	0.92474	0.94024	0.95372	0.95856
14.00	0.93289	0.93770	0.94889	0.95885	0.96248
15.00	0.94490	0.94834	0.95641	0.96372	0.96642
16.00	0.95463	0.95710	0.96292	0.96826	0.97025
17.00	0.96257	0.96434	0.96853	0.97242	0.97388
18.00	0.96907	0.97034	0.97335	0.97618	0.97724
19.00	0.97442	0.97533	0.97749	0.97953	0.98030
20.00	0.97883	0.97949	0.98103	0.98250	0.98305
21.00	0.98247	0.98294	0.98404	0.98510	0.98550
22.00	0.98548	0.98582	0.98660	0.98735	0.98764
23.00	0.98796	0.98820	0.98875	0.98928	0.98949
24.00	0.98996	0.99013	0.99053	0.99090	0.99105
25.00	0.99121	0.99135	0.99166	0.99196	0.99208

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	836.91	830.14	800.33	609.46	414.92
1.00	939.59	927.83	828.36	563.74	323.75
2.00	988.92	964.23	682.92	529.00	315.12
3.00	1010.24	971.33	657.21	502.37	312.93
4.00	1005.41	954.39	635.36	481.40	311.53
5.00	972.57	912.76	611.49	463.86	310.40
6.00	906.69	730.96	584.63	448.24	309.41
7.00	726.35	669.77	557.37	433.89	308.50
8.00	662.28	622.98	531.41	420.67	307.67
9.00	615.20	584.67	507.58	408.58	306.90
10.00	577.65	552.53	486.12	397.62	306.21
11.00	546.61	525.16	467.03	387.78	305.58
12.00	520.38	501.64	450.14	379.00	305.02
13.00	497.87	481.25	435.23	371.20	304.53
14.00	478.35	463.47	422.07	364.28	304.09
15.00	461.29	447.86	410.45	358.15	303.70
16.00	446.26	434.09	400.16	352.71	303.35
17.00	432.95	421.87	391.01	347.88	303.04
18.00	421.09	410.99	382.86	343.57	302.77
19.00	410.48	401.26	375.56	339.72	302.52
20.00	400.95	392.50	369.00	336.26	302.30
21.00	392.35	384.61	363.10	333.14	302.11
22.00	384.57	377.48	357.76	330.33	301.93
23.00	377.53	371.02	352.93	327.79	301.76
24.00	371.36	365.36	348.71	325.57	301.62
25.00	367.91	362.21	346.35	324.33	301.54

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.90508	0.99899
1.00	0.00000	0.00000	0.00000	0.97825	0.99567
2.00	0.00000	0.00000	0.77097	0.97872	0.99153
3.00	0.0	0.00000	0.86835	0.97460	0.98732
4.00	0.0	0.00000	0.89897	0.97091	0.98350
5.00	0.00001	0.39463	0.91545	0.96865	0.98045
6.00	0.52172	0.80621	0.92759	0.96795	0.97838
7.00	0.81821	0.87402	0.93781	0.96852	0.97731
8.00	0.88215	0.90782	0.94678	0.97003	0.97718
9.00	0.91481	0.92919	0.95468	0.97212	0.97777
10.00	0.93543	0.94428	0.96155	0.97454	0.97891
11.00	0.94980	0.95553	0.96750	0.97710	0.98042
12.00	0.96034	0.96420	0.97259	0.97963	0.98213
13.00	0.96835	0.97099	0.97692	0.98206	0.98391
14.00	0.97454	0.97638	0.98059	0.98432	0.98569
15.00	0.97940	0.98070	0.98368	0.98639	0.98738
16.00	0.98325	0.98416	0.98629	0.98823	0.98896
17.00	0.98631	0.98696	0.98847	0.98987	0.99040
18.00	0.98876	0.98923	0.99029	0.99130	0.99168
19.00	0.99073	0.99106	0.99182	0.99254	0.99281
20.00	0.99231	0.99255	0.99308	0.99360	0.99379
21.00	0.99357	0.99375	0.99413	0.99449	0.99463
22.00	0.99459	0.99472	0.99498	0.99525	0.99534
23.00	0.99541	0.99550	0.99569	0.99587	0.99595
24.00	0.99605	0.99612	0.99625	0.99638	0.99643
25.00	0.99644	0.99650	0.99660	0.99671	0.99674

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1033.05	1029.96	1014.76	638.05	414.71
1.00	1056.73	1045.70	977.36	559.60	323.35
2.00	1058.75	1037.38	684.70	519.16	314.50
3.00	1042.55	1013.51	628.39	490.01	312.16
4.00	1013.64	978.55	594.84	467.29	310.66
5.00	974.95	807.02	566.66	448.62	309.46
6.00	759.76	641.36	541.29	432.73	308.44
7.00	633.77	595.46	518.32	418.96	307.56
8.00	590.05	563.35	497.62	406.93	306.79
9.00	559.19	537.33	479.06	396.34	306.12
10.00	534.17	515.08	462.46	387.02	305.53
11.00	512.74	495.58	447.63	378.78	305.00
12.00	493.91	478.27	434.36	371.48	304.54
13.00	477.12	462.78	422.47	364.98	304.12
14.00	462.04	448.85	411.80	359.19	303.75
15.00	448.41	436.26	402.19	354.00	303.42
16.00	436.05	424.85	393.51	349.35	303.13
17.00	424.81	414.49	385.65	345.14	302.86
18.00	414.56	405.06	378.52	341.34	302.62
19.00	405.21	396.45	372.04	337.90	302.40
20.00	396.66	388.59	366.12	334.77	302.20
21.00	388.83	381.41	360.73	331.92	302.02
22.00	381.67	374.83	355.80	329.31	301.86
23.00	375.12	368.82	351.31	326.94	301.71
24.00	369.33	363.51	347.34	324.86	301.58
25.00	366.10	360.55	345.13	323.69	301.50

ITERATION NO. 300 TIME = 5.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.91551	0.91835	0.93239	0.99112	0.99734
1.00	0.75062	0.75935	0.80428	0.96573	0.98772
2.00	0.61476	0.63227	0.71311	0.93436	0.97193
3.00	0.51165	0.54279	0.67486	0.90636	0.95320
4.00	0.44350	0.49300	0.70177	0.88823	0.93549
5.00	0.40397	0.46837	0.71821	0.87636	0.92041
6.00	0.38488	0.45937	0.72649	0.86755	0.90794
7.00	0.38534	0.46842	0.73226	0.86078	0.89778
8.00	0.42097	0.52672	0.74245	0.85639	0.88987
9.00	0.50946	0.59823	0.75805	0.85480	0.88433
10.00	0.59733	0.65850	0.77631	0.85589	0.88120
11.00	0.66558	0.70814	0.79517	0.85923	0.88038
12.00	0.71874	0.74888	0.81352	0.86432	0.88163
13.00	0.76086	0.78259	0.83085	0.87070	0.88464
14.00	0.79491	0.81080	0.84699	0.87799	0.88906
15.00	0.82296	0.83469	0.86191	0.88587	0.89456
16.00	0.84643	0.85516	0.87565	0.89407	0.90083
17.00	0.86634	0.87286	0.88830	0.90238	0.90761
18.00	0.88342	0.88830	0.89992	0.91065	0.91466
19.00	0.89820	0.90185	0.91060	0.91874	0.92179
20.00	0.91109	0.91382	0.92038	0.92654	0.92886
21.00	0.92239	0.92443	0.92934	0.93397	0.93573
22.00	0.93232	0.93385	0.93752	0.94099	0.94231
23.00	0.94106	0.94220	0.94493	0.94753	0.94852
24.00	0.94861	0.94946	0.95150	0.95345	0.95419
25.00	0.95361	0.95431	0.95599	0.95758	0.95819

BULK CONCENTRATION AT REACTOR EXIT = 0.956855

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	683.79	681.22	668.15	608.51	414.98
1.00	785.66	776.81	732.32	570.07	324.12
2.00	864.77	846.52	764.97	545.77	316.07
3.00	918.03	886.97	759.53	527.42	314.38
4.00	944.93	899.37	718.70	509.26	313.20
5.00	950.50	893.99	686.06	492.18	312.12
6.00	940.19	876.61	659.00	476.90	311.15
7.00	914.53	845.22	633.88	463.11	310.28
8.00	865.43	784.50	606.96	450.08	309.45
9.00	787.66	720.08	578.46	437.35	308.66
10.00	715.25	664.90	550.32	424.90	307.88
11.00	657.09	618.21	523.82	412.95	307.13
12.00	609.83	578.69	499.54	401.68	306.42
13.00	570.78	545.07	477.66	391.25	305.76
14.00	537.99	516.26	458.14	381.72	305.16
15.00	510.12	491.45	440.84	373.12	304.62
16.00	486.23	469.98	425.57	365.40	304.14
17.00	465.60	451.34	412.11	358.54	303.70
18.00	447.71	435.09	400.27	352.44	303.32
19.00	432.12	420.90	389.85	347.04	302.98
20.00	418.49	408.46	380.68	342.27	302.67
21.00	406.54	397.54	372.59	338.06	302.41
22.00	396.02	387.92	365.45	334.32	302.17
23.00	386.76	379.45	359.16	331.03	301.96
24.00	378.83	372.19	353.76	328.20	301.78
25.00	374.37	368.10	350.72	326.61	301.69

BULK TEMPERATURE AT REACTOR EXIT = 332.73

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.57207	0.58198	0.62503	0.98561	0.99737
1.00	0.39697	0.40217	0.44182	0.96510	0.98786
2.00	0.30107	0.31621	0.37617	0.93509	0.97239
3.00	0.23407	0.26316	0.34752	0.90844	0.95423
4.00	0.19897	0.24017	0.66952	0.89113	0.93712
5.00	0.18510	0.23393	0.71147	0.87959	0.92253
6.00	0.18409	0.23587	0.72687	0.87095	0.91042
7.00	0.19404	0.24076	0.73600	0.86438	0.90057
8.00	0.21423	0.44483	0.74804	0.86024	0.89294
9.00	0.44193	0.59447	0.76444	0.85890	0.88767
10.00	0.59728	0.66541	0.78289	0.86019	0.88478
11.00	0.67374	0.71673	0.80163	0.86366	0.88417
12.00	0.72772	0.75722	0.81975	0.86882	0.88557
13.00	0.76926	0.79028	0.83679	0.87522	0.88868
14.00	0.80253	0.81783	0.85263	0.88247	0.89314
15.00	0.82985	0.84111	0.86724	0.89026	0.89863
16.00	0.85266	0.86103	0.88067	0.89834	0.90484
17.00	0.87199	0.87823	0.89300	0.90650	0.91151
18.00	0.88855	0.89321	0.90432	0.91459	0.91842
19.00	0.90287	0.90635	0.91469	0.92247	0.92539
20.00	0.91532	0.91793	0.92418	0.93004	0.93226
21.00	0.92622	0.92816	0.93284	0.93725	0.93891
22.00	0.93578	0.93723	0.94072	0.94402	0.94527
23.00	0.94418	0.94526	0.94785	0.95031	0.95125
24.00	0.95141	0.95222	0.95416	0.95600	0.95670
25.00	0.95609	0.95675	0.95833	0.95985	0.96042

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	832.84	827.15	801.33	610.85	414.99
1.00	939.70	932.19	887.26	570.13	324.11
2.00	1001.18	983.74	902.56	544.85	316.02
3.00	1038.15	1007.67	876.47	525.59	314.30
4.00	1049.91	1007.68	726.74	507.06	313.11
5.00	1043.20	992.95	685.34	489.96	312.03
6.00	1023.41	968.07	655.78	474.71	311.06
7.00	990.95	931.12	629.31	460.93	310.18
8.00	941.75	806.95	601.73	447.89	309.36
9.00	804.29	715.36	573.17	435.17	308.56
10.00	709.03	657.36	545.34	422.80	307.79
11.00	649.21	611.05	519.31	410.97	307.04
12.00	602.75	572.48	495.54	399.87	306.34
13.00	564.78	539.80	474.18	389.63	305.70
14.00	532.98	511.83	455.14	380.29	305.11
15.00	505.97	487.75	438.28	371.87	304.57
16.00	482.79	466.89	423.40	364.33	304.09
17.00	462.76	448.77	410.29	357.63	303.67
18.00	445.37	432.97	398.75	351.67	303.29
19.00	430.20	419.15	388.59	346.41	302.95
20.00	416.92	407.03	379.64	341.74	302.66
21.00	405.25	396.37	371.74	337.62	302.39
22.00	394.97	386.97	364.76	333.97	302.16
23.00	385.91	378.67	358.59	330.74	301.96
24.00	378.14	371.56	353.30	327.96	301.78
25.00	373.80	367.59	350.34	326.41	301.68

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.88824	0.99815
1.00	0.00000	0.00000	0.00000	0.96454	0.99162
2.00	0.00000	0.00000	0.0	0.95581	0.98215
3.00	0.00000	0.0	0.00980	0.94442	0.97204
4.00	0.00000	0.00000	0.70055	0.93555	0.96268
5.00	0.00000	0.0	0.78811	0.92880	0.95458
6.00	0.0	0.00000	0.81966	0.92393	0.94788
7.00	0.00000	0.00117	0.83838	0.92105	0.94275
8.00	0.00271	0.62552	0.85405	0.92025	0.93928
9.00	0.65035	0.76545	0.86869	0.92131	0.93748
10.00	0.77670	0.81860	0.88247	0.92386	0.93724
11.00	0.82835	0.85160	0.89528	0.92750	0.93833
12.00	0.86090	0.87587	0.90704	0.93189	0.94049
13.00	0.88473	0.89503	0.91771	0.93673	0.94346
14.00	0.90335	0.91068	0.92733	0.94179	0.94701
15.00	0.91839	0.92369	0.93597	0.94691	0.95090
16.00	0.93076	0.93463	0.94371	0.95193	0.95497
17.00	0.94107	0.94391	0.95062	0.95679	0.95909
18.00	0.94975	0.95184	0.95679	0.96139	0.96312
19.00	0.95710	0.95863	0.96228	0.96570	0.96699
20.00	0.96335	0.96448	0.96716	0.96970	0.97066
21.00	0.96868	0.96952	0.97148	0.97335	0.97406
22.00	0.97324	0.97386	0.97530	0.97668	0.97719
23.00	0.97715	0.97760	0.97865	0.97966	0.98005
24.00	0.98042	0.98076	0.98153	0.98227	0.98255
25.00	0.98251	0.98278	0.98340	0.98400	0.98423

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1040.67	1038.04	1025.47	645.00	414.85
1.00	1074.53	1066.83	1019.27	567.24	323.72
2.00	1089.48	1073.69	987.59	531.47	315.19
3.00	1088.99	1065.13	947.25	505.20	313.07
4.00	1075.24	1044.69	684.10	483.96	311.67
5.00	1050.61	1016.17	630.50	466.22	310.54
6.00	1018.52	980.68	596.96	450.86	309.56
7.00	978.65	938.19	568.58	437.05	308.68
8.00	933.38	689.40	542.39	424.33	307.87
9.00	676.84	614.61	518.18	412.53	307.13
10.00	607.21	573.00	496.07	401.65	306.44
11.00	566.91	541.18	476.11	391.69	305.81
12.00	536.05	514.76	458.25	382.65	305.24
13.00	510.50	492.16	442.34	374.51	304.72
14.00	488.68	472.55	428.20	367.22	304.26
15.00	469.76	455.39	415.66	360.70	303.85
16.00	453.18	440.28	404.52	354.88	303.47
17.00	438.57	426.93	394.62	349.70	303.15
18.00	425.63	415.09	385.81	345.07	302.85
19.00	414.12	404.55	377.95	340.94	302.59
20.00	403.83	395.13	370.92	337.24	302.35
21.00	394.63	386.68	364.61	333.93	302.15
22.00	386.35	379.10	358.95	330.95	301.96
23.00	378.92	372.29	353.87	328.28	301.79
24.00	372.44	366.35	349.44	325.95	301.64
25.00	368.83	363.05	346.97	324.65	301.56

ITERATION NO. 350 TIME = 7.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.91787	0.92054	0.93389	0.99104	0.99725
1.00	0.75582	0.76391	0.80466	0.96499	0.98715
2.00	0.61831	0.63415	0.70314	0.93033	0.96954
3.00	0.50593	0.53075	0.62774	0.89243	0.94580
4.00	0.42005	0.45294	0.57426	0.85519	0.91830
5.00	0.35944	0.39990	0.54575	0.82240	0.88998
6.00	0.32256	0.37286	0.56192	0.79881	0.86417
7.00	0.30587	0.36648	0.59093	0.78424	0.84293
8.00	0.30325	0.37124	0.61123	0.77491	0.82640
9.00	0.31224	0.38588	0.62600	0.76890	0.81401
10.00	0.34143	0.42878	0.64090	0.76573	0.80521
11.00	0.40932	0.49551	0.65948	0.76552	0.79968
12.00	0.49316	0.55625	0.68023	0.76809	0.79716
13.00	0.56258	0.60776	0.70150	0.77305	0.79737
14.00	0.61832	0.65112	0.72235	0.77990	0.79994
15.00	0.66368	0.68792	0.74232	0.78820	0.80450
16.00	0.70133	0.71949	0.76122	0.79754	0.81067
17.00	0.73316	0.74690	0.77900	0.80761	0.81808
18.00	0.76048	0.77096	0.79569	0.81813	0.82643
19.00	0.78427	0.79228	0.81136	0.82889	0.83543
20.00	0.80522	0.81136	0.82608	0.83973	0.84486
21.00	0.82385	0.82857	0.83992	0.85052	0.85452
22.00	0.84057	0.84420	0.85293	0.86115	0.86425
23.00	0.85564	0.85843	0.86515	0.87150	0.87391
24.00	0.86901	0.87116	0.87636	0.88128	0.88315
25.00	0.87781	0.87963	0.88401	0.88817	0.88976

BULK CONCENTRATION AT REACTOR EXIT = 0.886272

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	682.39	679.98	667.49	608.63	414.99
1.00	783.03	774.85	733.85	570.92	324.18
2.00	864.66	848.19	776.77	549.32	316.29
3.00	926.08	900.24	799.75	537.59	315.00
4.00	966.29	931.81	806.36	529.92	314.44
5.00	986.36	943.99	795.06	522.11	313.93
6.00	988.27	937.58	757.69	511.04	313.25
7.00	975.63	917.71	716.36	497.30	312.41
8.00	952.85	890.35	681.75	483.10	311.53
9.00	921.36	855.66	651.44	469.33	310.67
10.00	876.07	803.36	622.04	455.99	309.83
11.00	808.89	740.44	592.00	442.90	309.01
12.00	737.08	683.98	562.58	430.07	308.21
13.00	676.92	635.41	534.83	417.70	307.43
14.00	627.21	593.80	509.28	405.97	306.70
15.00	585.63	558.04	486.11	395.04	306.01
16.00	550.40	527.14	465.31	384.99	305.37
17.00	520.23	500.34	446.76	375.85	304.80
18.00	494.21	477.03	430.29	367.61	304.28
19.00	471.66	456.69	415.72	360.22	303.81
20.00	452.04	438.92	402.84	353.64	303.40
21.00	434.93	423.36	391.49	347.80	303.03
22.00	419.97	409.74	381.49	342.62	302.70
23.00	406.90	397.82	372.70	338.06	302.41
24.00	395.80	387.68	365.21	334.16	302.16
25.00	389.52	381.95	360.96	331.95	302.03

BULK TEMPERATURE AT REACTOR EXIT = 339.34

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.58692	0.59664	0.63970	0.98514	0.99725
1.00	0.40995	0.41576	0.45141	0.96385	0.98714
2.00	0.30518	0.32213	0.37945	0.92989	0.96958
3.00	0.22605	0.25280	0.33933	0.89272	0.94613
4.00	0.17845	0.21040	0.31861	0.85690	0.91935
5.00	0.15292	0.18943	0.31636	0.82668	0.89240
6.00	0.14335	0.18601	0.52000	0.80617	0.86846
7.00	0.14510	0.19335	0.59303	0.79333	0.84904
8.00	0.15424	0.20619	0.62171	0.78505	0.83404
9.00	0.17012	0.22474	0.63975	0.77983	0.82288
10.00	0.19893	0.35325	0.65702	0.77743	0.81509
11.00	0.35381	0.50684	0.67684	0.77793	0.81042
12.00	0.51014	0.57834	0.69795	0.78108	0.80862
13.00	0.58694	0.63080	0.71913	0.78645	0.80939
14.00	0.64229	0.67314	0.73964	0.79356	0.81239
15.00	0.68602	0.70857	0.75914	0.80196	0.81723
16.00	0.72200	0.73882	0.77750	0.81129	0.82353
17.00	0.75233	0.76502	0.79470	0.82124	0.83097
18.00	0.77834	0.78799	0.81080	0.83155	0.83924
19.00	0.80095	0.80832	0.82587	0.84204	0.84807
20.00	0.82085	0.82649	0.83999	0.85254	0.85726
21.00	0.83853	0.84285	0.85323	0.86295	0.86661
22.00	0.85437	0.85768	0.86565	0.87315	0.87599
23.00	0.86862	0.87116	0.87727	0.88305	0.88524
24.00	0.88123	0.88319	0.88790	0.89236	0.89406
25.00	0.88945	0.89109	0.89506	0.89882	0.90026

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	826.06	820.59	795.21	611.18	414.99
1.00	933.85	926.58	887.31	571.38	324.18
2.00	1001.18	984.12	916.44	549.27	316.28
3.00	1047.72	1020.68	921.65	536.80	314.95
4.00	1070.52	1035.80	909.64	527.94	314.32
5.00	1074.30	1032.80	877.70	518.48	313.73
6.00	1063.25	1015.17	764.72	506.00	312.98
7.00	1041.52	988.41	708.85	491.90	312.12
8.00	1012.22	955.71	672.12	477.77	311.24
9.00	975.37	914.24	641.06	464.16	310.38
10.00	925.04	820.00	611.05	450.97	309.55
11.00	816.91	726.57	581.07	438.01	308.74
12.00	720.70	667.79	552.19	425.39	307.95
13.00	659.90	620.43	525.24	413.28	307.19
14.00	612.09	580.58	500.59	401.88	306.47
15.00	572.57	546.52	478.33	391.30	305.80
16.00	539.16	517.15	458.41	381.61	305.19
17.00	510.58	491.70	440.68	372.83	304.63
18.00	485.92	469.56	424.97	364.93	304.13
19.00	464.55	450.26	411.09	357.88	303.69
20.00	445.96	433.40	398.84	351.60	303.29
21.00	429.73	418.64	388.04	346.03	302.93
22.00	415.54	405.71	378.53	341.10	302.62
23.00	403.15	394.40	370.18	336.76	302.34
24.00	392.60	384.77	363.06	333.04	302.10
25.00	386.68	379.35	359.05	330.95	301.97

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.87386	0.99768
1.00	0.00000	0.00000	0.00000	0.95597	0.98915
2.00	0.00000	0.00000	0.00000	0.93885	0.97527
3.00	0.00000	0.00000	0.00000	0.91555	0.95826
4.00	0.00000	0.00000	0.0	0.89527	0.94067
5.00	0.00000	0.00000	0.00274	0.88047	0.92461
6.00	0.00000	0.00000	0.56437	0.87064	0.91117
7.00	0.00000	0.0	0.69305	0.86421	0.90056
8.00	0.0	0.00000	0.73584	0.86036	0.89258
9.00	0.00000	0.00053	0.76064	0.85883	0.88705
10.00	0.00125	0.50777	0.78058	0.85953	0.88381
11.00	0.54196	0.68179	0.79887	0.86222	0.88269
12.00	0.69503	0.74256	0.81606	0.86652	0.88345
13.00	0.75389	0.78055	0.83216	0.87204	0.88582
14.00	0.79158	0.80927	0.84714	0.87843	0.88949
15.00	0.82009	0.83268	0.86099	0.88539	0.89417
16.00	0.84316	0.85240	0.87376	0.89268	0.89959
17.00	0.86244	0.86933	0.88550	0.90011	0.90551
18.00	0.87887	0.88405	0.89630	0.90755	0.91173
19.00	0.89305	0.89695	0.90625	0.91487	0.91810
20.00	0.90541	0.90836	0.91541	0.92199	0.92448
21.00	0.91627	0.91849	0.92383	0.92885	0.93075
22.00	0.92586	0.92754	0.93158	0.93539	0.93683
23.00	0.93436	0.93563	0.93868	0.94157	0.94266
24.00	0.94176	0.94273	0.94504	0.94723	0.94807
25.00	0.94653	0.94733	0.94925	0.95108	0.95178

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1042.54	1040.20	1028.98	650.71	414.92
1.00	1080.47	1074.47	1040.10	572.31	323.96
2.00	1102.28	1089.51	1026.63	541.70	315.76
3.00	1110.98	1090.73	1001.18	521.43	314.01
4.00	1106.62	1079.86	968.21	504.70	312.91
5.00	1091.45	1060.03	931.00	489.00	311.93
6.00	1068.45	1033.56	708.83	473.97	310.99
7.00	1038.52	1001.17	640.19	459.85	310.10
8.00	1003.24	964.31	602.50	446.62	309.26
9.00	962.91	922.33	572.11	434.07	308.48
10.00	918.09	710.79	544.65	422.10	307.72
11.00	695.00	622.87	519.39	410.71	307.00
12.00	614.55	577.61	496.32	400.01	306.33
13.00	570.61	543.38	475.48	390.07	305.70
14.00	537.24	515.03	456.79	380.96	305.13
15.00	509.68	490.82	440.13	372.69	304.61
16.00	486.23	469.86	425.34	365.23	304.13
17.00	465.98	451.61	412.22	358.56	303.71
18.00	448.36	435.64	400.62	352.59	303.33
19.00	432.94	421.62	390.35	347.28	302.99
20.00	419.40	409.28	381.25	342.56	302.69
21.00	407.47	398.38	373.20	338.36	302.43
22.00	396.93	388.75	366.05	334.63	302.19
23.00	387.62	380.23	359.73	331.32	301.98
24.00	379.61	372.91	354.29	328.47	301.80
25.00	375.15	368.82	351.24	326.88	301.70

ITERATION NO. 400 TIME = 8.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.92062	0.92332	0.93665	0.99129	0.99731
1.00	0.76207	0.77042	0.81118	0.96595	0.98744
2.00	0.62551	0.64207	0.71150	0.93186	0.97003
3.00	0.51175	0.53726	0.63477	0.89372	0.94612
4.00	0.42279	0.45563	0.57523	0.85443	0.91737
5.00	0.35642	0.39462	0.52925	0.81585	0.88564
6.00	0.30883	0.35086	0.49540	0.77953	0.85275
7.00	0.27682	0.32211	0.47582	0.74734	0.82065
8.00	0.25889	0.30883	0.48222	0.72227	0.79152
9.00	0.25374	0.30999	0.50972	0.70528	0.76708
10.00	0.25819	0.31944	0.53005	0.69391	0.74766
11.00	0.27087	0.33612	0.54567	0.68637	0.73285
12.00	0.29798	0.37140	0.56062	0.68200	0.72212
13.00	0.35319	0.42946	0.57790	0.68070	0.71510
14.00	0.42537	0.48213	0.59686	0.68232	0.71145
15.00	0.48618	0.52796	0.61644	0.68648	0.71085
16.00	0.53644	0.56751	0.63596	0.69279	0.71294
17.00	0.57846	0.60190	0.65508	0.70085	0.71734
18.00	0.61426	0.63216	0.67363	0.71029	0.72367
19.00	0.64535	0.65915	0.69156	0.72080	0.73159
20.00	0.67280	0.68350	0.70888	0.73212	0.74077
21.00	0.69737	0.70570	0.72560	0.74402	0.75091
22.00	0.71964	0.72614	0.74174	0.75630	0.76178
23.00	0.73996	0.74504	0.75728	0.76877	0.77311
24.00	0.75821	0.76221	0.77186	0.78096	0.78441
25.00	0.77040	0.77383	0.78210	0.78992	0.79288

BULK CONCENTRATION AT REACTOR EXIT = 0.786340

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	680.63	678.21	665.78	608.50	414.98
1.00	779.12	770.85	730.04	570.46	324.15
2.00	860.58	843.87	772.77	548.85	316.27
3.00	923.93	898.11	798.53	537.91	315.02
4.00	967.95	934.30	812.14	532.39	314.59
5.00	994.32	954.54	816.17	528.97	314.35
6.00	1005.75	961.26	811.44	525.46	314.12
7.00	1004.59	956.20	796.39	520.16	313.79
8.00	992.38	939.76	764.86	511.45	313.26
9.00	970.82	913.85	723.75	499.50	312.54
10.00	942.37	882.55	688.28	486.20	311.71
11.00	907.91	846.19	656.71	472.70	310.87
12.00	863.75	798.07	626.63	459.36	310.04
13.00	803.60	739.59	596.67	446.18	309.21
14.00	737.58	686.79	567.57	433.28	308.40
15.00	681.14	640.42	540.09	420.82	307.62
16.00	633.38	599.99	514.66	408.99	306.88
17.00	592.64	564.70	491.43	397.92	306.18
18.00	557.56	533.80	470.41	387.69	305.54
19.00	527.12	506.68	451.51	378.33	304.95
20.00	500.57	482.84	434.59	369.83	304.41
21.00	477.32	461.84	419.51	362.18	303.93
22.00	456.92	443.35	406.09	355.32	303.50
23.00	439.03	427.10	394.22	349.21	303.11
24.00	423.79	413.22	384.03	343.93	302.78
25.00	415.05	405.25	378.18	340.90	302.59

BULK TEMPERATURE AT REACTOR EXIT = 350.44

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.60582	0.61579	0.66009	0.98512	0.99732
1.00	0.42480	0.43209	0.47333	0.96475	0.98738
2.00	0.31335	0.33365	0.40237	0.93106	0.96988
3.00	0.22842	0.25697	0.35730	0.89290	0.94585
4.00	0.17636	0.20812	0.32645	0.85358	0.91702
5.00	0.14522	0.17888	0.30611	0.81515	0.88530
6.00	0.12745	0.16282	0.29553	0.77926	0.85258
7.00	0.11918	0.15669	0.29664	0.74784	0.82088
8.00	0.11901	0.15992	0.34801	0.72368	0.79234
9.00	0.12593	0.17088	0.48704	0.70742	0.76853
10.00	0.13797	0.18621	0.52503	0.69659	0.74972
11.00	0.15450	0.20536	0.54657	0.68951	0.73546
12.00	0.17956	0.25135	0.56421	0.68558	0.72523
13.00	0.24763	0.41466	0.58281	0.68473	0.71867
14.00	0.41479	0.48415	0.60241	0.68673	0.71545
15.00	0.48994	0.53398	0.62231	0.69125	0.71524
16.00	0.54327	0.57448	0.64201	0.69785	0.71766
17.00	0.58586	0.60902	0.66123	0.70614	0.72233
18.00	0.62164	0.63921	0.67983	0.71576	0.72889
19.00	0.65255	0.66606	0.69778	0.72640	0.73697
20.00	0.67980	0.69026	0.71508	0.73781	0.74627
21.00	0.70418	0.71232	0.73175	0.74975	0.75649
22.00	0.72625	0.73260	0.74782	0.76204	0.76739
23.00	0.74638	0.75134	0.76327	0.77448	0.77871
24.00	0.76444	0.76834	0.77774	0.78661	0.78997
25.00	0.77614	0.77948	0.78754	0.79517	0.79806

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	817.24	811.70	785.92	611.18	414.99
1.00	926.04	918.22	877.28	571.05	324.16
2.00	996.74	978.45	907.89	549.28	316.28
3.00	1047.62	1020.43	919.76	538.29	315.04
4.00	1075.57	1042.25	920.29	532.64	314.60
5.00	1086.42	1048.35	912.04	528.90	314.34
6.00	1084.51	1042.55	895.22	524.88	314.09
7.00	1072.57	1027.12	867.44	518.91	313.72
8.00	1052.14	1003.07	809.89	509.62	313.17
9.00	1024.80	972.39	728.86	497.40	312.43
10.00	992.27	937.45	687.04	484.02	311.61
11.00	954.83	897.33	653.37	470.50	310.77
12.00	908.87	836.78	622.35	457.16	309.93
13.00	836.27	740.10	592.10	444.00	309.11
14.00	736.17	681.60	563.05	431.15	308.31
15.00	675.21	634.38	535.79	418.78	307.53
16.00	627.05	594.20	510.66	407.07	306.79
17.00	586.77	559.42	487.76	396.13	306.10
18.00	552.29	529.07	467.08	386.04	305.47
19.00	522.45	502.47	448.50	376.83	304.88
20.00	496.43	479.10	431.90	368.48	304.35
21.00	473.67	458.54	417.11	360.96	303.88
22.00	453.72	440.45	403.97	354.24	303.45
23.00	436.23	424.55	392.35	348.25	303.07
24.00	421.33	410.98	382.39	343.09	302.74
25.00	412.93	403.32	376.75	340.16	302.55

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.85967	0.99747
1.00	0.00000	0.00000	0.00000	0.95148	0.98803
2.00	0.00000	0.00000	0.00000	0.93027	0.97185
3.00	0.00000	0.00000	0.00000	0.89943	0.95049
4.00	0.00000	0.00000	0.00000	0.86832	0.92611
5.00	0.00000	0.00000	0.00000	0.84020	0.90091
6.00	0.00000	0.00000	0.00000	0.81686	0.87687
7.00	0.00000	0.00000	0.00005	0.79931	0.85559
8.00	0.00000	0.00000	0.24684	0.78751	0.83805
9.00	0.00000	0.00000	0.56405	0.78016	0.82443
10.00	0.00000	0.00000	0.63117	0.77609	0.81447
11.00	0.00000	0.00010	0.66404	0.77476	0.80779
12.00	0.00023	0.30484	0.68763	0.77591	0.80406
13.00	0.36049	0.57149	0.70821	0.77929	0.80296
14.00	0.58660	0.64451	0.72741	0.78455	0.80418
15.00	0.65657	0.68733	0.74558	0.79130	0.80739
16.00	0.69920	0.71947	0.76279	0.79918	0.81223
17.00	0.73149	0.74609	0.77907	0.80789	0.81838
18.00	0.75816	0.76907	0.79443	0.81717	0.82554
19.00	0.78104	0.78934	0.80893	0.82681	0.83345
20.00	0.80109	0.80746	0.82263	0.83663	0.84187
21.00	0.81890	0.82381	0.83556	0.84651	0.85062
22.00	0.83489	0.83868	0.84778	0.85631	0.85953
23.00	0.84932	0.85225	0.85929	0.86594	0.86845
24.00	0.86212	0.86440	0.86989	0.87507	0.87704
25.00	0.87036	0.87229	0.87695	0.88137	0.88305

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1042.02	1039.84	1029.22	656.13	414.95
1.00	1081.65	1076.46	1048.65	575.09	324.08
2.00	1107.66	1096.30	1045.89	547.61	316.07
3.00	1122.72	1104.69	1032.70	532.20	314.62
4.00	1125.76	1102.05	1012.08	521.45	313.89
5.00	1118.53	1090.34	986.07	511.87	313.29
6.00	1103.12	1071.37	955.12	501.67	312.66
7.00	1080.90	1046.46	920.52	490.11	311.95
8.00	1053.54	1017.31	801.65	477.39	311.17
9.00	1021.93	984.36	666.38	464.28	310.36
10.00	986.45	948.04	619.15	451.34	309.55
11.00	947.40	908.26	585.20	438.74	308.76
12.00	905.02	764.20	555.88	426.55	307.99
13.00	741.21	642.97	529.26	414.84	307.26
14.00	633.96	592.22	504.98	403.75	306.56
15.00	584.77	555.22	482.95	393.38	305.91
16.00	548.50	524.75	463.10	383.81	305.30
17.00	518.69	498.69	445.32	375.06	304.75
18.00	493.28	476.06	429.45	367.13	304.25
19.00	471.29	456.29	415.34	360.00	303.80
20.00	452.12	438.96	402.82	353.61	303.39
21.00	435.35	423.73	391.72	347.90	303.03
22.00	420.64	410.34	381.90	342.83	302.71
23.00	407.73	398.57	373.24	338.33	302.43
24.00	396.72	388.52	365.82	334.47	302.18
25.00	390.57	382.90	361.66	332.30	302.04

ITERATION NO. 450 TIME = 8.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.92323	0.92604	0.93953	0.99161	0.99742
1.00	0.76799	0.77682	0.81870	0.96726	0.98791
2.00	0.63281	0.65034	0.72197	0.93434	0.97110
3.00	0.51904	0.54568	0.64656	0.89723	0.94787
4.00	0.42943	0.46340	0.58704	0.85858	0.91970
5.00	0.36186	0.40107	0.53972	0.81998	0.88815
6.00	0.31231	0.35497	0.50213	0.78248	0.85467
7.00	0.27690	0.32168	0.47275	0.74685	0.82054
8.00	0.25259	0.29869	0.45133	0.71389	0.78694
9.00	0.23757	0.28495	0.44032	0.68486	0.75514
10.00	0.23136	0.28139	0.44919	0.66177	0.72658
11.00	0.23336	0.28714	0.46920	0.64507	0.70234
12.00	0.24174	0.29850	0.48494	0.63292	0.68256
13.00	0.25653	0.31592	0.49720	0.62409	0.66690
14.00	0.28397	0.35035	0.50925	0.61815	0.65498
15.00	0.33381	0.39657	0.52303	0.61502	0.64648
16.00	0.39113	0.43905	0.53798	0.61454	0.64116
17.00	0.44024	0.47613	0.55344	0.61645	0.63873
18.00	0.48126	0.50841	0.56902	0.62045	0.63891
19.00	0.51600	0.53682	0.58451	0.62622	0.64141
20.00	0.54606	0.56220	0.59983	0.63352	0.64592
21.00	0.57261	0.58522	0.61500	0.64210	0.65217
22.00	0.59649	0.60640	0.63000	0.65175	0.65989
23.00	0.61829	0.62611	0.64484	0.66226	0.66881
24.00	0.63793	0.64415	0.65911	0.67312	0.67841
25.00	0.65085	0.65623	0.66919	0.68137	0.68598

BULK CONCENTRATION AT REACTOR EXIT = 0.675787

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	678.92	676.44	663.91	608.30	414.97
1.00	775.25	766.69	725.22	569.68	324.11
2.00	855.84	838.56	766.19	547.48	316.19
3.00	919.41	892.98	791.57	536.20	314.92
4.00	964.41	930.27	806.11	530.78	314.50
5.00	992.60	952.56	812.58	528.09	314.30
6.00	1006.95	962.65	812.58	526.20	314.17
7.00	1010.26	962.99	806.92	523.90	314.03
8.00	1004.67	955.28	795.50	520.32	313.81
9.00	991.50	940.27	776.53	514.65	313.46
10.00	971.37	917.79	745.19	505.96	312.94
11.00	945.17	889.17	708.93	494.65	312.25
12.00	914.33	856.82	676.34	482.21	311.48
13.00	878.78	820.25	646.73	469.50	310.69
14.00	834.98	773.51	618.22	456.83	309.89
15.00	778.88	722.05	590.05	444.28	309.11
16.00	721.38	674.90	562.83	431.98	308.34
17.00	671.14	632.98	537.10	420.10	307.59
18.00	627.82	595.89	513.16	408.79	306.88
19.00	590.21	563.04	491.14	398.15	306.21
20.00	557.29	533.88	471.04	388.26	305.58
21.00	528.31	507.96	452.80	379.16	305.01
22.00	502.69	484.89	436.32	370.83	304.48
23.00	480.05	464.41	421.53	363.30	304.01
24.00	460.58	446.74	408.68	356.70	303.59
25.00	449.42	436.60	401.27	352.89	303.36

BULK TEMPERATURE AT REACTOR EXIT = 365.35

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.62113	0.63141	0.67664	0.98531	0.99742
1.00	0.43591	0.44449	0.49350	0.96608	0.98784
2.00	0.32084	0.34359	0.42392	0.93349	0.97091
3.00	0.23357	0.26357	0.37823	0.89627	0.94751
4.00	0.17986	0.21252	0.34578	0.85741	0.91915
5.00	0.14702	0.18108	0.32286	0.81863	0.88741
6.00	0.12718	0.16231	0.30739	0.78103	0.85379
7.00	0.11592	0.15221	0.29860	0.74549	0.81962
8.00	0.11096	0.14864	0.29731	0.71292	0.78617
9.00	0.11135	0.15080	0.30733	0.68469	0.75477
10.00	0.11704	0.15914	0.38331	0.66272	0.72687
11.00	0.12748	0.17272	0.45602	0.64692	0.70342
12.00	0.14153	0.18997	0.48301	0.63552	0.68444
13.00	0.16001	0.21185	0.49963	0.62741	0.66958
14.00	0.18740	0.29868	0.51406	0.62220	0.65845
15.00	0.28927	0.39254	0.52921	0.61983	0.65073
16.00	0.39034	0.44501	0.54503	0.62009	0.64618
17.00	0.44799	0.48486	0.56113	0.62270	0.64449
18.00	0.49113	0.51801	0.57721	0.62735	0.64538
19.00	0.52643	0.54675	0.59312	0.63373	0.64853
20.00	0.55664	0.57231	0.60884	0.64157	0.65364
21.00	0.58326	0.59548	0.62434	0.65064	0.66042
22.00	0.60721	0.61680	0.63965	0.66073	0.66862
23.00	0.62907	0.63663	0.65474	0.67160	0.67795
24.00	0.64876	0.65477	0.66922	0.68276	0.68788
25.00	0.66138	0.66657	0.67909	0.69087	0.69533

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	810.00	804.31	778.11	611.05	414.98
1.00	919.85	911.39	866.90	570.29	324.12
2.00	991.92	972.43	896.57	548.00	316.21
3.00	1044.09	1016.24	909.24	536.80	314.95
4.00	1073.57	1040.01	911.99	531.46	314.53
5.00	1086.65	1048.81	907.62	528.75	314.34
6.00	1087.95	1046.82	897.47	526.72	314.20
7.00	1080.49	1036.72	881.88	524.11	314.04
8.00	1066.07	1020.04	859.99	520.03	313.79
9.00	1045.65	997.48	828.53	513.65	313.40
10.00	1019.73	969.21	766.09	504.25	312.84
11.00	989.19	936.51	710.44	492.54	312.13
12.00	954.97	900.39	673.74	479.88	311.35
13.00	916.34	858.86	642.50	467.05	310.55
14.00	869.38	787.00	613.12	454.29	309.75
15.00	788.84	718.00	584.61	441.69	308.96
16.00	715.65	667.65	557.35	429.38	308.19
17.00	663.01	625.31	531.77	417.53	307.45
18.00	619.67	588.54	508.07	406.30	306.74
19.00	582.58	556.19	486.34	395.77	306.08
20.00	550.29	527.58	466.56	386.02	305.46
21.00	521.93	502.20	448.66	377.06	304.90
22.00	496.90	479.64	432.52	368.90	304.38
23.00	474.81	459.64	418.06	361.52	303.91
24.00	455.84	442.42	405.51	355.07	303.50
25.00	445.12	432.68	398.39	351.40	303.27

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.84913	0.99745
1.00	0.00000	0.00000	0.00000	0.95039	0.98788
2.00	0.00000	0.00000	0.00000	0.92832	0.97118
3.00	0.00000	0.00000	0.00000	0.89517	0.94854
4.00	0.00000	0.00000	0.00000	0.86011	0.92177
5.00	0.00000	0.00000	0.00000	0.82618	0.89277
6.00	0.00000	0.00000	0.00000	0.79500	0.86327
7.00	0.00000	0.00000	0.00000	0.76773	0.83483
8.00	0.00000	0.00000	0.0	0.74528	0.80878
9.00	0.00000	0.00000	0.00058	0.72831	0.78620
10.00	0.00000	0.00000	0.29384	0.71661	0.76771
11.00	0.00000	0.00000	0.50903	0.70903	0.75333
12.00	0.00000	0.0	0.56769	0.70465	0.74273
13.00	0.0	0.00202	0.59795	0.70300	0.73554
14.00	0.00354	0.35056	0.61999	0.70385	0.73142
15.00	0.37815	0.51971	0.63925	0.70694	0.73006
16.00	0.53166	0.58143	0.65727	0.71196	0.73114
17.00	0.59200	0.62003	0.67452	0.71856	0.73432
18.00	0.63094	0.64993	0.69112	0.72645	0.73929
19.00	0.66136	0.67530	0.70711	0.73536	0.74574
20.00	0.68713	0.69773	0.72254	0.74504	0.75339
21.00	0.70981	0.71800	0.73743	0.75531	0.76199
22.00	0.73019	0.73657	0.75182	0.76599	0.77131
23.00	0.74873	0.75371	0.76569	0.77691	0.78114
24.00	0.76533	0.76926	0.77873	0.78764	0.79101
25.00	0.77594	0.77932	0.78747	0.79515	0.79807

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1040.55	1038.40	1027.88	660.03	414.96
1.00	1080.60	1075.60	1049.71	575.81	324.10
2.00	1108.37	1097.31	1050.54	549.29	316.15
3.00	1126.34	1109.06	1042.39	535.78	314.82
4.00	1133.09	1110.63	1028.09	527.84	314.26
5.00	1130.30	1103.72	1009.33	521.87	313.88
6.00	1119.81	1090.00	986.49	515.87	313.51
7.00	1102.97	1070.68	959.82	508.72	313.07
8.00	1081.07	1046.92	929.29	499.81	312.53
9.00	1054.93	1019.29	895.23	489.03	311.87
10.00	1025.23	988.63	761.83	476.86	311.13
11.00	992.57	955.40	661.40	464.14	310.34
12.00	957.07	919.46	616.99	451.43	309.55
13.00	918.67	879.89	583.90	438.96	308.77
14.00	876.35	723.76	555.14	426.85	308.01
15.00	710.74	636.65	529.02	415.22	307.28
16.00	629.05	590.17	505.16	404.18	306.58
17.00	583.47	554.77	483.44	393.85	305.94
18.00	548.53	525.09	463.77	384.28	305.33
19.00	519.31	499.40	446.05	375.51	304.78
20.00	494.10	476.88	430.16	367.53	304.27
21.00	472.08	457.04	415.94	360.32	303.82
22.00	452.74	439.53	403.25	353.83	303.41
23.00	435.76	424.10	391.99	348.04	303.04
24.00	421.24	410.88	382.30	343.03	302.72
25.00	413.10	403.46	376.84	340.19	302.54

ITERATION NO. 500 TIME = 10.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.92555	0.92849	0.94218	0.99193	0.99752
1.00	0.77315	0.78250	0.82581	0.96856	0.98839
2.00	0.63945	0.65792	0.73190	0.93683	0.97222
3.00	0.52618	0.55396	0.65810	0.90091	0.94980
4.00	0.43667	0.47188	0.59939	0.86334	0.92253
5.00	0.36889	0.40942	0.55239	0.82563	0.89185
6.00	0.31890	0.36290	0.51467	0.78873	0.85908
7.00	0.28274	0.32880	0.48443	0.75324	0.82534
8.00	0.25717	0.30430	0.46045	0.71962	0.79156
9.00	0.23981	0.28741	0.44214	0.68827	0.75852
10.00	0.22917	0.27699	0.43014	0.65980	0.72702
11.00	0.22467	0.27321	0.42857	0.63533	0.69795
12.00	0.22633	0.27687	0.44167	0.61608	0.67225
13.00	0.23337	0.28593	0.45479	0.60124	0.65034
14.00	0.24492	0.29889	0.46465	0.58958	0.63208
15.00	0.26290	0.31918	0.47288	0.58049	0.61716
16.00	0.29402	0.35403	0.48185	0.57379	0.60531
17.00	0.34038	0.39015	0.49199	0.56943	0.59632
18.00	0.38436	0.42238	0.50280	0.56726	0.58998
19.00	0.42144	0.45036	0.51390	0.56707	0.58609
20.00	0.45249	0.47473	0.52507	0.56863	0.58443
21.00	0.47893	0.49622	0.53624	0.57176	0.58480
22.00	0.50193	0.51551	0.54741	0.57627	0.58696
23.00	0.52236	0.53310	0.55859	0.58198	0.59070
24.00	0.54037	0.54896	0.56948	0.58850	0.59564
25.00	0.55166	0.55913	0.57704	0.59374	0.60003

BULK CONCENTRATION AT REACTOR EXIT = 0.586054

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	677.41	674.85	662.20	608.10	414.96
1.00	771.87	762.97	720.61	568.89	324.06
2.00	851.44	833.57	759.74	546.01	316.10
3.00	914.62	887.51	784.12	534.14	314.80
4.00	959.60	924.74	798.34	528.32	314.35
5.00	988.16	947.40	805.05	525.48	314.14
6.00	1003.30	958.36	805.94	523.77	314.02
7.00	1007.98	960.22	802.09	522.07	313.92
8.00	1004.55	954.96	794.11	519.73	313.77
9.00	994.70	943.93	782.19	516.28	313.56
10.00	979.46	927.86	765.68	511.29	313.26
11.00	959.29	906.69	741.98	504.20	312.83
12.00	934.42	880.35	710.09	494.68	312.25
13.00	905.61	850.43	679.20	483.63	311.57
14.00	873.45	817.83	651.03	472.02	310.84
15.00	836.72	780.29	624.55	460.31	310.11
16.00	791.86	734.96	598.55	448.65	309.38
17.00	739.60	690.52	573.07	437.12	308.66
18.00	690.84	650.01	548.59	425.85	307.95
19.00	647.99	613.65	525.48	414.98	307.27
20.00	610.44	581.09	503.91	404.62	306.61
21.00	577.31	551.90	483.97	394.86	306.00
22.00	547.89	525.68	465.65	385.75	305.42
23.00	521.72	502.17	448.94	377.34	304.89
24.00	499.05	481.71	434.23	369.87	304.42
25.00	486.16	470.04	425.79	365.56	304.15

BULK TEMPERATURE AT REACTOR EXIT = 381.17

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.63514	0.64568	0.69127	0.98554	0.99751
1.00	0.44527	0.45509	0.51262	0.96742	0.98832
2.00	0.32779	0.35265	0.44388	0.93603	0.97203
3.00	0.23925	0.27076	0.39819	0.90000	0.94945
4.00	0.18467	0.21872	0.36534	0.86219	0.92197
5.00	0.15104	0.18636	0.34194	0.82423	0.89105
6.00	0.13039	0.16658	0.32570	0.78707	0.85804
7.00	0.11815	0.15522	0.31521	0.75137	0.82407
8.00	0.11179	0.14993	0.30975	0.71763	0.79011
9.00	0.10995	0.14936	0.30948	0.68633	0.75700
10.00	0.11209	0.15285	0.31651	0.65822	0.72560
11.00	0.11817	0.16066	0.34012	0.63449	0.69688
12.00	0.12820	0.17324	0.41933	0.61608	0.67173
13.00	0.14156	0.18951	0.44885	0.60196	0.65047
14.00	0.15813	0.20968	0.46408	0.59096	0.63291
15.00	0.18089	0.24023	0.47500	0.58256	0.61872
16.00	0.21772	0.33811	0.48567	0.57661	0.60764
17.00	0.32764	0.39148	0.49694	0.57305	0.59945
18.00	0.38788	0.42853	0.50860	0.57168	0.59394
19.00	0.42910	0.45817	0.52042	0.57229	0.59089
20.00	0.46144	0.48326	0.53225	0.57466	0.59007
21.00	0.48843	0.50524	0.54406	0.57857	0.59126
22.00	0.51182	0.52497	0.55585	0.58385	0.59423
23.00	0.53261	0.54299	0.56764	0.59029	0.59876
24.00	0.55099	0.55928	0.57910	0.59750	0.60442
25.00	0.56238	0.56959	0.58688	0.60302	0.60910

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	803.39	797.56	771.17	610.88	414.96
1.00	914.56	905.44	856.94	569.47	324.08
2.00	987.31	966.72	885.57	546.51	316.12
3.00	1039.88	1011.20	898.00	534.74	314.83
4.00	1069.80	1035.50	901.12	529.06	314.39
5.00	1083.59	1045.15	897.63	526.33	314.19
6.00	1086.01	1044.49	889.13	524.67	314.07
7.00	1080.25	1036.38	876.46	522.96	313.97
8.00	1068.33	1022.57	859.95	520.48	313.81
9.00	1051.45	1004.10	839.27	516.74	313.59
10.00	1030.24	981.47	812.75	511.27	313.26
11.00	1004.94	954.66	774.37	503.53	312.79
12.00	975.83	923.83	716.01	493.45	312.18
13.00	943.56	889.98	678.78	482.06	311.48
14.00	908.18	852.74	648.45	470.22	310.74
15.00	867.62	806.59	620.81	458.32	310.00
16.00	815.91	735.98	594.11	446.50	309.26
17.00	738.62	685.11	568.28	434.85	308.53
18.00	684.13	643.12	543.69	423.51	307.82
19.00	640.27	606.58	520.59	412.61	307.13
20.00	602.80	574.23	499.14	402.27	306.48
21.00	570.04	545.37	479.36	392.56	305.87
22.00	541.07	519.53	461.25	383.53	305.30
23.00	515.34	496.40	444.77	375.22	304.78
24.00	493.09	476.30	430.29	367.85	304.31
25.00	480.56	464.94	422.06	363.64	304.04

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.84048	0.99750
1.00	0.00000	0.00000	0.00000	0.95075	0.98809
2.00	0.00000	0.00000	0.00000	0.92894	0.97152
3.00	0.00000	0.00000	0.00000	0.89542	0.94879
4.00	0.00000	0.00000	0.00000	0.85919	0.92148
5.00	0.00000	0.00000	0.00000	0.82312	0.89126
6.00	0.00000	0.00000	0.00000	0.78864	0.85964
7.00	0.00000	0.00000	0.00000	0.75669	0.82797
8.00	0.00000	0.00000	0.00000	0.72801	0.79739
9.00	0.00000	0.00000	0.00000	0.70329	0.76893
10.00	0.00000	0.00000	0.00004	0.68318	0.74350
11.00	0.00000	0.00000	0.03369	0.66798	0.72177
12.00	0.00000	0.00000	0.39128	0.65710	0.70398
13.00	0.00000	0.00000	0.48934	0.64956	0.68997
14.00	0.00000	0.00003	0.52782	0.64477	0.67941
15.00	0.00002	0.06468	0.55071	0.64247	0.67198
16.00	0.08071	0.39630	0.56855	0.64246	0.66741
17.00	0.40670	0.49011	0.58454	0.64452	0.66541
18.00	0.49771	0.53572	0.59970	0.64838	0.66572
19.00	0.54367	0.56704	0.61437	0.65379	0.66806
20.00	0.57581	0.59227	0.62867	0.66049	0.67217
21.00	0.60184	0.61419	0.64267	0.66829	0.67778
22.00	0.62442	0.63396	0.65643	0.67699	0.68467
23.00	0.64466	0.65213	0.66993	0.68641	0.69260
24.00	0.66270	0.66862	0.68283	0.69610	0.70110
25.00	0.67403	0.67915	0.69147	0.70303	0.70741

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1038.76	1036.58	1026.00	663.17	414.96
1.00	1078.90	1073.85	1048.21	575.65	324.09
2.00	1107.42	1096.25	1050.11	549.21	316.14
3.00	1126.76	1109.61	1044.02	536.26	314.84
4.00	1135.35	1113.30	1032.72	529.47	314.35
5.00	1134.95	1109.01	1017.74	525.24	314.07
6.00	1127.36	1098.45	999.60	521.57	313.84
7.00	1114.02	1082.88	978.53	517.28	313.58
8.00	1096.09	1063.27	954.45	511.68	313.24
9.00	1074.30	1040.15	927.11	504.36	312.80
10.00	1049.17	1014.03	896.32	495.14	312.25
11.00	1021.21	985.35	851.65	484.21	311.58
12.00	990.80	954.50	699.73	472.25	310.84
13.00	958.11	921.49	640.82	459.97	310.08
14.00	922.96	885.90	604.17	447.76	309.32
15.00	885.13	825.94	574.26	435.78	308.57
16.00	817.91	679.99	547.53	424.15	307.84
17.00	673.49	620.42	523.05	412.98	307.14
18.00	614.89	580.59	500.58	402.39	306.47
19.00	575.25	548.42	480.02	392.47	305.84
20.00	543.24	520.78	461.30	383.26	305.26
21.00	515.84	496.49	444.33	374.78	304.73
22.00	491.86	474.98	429.00	367.04	304.24
23.00	470.74	455.90	415.24	360.02	303.80
24.00	452.61	439.45	403.28	353.89	303.41
25.00	442.44	430.21	396.53	350.41	303.19

ITERATION NO. 550 TIME = 11.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.92763	0.93068	0.94456	0.99222	0.99761
1.00	0.77758	0.78747	0.83237	0.96975	0.98883
2.00	0.64523	0.66460	0.74090	0.93910	0.97325
3.00	0.53264	0.56147	0.66860	0.90429	0.95160
4.00	0.44346	0.47986	0.61084	0.86779	0.92521
5.00	0.37583	0.41767	0.56452	0.83109	0.89547
6.00	0.32588	0.37129	0.52735	0.79512	0.86365
7.00	0.28968	0.33722	0.49753	0.76047	0.83081
8.00	0.26396	0.31262	0.47372	0.72749	0.79779
9.00	0.24625	0.29535	0.45492	0.69645	0.76528
10.00	0.23479	0.28390	0.44052	0.66756	0.73382
11.00	0.22846	0.27736	0.43065	0.64115	0.70392
12.00	0.22681	0.27573	0.42765	0.61790	0.67616
13.00	0.22992	0.27977	0.43600	0.59873	0.65119
14.00	0.23740	0.28836	0.44581	0.58327	0.62936
15.00	0.24855	0.30001	0.45298	0.57055	0.61062
16.00	0.26402	0.31592	0.45847	0.55998	0.59469
17.00	0.28787	0.34223	0.46408	0.55138	0.58135
18.00	0.32398	0.37225	0.47056	0.54470	0.57042
19.00	0.36180	0.39925	0.47762	0.53984	0.56172
20.00	0.39385	0.42255	0.48492	0.53665	0.55512
21.00	0.42036	0.44253	0.49226	0.53498	0.55044
22.00	0.44248	0.45979	0.49957	0.53467	0.54752
23.00	0.46125	0.47490	0.50682	0.53557	0.54619
24.00	0.47710	0.48802	0.51385	0.53746	0.54625
25.00	0.48654	0.49605	0.51869	0.53955	0.54736

BULK CONCENTRATION AT REACTOR EXIT = 0.529901

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	676.06	673.43	660.66	607.92	414.95
1.00	768.97	759.72	716.37	568.16	324.02
2.00	847.59	829.16	753.89	544.66	316.02
3.00	910.26	882.48	777.27	532.20	314.68
4.00	954.93	919.34	790.88	525.89	314.20
5.00	983.35	941.82	797.26	522.69	313.97
6.00	998.53	952.80	798.04	520.74	313.84
7.00	1003.45	954.91	794.35	518.98	313.72
8.00	1000.57	950.25	786.98	516.80	313.59
9.00	991.71	940.32	776.47	513.84	313.41
10.00	978.14	926.16	763.07	509.87	313.17
11.00	960.61	908.33	746.51	504.69	312.85
12.00	939.45	886.82	725.20	497.94	312.44
13.00	914.74	861.36	697.19	489.28	311.91
14.00	886.88	832.92	669.13	479.29	311.29
15.00	856.38	802.44	643.29	468.73	310.64
16.00	822.76	769.04	619.06	458.05	309.97
17.00	783.72	729.56	595.44	447.40	309.30
18.00	737.96	689.07	572.18	436.85	308.64
19.00	692.81	651.59	549.66	426.47	307.99
20.00	652.53	617.57	528.20	416.39	307.35
21.00	616.92	586.83	507.99	406.71	306.74
22.00	585.28	559.06	489.12	397.50	306.16
23.00	557.07	533.98	471.68	388.85	305.62
24.00	532.55	512.01	456.14	381.06	305.12
25.00	518.63	499.49	447.19	376.54	304.84

BULK TEMPERATURE AT REACTOR EXIT = 394.99

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.64959	0.66030	0.70552	0.98581	0.99762
1.00	0.45402	0.46512	0.53282	0.96880	0.98882
2.00	0.33464	0.36157	0.46416	0.93862	0.97319
3.00	0.24517	0.27836	0.41857	0.90385	0.95148
4.00	0.18997	0.22574	0.38578	0.86728	0.92500
5.00	0.15589	0.19295	0.36262	0.83046	0.89515
6.00	0.13490	0.17281	0.34678	0.79434	0.86320
7.00	0.12236	0.16110	0.33665	0.75952	0.83021
8.00	0.11562	0.15535	0.33111	0.72638	0.79703
9.00	0.11318	0.15412	0.32947	0.69518	0.76435
10.00	0.11424	0.15653	0.33143	0.66617	0.73275
11.00	0.11850	0.16211	0.33760	0.63973	0.70274
12.00	0.12596	0.17105	0.35250	0.61656	0.67494
13.00	0.13676	0.18406	0.40696	0.59752	0.65000
14.00	0.15067	0.20064	0.43550	0.58218	0.62825
15.00	0.16749	0.22020	0.44823	0.56957	0.60960
16.00	0.18846	0.24474	0.45608	0.55914	0.59380
17.00	0.21771	0.30856	0.46289	0.55070	0.58062
18.00	0.28942	0.36294	0.47003	0.54421	0.56986
19.00	0.35304	0.39656	0.47750	0.53956	0.56137
20.00	0.39170	0.42210	0.48510	0.53660	0.55499
21.00	0.42033	0.44294	0.49269	0.53517	0.55055
22.00	0.44325	0.46063	0.50024	0.53511	0.54789
23.00	0.46241	0.47602	0.50773	0.53628	0.54683
24.00	0.47851	0.48936	0.51499	0.53842	0.54716
25.00	0.48787	0.49732	0.51979	0.54050	0.54825

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	796.68	790.75	764.46	610.71	414.95
1.00	909.63	899.83	846.57	568.62	324.03
2.00	982.79	961.10	874.46	544.96	316.03
3.00	1035.47	1005.83	886.41	532.52	314.70
4.00	1065.46	1030.18	889.30	526.28	314.22
5.00	1079.38	1039.97	885.71	523.16	314.00
6.00	1082.05	1039.62	877.30	521.29	313.87
7.00	1076.76	1032.07	865.10	519.60	313.76
8.00	1065.67	1019.24	849.79	517.46	313.63
9.00	1050.19	1002.34	831.72	514.51	313.45
10.00	1031.12	982.08	810.90	510.49	313.21
11.00	1008.89	958.82	786.65	505.18	312.88
12.00	983.61	932.51	755.78	498.20	312.46
13.00	955.35	902.92	707.92	489.33	311.92
14.00	924.42	870.68	672.46	479.18	311.29
15.00	891.02	836.13	644.28	468.50	310.63
16.00	854.24	797.27	618.96	457.72	309.96
17.00	811.10	740.78	594.71	446.97	309.28
18.00	749.03	690.75	571.11	436.32	308.62
19.00	693.94	650.67	548.38	425.87	307.96
20.00	651.17	615.81	526.81	415.73	307.32
21.00	614.83	584.81	506.53	406.01	306.71
22.00	583.00	556.97	487.64	396.78	306.13
23.00	554.78	531.90	470.20	388.12	305.58
24.00	530.30	509.98	454.67	380.32	305.09
25.00	516.60	497.64	445.86	375.86	304.81

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.83277	0.99759
1.00	0.00000	0.00000	0.00000	0.95195	0.98847
2.00	0.00000	0.00000	0.00000	0.93090	0.97236
3.00	0.00000	0.00000	0.00000	0.89792	0.95011
4.00	0.00000	0.00000	0.00000	0.86183	0.92314
5.00	0.00000	0.00000	0.00000	0.82540	0.89298
6.00	0.00000	0.00000	0.00000	0.78993	0.86099
7.00	0.00000	0.00000	0.00000	0.75624	0.82835
8.00	0.00000	0.00000	0.00000	0.72486	0.79603
9.00	0.00000	0.00000	0.00000	0.69624	0.76487
10.00	0.00000	0.00000	0.00001	0.67085	0.73561
11.00	0.00000	0.00000	0.00010	0.64917	0.70891
12.00	0.00000	0.00000	0.00638	0.63166	0.68536
13.00	0.00000	0.00000	0.28707	0.61813	0.66527
14.00	0.00000	0.00000	0.42873	0.60778	0.64862
15.00	0.00000	0.00003	0.47468	0.59997	0.63515
16.00	0.00001	0.00517	0.49778	0.59442	0.62459
17.00	0.00459	0.25719	0.51345	0.59099	0.61669
18.00	0.25826	0.40812	0.52641	0.58951	0.61124
19.00	0.41038	0.46409	0.53827	0.58981	0.60802
20.00	0.46751	0.49662	0.54961	0.59167	0.60683
21.00	0.50124	0.52045	0.56066	0.59493	0.60744
22.00	0.52615	0.54015	0.57155	0.59938	0.60966
23.00	0.54673	0.55743	0.58230	0.60486	0.61327
24.00	0.56429	0.57272	0.59266	0.61103	0.61791
25.00	0.57484	0.58214	0.59954	0.61568	0.62175

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1036.71	1034.47	1023.80	665.92	414.95
1.00	1076.90	1071.69	1045.46	574.99	324.05
2.00	1105.68	1094.21	1047.40	548.20	316.09
3.00	1125.59	1108.28	1042.00	535.16	314.77
4.00	1135.04	1112.94	1032.03	528.61	314.30
5.00	1135.82	1109.97	1018.88	525.02	314.06
6.00	1129.80	1101.14	1003.18	522.43	313.89
7.00	1118.52	1087.79	985.29	519.66	313.72
8.00	1103.13	1070.90	965.28	516.06	313.51
9.00	1084.41	1051.06	943.04	511.21	313.22
10.00	1062.87	1028.70	918.31	504.85	312.84
11.00	1038.86	1004.06	890.60	496.83	312.35
12.00	1012.65	977.35	857.73	487.16	311.76
13.00	984.48	948.84	731.22	476.27	311.09
14.00	954.47	918.60	657.05	464.85	310.38
15.00	922.47	886.28	617.84	453.34	309.66
16.00	888.06	849.61	587.77	441.96	308.95
17.00	849.59	728.86	561.43	430.80	308.25
18.00	726.95	648.30	537.32	419.98	307.57
19.00	645.46	603.62	515.04	409.60	306.92
20.00	600.30	569.60	494.45	399.74	306.30
21.00	566.01	540.87	475.50	390.48	305.72
22.00	537.19	515.67	458.14	381.85	305.17
23.00	512.09	493.29	442.33	373.90	304.67
24.00	490.53	473.89	428.42	366.84	304.22
25.00	478.49	463.01	420.56	362.82	303.97

ITERATION NO. 600 TIME = 11.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.92939	0.93255	0.94658	0.99247	0.99769
1.00	0.78132	0.79174	0.83821	0.97080	0.98922
2.00	0.65018	0.67037	0.74884	0.94110	0.97415
3.00	0.53824	0.56803	0.67781	0.90726	0.95318
4.00	0.44944	0.48693	0.62092	0.87171	0.92757
5.00	0.38207	0.42509	0.57531	0.83594	0.89869
6.00	0.33232	0.37902	0.53883	0.80088	0.86776
7.00	0.29632	0.34528	0.50975	0.76712	0.83583
8.00	0.27083	0.32102	0.48669	0.73504	0.80373
9.00	0.25335	0.30408	0.46857	0.70484	0.77211
10.00	0.24206	0.29288	0.45457	0.67666	0.74145
11.00	0.23571	0.28629	0.44409	0.65060	0.71213
12.00	0.23349	0.28364	0.43714	0.62685	0.68448
13.00	0.23513	0.28502	0.43574	0.60587	0.65889
14.00	0.24071	0.29100	0.44256	0.58827	0.63580
15.00	0.24992	0.30052	0.44949	0.57359	0.61538
16.00	0.26220	0.31243	0.45427	0.56109	0.59753
17.00	0.27796	0.32751	0.45774	0.55033	0.58201
18.00	0.29996	0.35005	0.46126	0.54116	0.56861
19.00	0.33078	0.37519	0.46542	0.53354	0.55719
20.00	0.36285	0.39759	0.46995	0.52738	0.54760
21.00	0.38986	0.41663	0.47456	0.52257	0.53971
22.00	0.41184	0.43262	0.47910	0.51897	0.53339
23.00	0.42976	0.44608	0.48349	0.51645	0.52850
24.00	0.44421	0.45722	0.48760	0.51491	0.52499
25.00	0.45218	0.46353	0.49024	0.51453	0.52354

BULK CONCENTRATION AT REACTOR EXIT = 0.503219

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	674.93	672.22	659.36	607.75	414.94
1.00	766.53	756.96	712.63	567.51	323.99
2.00	844.33	825.38	748.78	543.47	315.95
3.00	906.50	878.13	771.32	530.50	314.58
4.00	950.84	914.59	784.35	523.75	314.07
5.00	979.01	936.77	790.28	520.16	313.81
6.00	993.99	947.52	790.68	517.90	313.66
7.00	998.78	949.45	786.66	515.89	313.53
8.00	995.83	944.70	779.08	513.53	313.39
9.00	987.05	934.84	768.57	510.51	313.20
10.00	973.78	921.01	755.60	506.67	312.97
11.00	956.95	903.99	740.46	501.93	312.68
12.00	937.13	884.19	723.03	496.19	312.33
13.00	914.50	861.56	701.93	489.21	311.90
14.00	889.10	835.89	676.14	480.78	311.38
15.00	861.25	808.00	650.94	471.40	310.80
16.00	831.32	778.63	627.60	461.67	310.20
17.00	798.99	747.16	605.59	451.88	309.58
18.00	762.65	711.34	584.13	442.16	308.97
19.00	721.40	674.83	563.03	432.54	308.37
20.00	680.58	640.88	542.57	423.09	307.78
21.00	643.89	609.93	523.02	413.89	307.20
22.00	611.28	581.82	504.53	405.03	306.64
23.00	582.24	556.34	487.25	396.59	306.11
24.00	557.01	533.95	471.71	388.90	305.62
25.00	542.85	521.31	462.83	384.47	305.35

BULK TEMPERATURE AT REACTOR EXIT = 405.09

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.66009	0.67080	0.71522	0.98604	0.99770
1.00	0.46008	0.47217	0.54838	0.96986	0.98920
2.00	0.33980	0.36824	0.47932	0.94061	0.97408
3.00	0.24983	0.28437	0.43379	0.90680	0.95304
4.00	0.19427	0.23147	0.40122	0.87118	0.92734
5.00	0.15998	0.19854	0.37853	0.83530	0.89835
6.00	0.13891	0.17841	0.36340	0.80011	0.86730
7.00	0.12640	0.16681	0.35416	0.76621	0.83523
8.00	0.11976	0.16124	0.34959	0.73395	0.80297
9.00	0.11743	0.16020	0.34877	0.70357	0.77117
10.00	0.11854	0.16278	0.35101	0.67521	0.74033
11.00	0.12265	0.16839	0.35581	0.64899	0.71083
12.00	0.12960	0.17674	0.36359	0.62514	0.68303
13.00	0.13946	0.18820	0.38017	0.60418	0.65736
14.00	0.15239	0.20348	0.42387	0.58667	0.63424
15.00	0.16832	0.22201	0.44173	0.57206	0.61385
16.00	0.18725	0.24314	0.45013	0.55964	0.59605
17.00	0.21021	0.26902	0.45526	0.54897	0.58061
18.00	0.24090	0.32381	0.45970	0.53993	0.56733
19.00	0.30233	0.36732	0.46441	0.53248	0.55605
20.00	0.35515	0.39496	0.46930	0.52652	0.54664
21.00	0.38766	0.41585	0.47420	0.52192	0.53897
22.00	0.41148	0.43262	0.47899	0.51856	0.53289
23.00	0.43013	0.44647	0.48362	0.51630	0.52827
24.00	0.44494	0.45788	0.48798	0.51503	0.52503
25.00	0.45298	0.46424	0.49070	0.51475	0.52369

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	791.76	785.81	759.84	610.56	414.94
1.00	906.17	895.84	838.59	567.97	323.99
2.00	979.43	956.92	866.16	543.77	315.96
3.00	1032.10	1001.69	877.76	530.82	314.60
4.00	1062.05	1025.96	880.32	524.12	314.09
5.00	1075.90	1035.65	876.38	520.61	313.84
6.00	1078.49	1035.19	867.58	518.42	313.69
7.00	1073.14	1027.57	855.01	516.49	313.57
8.00	1062.06	1014.76	839.46	514.20	313.43
9.00	1046.75	998.03	821.46	511.24	313.25
10.00	1028.12	978.22	801.40	507.44	313.02
11.00	1006.74	955.87	779.45	502.69	312.73
12.00	982.86	931.18	755.09	496.86	312.37
13.00	956.53	903.99	724.72	489.69	311.93
14.00	927.76	874.07	683.33	481.07	311.40
15.00	896.75	842.01	653.62	471.55	310.81
16.00	863.57	808.12	628.66	461.68	310.20
17.00	827.46	770.66	605.78	451.78	309.58
18.00	785.99	720.22	583.77	441.94	308.96
19.00	730.64	676.28	562.30	432.20	308.35
20.00	681.58	640.16	541.59	422.65	307.75
21.00	642.71	608.42	521.86	413.36	307.17
22.00	609.39	579.99	503.25	404.42	306.61
23.00	580.09	554.39	485.88	395.93	306.07
24.00	554.78	531.94	470.29	388.20	305.59
25.00	540.71	519.37	461.45	383.78	305.31

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.82747	0.99767
1.00	0.00000	0.00000	0.00000	0.95326	0.98885
2.00	0.00000	0.00000	0.00000	0.93297	0.97321
3.00	0.00000	0.00000	0.00000	0.90073	0.95154
4.00	0.00000	0.00000	0.00000	0.86525	0.92517
5.00	0.00000	0.00000	0.00000	0.82923	0.89554
6.00	0.00000	0.00000	0.00000	0.79395	0.86395
7.00	0.00000	0.00000	0.00000	0.76014	0.83151
8.00	0.00000	0.00000	0.00000	0.72827	0.79911
9.00	0.00000	0.00000	0.00000	0.69866	0.76746
10.00	0.00000	0.00000	0.00001	0.67159	0.73718
11.00	0.00000	0.00000	0.00004	0.64736	0.70879
12.00	0.00000	0.00000	0.00047	0.62637	0.68278
13.00	0.00000	0.00000	0.01831	0.60897	0.65959
14.00	0.00000	0.00000	0.30918	0.59499	0.63946
15.00	0.00000	0.00001	0.41814	0.58370	0.62234
16.00	0.00000	0.00014	0.45610	0.57459	0.60799
17.00	0.00007	0.00673	0.47511	0.56742	0.59618
18.00	0.00460	0.23199	0.48757	0.56208	0.58670
19.00	0.21852	0.37834	0.49750	0.55845	0.57938
20.00	0.37491	0.43207	0.50635	0.55639	0.57403
21.00	0.43158	0.46189	0.51466	0.55573	0.57050
22.00	0.46306	0.48271	0.52268	0.55633	0.56860
23.00	0.48507	0.49924	0.53051	0.55803	0.56817
24.00	0.50212	0.51298	0.53799	0.56058	0.56898
25.00	0.51165	0.52100	0.54285	0.56282	0.57028

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	1034.98	1032.71	1021.99	667.79	414.94
1.00	1075.29	1069.92	1042.84	574.28	324.02
2.00	1104.07	1092.29	1044.51	547.06	316.02
3.00	1124.11	1106.54	1039.15	533.67	314.69
4.00	1133.79	1111.48	1029.52	526.95	314.20
5.00	1134.95	1108.94	1016.94	523.38	313.96
6.00	1129.49	1100.72	1002.09	521.01	313.80
7.00	1118.98	1088.23	985.37	518.71	313.66
8.00	1104.66	1072.48	967.00	515.83	313.49
9.00	1087.33	1054.16	947.02	512.00	313.26
10.00	1067.58	1033.69	925.36	507.01	312.97
11.00	1045.76	1011.38	901.71	500.71	312.58
12.00	1022.08	987.31	875.39	492.97	312.11
13.00	996.69	961.61	840.07	483.81	311.55
14.00	969.76	934.46	711.57	473.60	310.92
15.00	941.32	905.91	649.79	462.94	310.26
16.00	911.19	875.50	614.25	452.21	309.59
17.00	878.88	840.41	586.35	441.57	308.93
18.00	842.55	730.03	561.69	431.11	308.27
19.00	734.49	651.59	538.98	420.93	307.63
20.00	651.76	608.03	517.86	411.10	307.01
21.00	606.83	575.03	498.23	401.71	306.42
22.00	573.19	547.19	480.04	392.84	305.86
23.00	545.07	522.75	463.30	384.53	305.34
24.00	521.27	501.62	448.43	377.07	304.87
25.00	508.11	489.82	440.04	372.82	304.60

ITERATION NO. 700 TIME = 13.9999 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.93211	0.93545	0.94965	0.99288	0.99782
1.00	0.78698	0.79833	0.84762	0.97247	0.98984
2.00	0.65781	0.67938	0.76157	0.94429	0.97560
3.00	0.54699	0.57838	0.69241	0.91198	0.95569
4.00	0.45888	0.49811	0.63679	0.87789	0.93130
5.00	0.39196	0.43689	0.59227	0.84354	0.90373
6.00	0.34261	0.39140	0.55692	0.80990	0.87419
7.00	0.30709	0.35832	0.52914	0.77760	0.84371
8.00	0.28221	0.33491	0.50759	0.74703	0.81313
9.00	0.26553	0.31901	0.49117	0.71842	0.78308
10.00	0.25522	0.30905	0.47896	0.69190	0.75406
11.00	0.25001	0.30384	0.47018	0.66751	0.72641
12.00	0.24897	0.30250	0.46415	0.64522	0.70034
13.00	0.25148	0.30445	0.46048	0.62503	0.67604
14.00	0.25726	0.30959	0.46004	0.60708	0.65364
15.00	0.26635	0.31826	0.46480	0.59167	0.63335
16.00	0.27853	0.32970	0.46915	0.57841	0.61520
17.00	0.29331	0.34288	0.47203	0.56680	0.59905
18.00	0.31037	0.35745	0.47395	0.55651	0.58470
19.00	0.33034	0.37523	0.47570	0.54739	0.57197
20.00	0.35450	0.39538	0.47776	0.53937	0.56070
21.00	0.38068	0.41327	0.47998	0.53240	0.55078
22.00	0.40292	0.42821	0.48213	0.52636	0.54208
23.00	0.42063	0.44039	0.48405	0.52115	0.53451
24.00	0.43426	0.44997	0.48563	0.51677	0.52812
25.00	0.44110	0.45479	0.48632	0.51428	0.52453

BULK CONCENTRATION AT REACTOR EXIT = 0.501112

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	673.18	670.36	657.40	607.50	414.93
1.00	762.88	752.72	706.64	566.50	323.93
2.00	839.37	819.55	740.68	541.60	315.84
3.00	900.75	871.39	762.03	527.85	314.42
4.00	944.56	907.25	774.27	520.44	313.87
5.00	972.34	928.97	779.55	516.27	313.57
6.00	986.96	939.29	779.30	513.51	313.39
7.00	991.36	940.75	774.58	511.03	313.23
8.00	987.97	935.47	766.22	508.24	313.06
9.00	978.69	925.02	754.91	504.81	312.85
10.00	964.93	910.61	741.22	500.61	312.59
11.00	947.67	893.11	725.68	495.63	312.29
12.00	927.66	873.16	708.70	489.91	311.94
13.00	905.37	851.21	690.52	483.50	311.54
14.00	881.02	827.31	670.52	476.34	311.10
15.00	854.65	801.34	647.71	468.32	310.60
16.00	826.49	773.89	625.72	459.77	310.07
17.00	796.88	745.63	605.21	451.06	309.53
18.00	766.05	716.75	585.85	442.41	308.99
19.00	733.52	686.10	567.17	433.90	308.45
20.00	698.67	654.59	548.92	425.55	307.93
21.00	663.28	625.10	531.24	417.37	307.41
22.00	631.06	598.10	514.33	409.43	306.92
23.00	602.39	573.56	498.34	401.80	306.43
24.00	577.61	551.98	483.85	394.78	305.99
25.00	563.98	539.99	475.68	390.78	305.74

BULK TEMPERATURE AT REACTOR EXIT = 413.43

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.67790	0.68830	0.73011	0.98644	0.99784
1.00	0.46939	0.48322	0.57675	0.97166	0.98985
2.00	0.34823	0.37925	0.50567	0.94398	0.97559
3.00	0.25751	0.29446	0.45964	0.91176	0.95566
4.00	0.20137	0.24109	0.42718	0.87769	0.93125
5.00	0.16678	0.20797	0.40519	0.84333	0.90365
6.00	0.14568	0.18798	0.39135	0.80966	0.87407
7.00	0.13339	0.17685	0.38394	0.77733	0.84356
8.00	0.12723	0.17206	0.38161	0.74671	0.81293
9.00	0.12561	0.17211	0.38327	0.71805	0.78283
10.00	0.12766	0.17608	0.38796	0.69146	0.75375
11.00	0.13287	0.18338	0.39481	0.66699	0.72602
12.00	0.14102	0.19355	0.40298	0.64461	0.69987
13.00	0.15198	0.20640	0.41201	0.62433	0.67547
14.00	0.16584	0.22222	0.42474	0.60630	0.65299
15.00	0.18287	0.24165	0.45373	0.59083	0.63261
16.00	0.20321	0.26406	0.46418	0.57752	0.61438
17.00	0.22676	0.28824	0.46909	0.56585	0.59816
18.00	0.25336	0.31358	0.47190	0.55550	0.58375
19.00	0.28351	0.34880	0.47408	0.54632	0.57096
20.00	0.32243	0.38669	0.47635	0.53827	0.55964
21.00	0.37047	0.40931	0.47868	0.53126	0.54967
22.00	0.39861	0.42591	0.48088	0.52519	0.54093
23.00	0.41823	0.43872	0.48282	0.51995	0.53333
24.00	0.43255	0.44855	0.48439	0.51556	0.52691
25.00	0.43959	0.45346	0.48510	0.51307	0.52333

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	783.50	777.64	752.76	610.31	414.93
1.00	900.84	889.56	824.29	566.89	323.93
2.00	974.01	950.11	851.96	541.78	315.85
3.00	1026.66	994.90	863.33	528.00	314.43
4.00	1056.59	1019.08	865.54	520.59	313.87
5.00	1070.34	1028.61	861.06	516.44	313.58
6.00	1072.71	1027.86	851.48	513.70	313.40
7.00	1067.02	1019.81	837.93	511.25	313.24
8.00	1055.53	1006.46	821.26	508.48	313.07
9.00	1039.74	989.13	802.14	505.08	312.87
10.00	1020.65	968.70	781.16	500.92	312.61
11.00	998.91	945.81	758.88	495.98	312.31
12.00	974.95	920.91	735.78	490.30	311.96
13.00	949.02	894.24	712.05	483.91	311.57
14.00	921.19	865.72	685.88	476.75	311.13
15.00	891.38	835.07	652.67	468.71	310.63
16.00	859.67	802.84	628.08	460.13	310.10
17.00	826.24	769.75	606.64	451.40	309.55
18.00	791.16	735.95	586.83	442.72	309.01
19.00	753.95	697.09	567.88	434.18	308.47
20.00	711.89	658.18	549.45	425.78	307.95
21.00	667.36	626.64	531.64	417.57	307.43
22.00	632.63	598.86	514.62	409.59	306.93
23.00	603.08	573.96	498.55	401.92	306.45
24.00	577.95	552.20	483.99	394.86	306.00
25.00	564.23	540.17	475.80	390.85	305.75

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.82005	0.99782
1.00	0.00000	0.00000	0.00000	0.95591	0.98956
2.00	0.00000	0.00000	0.00000	0.93708	0.97486
3.00	0.00000	0.00000	0.00000	0.90641	0.95437
4.00	0.00000	0.00000	0.00000	0.87242	0.92932
5.00	0.00000	0.00000	0.00000	0.83776	0.90105
6.00	0.00000	0.00000	0.00000	0.80368	C.87081
7.00	0.00000	0.00000	0.00000	0.77092	0.83963
8.00	0.00000	0.00000	0.00000	0.73990	0.80835
9.00	0.00000	0.00000	0.00000	0.71087	0.77763
10.00	0.00000	0.00000	0.00001	0.68396	0.74796
11.00	0.00000	0.00000	0.00005	0.65926	0.71972
12.00	0.00000	0.00000	0.00029	0.63682	0.69320
13.00	0.00000	0.00000	0.00187	0.61681	0.66863
14.00	0.00000	0.00000	0.02408	0.59945	0.64627
15.00	0.00000	0.00000	0.31506	0.58480	0.62629
16.00	0.00000	0.00004	0.41330	0.57231	0.60867
17.00	0.00002	0.00039	0.44628	0.56151	0.59322
18.00	0.00017	0.00409	0.46154	0.55216	0.57973
19.00	0.00216	0.11329	0.47030	0.54415	0.56803
20.00	0.06813	0.32733	0.47642	0.53742	0.55797
21.00	0.30671	0.39502	0.48126	0.53186	0.54943
22.00	0.38601	0.42648	0.48537	0.52736	0.54226
23.00	0.42121	0.44528	0.48899	0.52380	0.53636
24.00	0.44139	0.45801	0.49215	0.52111	0.53170
25.00	0.45047	0.46426	0.49394	0.51980	0.52933

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1031.88	1029.56	1018.90	670.39	414.92
1.00	1072.64	1066.93	1037.73	572.83	323.95
2.00	1101.18	1088.82	1038.86	544.74	315.90
3.00	1121.13	1103.02	1033.22	530.54	314.51
4.00	1130.82	1107.96	1023.58	523.18	313.98
5.00	1132.07	1105.53	1011.13	519.16	313.70
6.00	1126.81	1097.55	996.57	516.54	313.53
7.00	1116.66	1085.45	980.37	514.17	313.39
8.00	1102.88	1070.31	962.83	511.44	313.22
9.00	1086.39	1052.90	944.17	508.02	313.02
10.00	1067.85	1033.73	924.58	503.76	312.76
11.00	1047.70	1013.19	904.14	498.62	312.45
12.00	1026.23	991.53	882.76	492.58	312.08
13.00	1003.62	968.84	859.66	485.61	311.66
14.00	979.96	945.12	826.65	477.64	311.17
15.00	955.31	920.46	699.31	468.81	310.63
16.00	929.78	895.04	642.87	459.56	310.05
17.00	903.29	868.70	610.80	450.22	309.47
18.00	875.55	839.70	585.86	440.96	308.88
19.00	845.41	771.77	563.91	431.85	308.31
20.00	790.86	670.17	543.61	422.91	307.75
21.00	679.03	622.46	524.59	414.22	307.21
22.00	626.39	589.35	506.74	405.82	306.68
23.00	591.55	562.41	490.09	397.80	306.17
24.00	564.59	539.78	475.12	390.47	305.71
25.00	550.31	527.42	466.70	386.31	305.45

ITERATION NO. 800 TIME = 16.0000 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.93400	0.93748	0.95172	0.99317	0.99792
1.00	0.79092	0.80306	0.85459	0.97370	0.99029
2.00	0.66321	0.68588	0.77107	0.94665	0.97665
3.00	0.55325	0.58588	0.70315	0.91543	0.95752
4.00	0.46564	0.50619	0.64826	0.88237	0.93399
5.00	0.39903	0.44534	0.60431	0.84899	0.90734
6.00	0.34992	0.40017	0.56957	0.81628	0.87874
7.00	0.31468	0.36748	0.54252	0.78491	0.84923
8.00	0.29019	0.34458	0.52186	0.75531	0.81964
9.00	0.27405	0.32940	0.50649	0.72773	0.79062
10.00	0.26451	0.32037	0.49551	0.70231	0.76269
11.00	0.26031	0.31636	0.48810	0.67910	0.73619
12.00	0.26056	0.31651	0.48360	0.65810	0.71136
13.00	0.26467	0.32021	0.48144	0.63924	0.68835
14.00	0.27224	0.32710	0.48143	0.62250	0.66726
15.00	0.28317	0.33722	0.48502	0.60798	0.64816
16.00	0.29732	0.35018	0.48928	0.59550	0.63106
17.00	0.31423	0.36500	0.49229	0.58458	0.61586
18.00	0.33331	0.38092	0.49450	0.57494	0.60234
19.00	0.35409	0.39772	0.49638	0.56638	0.59033
20.00	0.37659	0.41640	0.49837	0.55882	0.57968
21.00	0.40058	0.43379	0.50049	0.55218	0.57023
22.00	0.42249	0.44839	0.50252	0.54637	0.56188
23.00	0.44005	0.46028	0.50429	0.54127	0.55453
24.00	0.45351	0.46958	0.50567	0.53689	0.54822
25.00	0.46015	0.47419	0.50621	0.53435	0.54463

BULK CONCENTRATION AT REACTOR EXIT = 0.521044

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	671.97	669.07	656.08	607.32	414.92
1.00	760.35	749.70	702.24	565.76	323.89
2.00	835.89	815.39	734.69	540.24	315.76
3.00	896.69	866.58	755.28	525.94	314.30
4.00	940.17	902.06	767.11	518.08	313.72
5.00	967.74	923.56	772.10	513.56	313.41
6.00	982.20	933.68	771.57	510.50	313.20
7.00	986.42	934.93	766.51	507.77	313.03
8.00	982.79	929.35	757.73	504.72	312.84
9.00	973.17	918.50	745.91	501.02	312.61
10.00	958.94	903.55	731.64	496.54	312.34
11.00	941.10	885.38	715.45	491.27	312.01
12.00	920.34	864.63	697.79	485.24	311.64
13.00	897.20	841.78	679.07	478.56	311.23
14.00	871.99	817.15	659.42	471.30	310.78
15.00	844.86	790.74	637.98	463.44	310.30
16.00	815.98	762.90	616.70	455.13	309.78
17.00	785.71	734.32	596.80	446.72	309.25
18.00	754.49	705.51	578.03	438.39	308.73
19.00	722.63	676.62	560.13	430.24	308.22
20.00	690.13	647.06	542.82	422.30	307.72
21.00	657.22	618.93	526.11	414.58	307.24
22.00	626.26	593.18	510.15	407.12	306.77
23.00	598.72	569.81	495.10	399.97	306.32
24.00	575.02	549.32	481.50	393.41	305.91
25.00	562.11	538.04	473.88	389.71	305.67

BULK TEMPERATURE AT REACTOR EXIT = 412.29

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.68914	0.69908	0.73834	0.98675	0.99793
1.00	0.47479	0.48987	0.59703	0.97287	0.99029
2.00	0.35383	0.38660	0.52405	0.94629	0.97662
3.00	0.26269	0.30137	0.47711	0.91514	0.95744
4.00	0.20619	0.24765	0.44432	0.88208	0.93388
5.00	0.17136	0.21435	0.42242	0.84866	0.90718
6.00	0.15020	0.19439	0.40910	0.81592	0.87853
7.00	0.13804	0.18352	0.40256	0.78451	0.84897
8.00	0.13219	0.17925	0.40140	0.75487	0.81933
9.00	0.13110	0.18011	0.40446	0.72724	0.79027
10.00	0.13392	0.18523	0.41074	0.70177	0.76228
11.00	0.14022	0.19407	0.41932	0.67851	0.73572
12.00	0.14979	0.20626	0.42938	0.65743	0.71082
13.00	0.16260	0.22156	0.44025	0.63849	0.68773
14.00	0.17869	0.23998	0.45190	0.62166	0.66654
15.00	0.19831	0.26192	0.47476	0.60705	0.64735
16.00	0.22168	0.28707	0.48492	0.59449	0.63017
17.00	0.24868	0.31415	0.48953	0.58350	0.61487
18.00	0.27870	0.34186	0.49240	0.57378	0.60127
19.00	0.31090	0.36990	0.49457	0.56514	0.58917
20.00	0.34481	0.40606	0.49668	0.55751	0.57843
21.00	0.38654	0.42915	0.49884	0.55079	0.56890
22.00	0.41704	0.44545	0.50087	0.54490	0.56047
23.00	0.43682	0.45798	0.50261	0.53973	0.55304
24.00	0.45106	0.46755	0.50397	0.53529	0.54666
25.00	0.45794	0.47224	0.50449	0.53273	0.54304

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	778.27	772.58	748.79	610.13	414.92
1.00	897.68	885.71	814.13	566.15	323.89
2.00	970.46	945.59	842.13	540.44	315.77
3.00	1023.10	990.37	853.67	526.12	314.31
4.00	1053.06	1014.57	855.91	518.27	313.73
5.00	1066.81	1024.09	851.33	513.77	313.42
6.00	1069.13	1023.26	841.49	510.71	313.22
7.00	1063.32	1015.03	827.51	507.99	313.04
8.00	1051.60	1001.36	810.26	504.95	312.85
9.00	1035.45	983.55	790.45	501.27	312.63
10.00	1015.87	962.47	768.70	496.81	312.36
11.00	993.48	938.74	745.58	491.56	312.03
12.00	968.71	912.79	721.64	485.57	311.67
13.00	941.82	884.94	697.31	478.92	311.26
14.00	912.95	855.33	672.61	471.69	310.81
15.00	882.08	823.82	642.75	463.84	310.32
16.00	849.24	790.71	618.89	455.54	309.81
17.00	814.63	756.83	598.25	447.13	309.28
18.00	778.69	722.93	579.17	438.80	308.76
19.00	741.89	689.06	561.09	430.64	308.25
20.00	704.34	651.85	543.68	422.69	307.75
21.00	663.53	621.21	526.89	414.95	307.26
22.00	628.86	594.64	510.86	407.47	306.79
23.00	600.27	570.90	495.76	400.30	306.34
24.00	576.14	550.21	482.09	393.72	305.93
25.00	563.08	538.85	474.44	390.00	305.69

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.81661	0.99793
1.00	0.00000	0.00000	0.00000	0.95789	0.99008
2.00	0.00000	0.00000	0.00000	0.94013	0.97607
3.00	0.00000	0.00000	0.00000	0.91063	0.95645
4.00	0.00000	0.00000	0.00000	0.87778	0.93239
5.00	0.00000	0.00000	0.00000	0.84420	0.90518
6.00	0.00000	0.00000	0.00000	0.81116	0.87601
7.00	0.00000	0.00000	0.00000	0.77943	0.84592
8.00	0.00000	0.00000	0.00000	0.74944	0.81575
9.00	0.00000	0.00000	0.00000	0.72146	0.78614
10.00	0.00000	0.00000	0.00001	0.69560	0.75760
11.00	0.00000	0.00000	0.00007	0.67193	0.73048
12.00	0.00000	0.00000	0.00042	0.65042	0.70501
13.00	0.00000	0.00000	0.00224	0.63106	0.68136
14.00	0.00000	0.00000	0.01401	0.61390	0.65967
15.00	0.00000	0.00001	0.27578	0.59910	0.64005
16.00	0.00000	0.00005	0.41845	0.58638	0.62254
17.00	0.00002	0.00037	0.45590	0.57527	0.60698
18.00	0.00016	0.00268	0.47197	0.56547	0.59319
19.00	0.00130	0.02366	0.48036	0.55680	0.58098
20.00	0.01193	0.26641	0.48566	0.54920	0.57020
21.00	0.20422	0.38159	0.48951	0.54259	0.56071
22.00	0.36262	0.42321	0.49250	0.53686	0.55239
23.00	0.41328	0.44499	0.49486	0.53192	0.54514
24.00	0.43786	0.45832	0.49668	0.52776	0.53902
25.00	0.44774	0.46428	0.49750	0.52542	0.53561

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1029.68	1027.37	1016.94	671.55	414.91
1.00	1070.97	1064.99	1033.82	571.76	323.90
2.00	1099.22	1086.44	1034.70	543.01	315.80
3.00	1119.02	1100.50	1028.88	528.21	314.37
4.00	1128.62	1105.34	1019.14	520.33	313.81
5.00	1129.83	1102.86	1006.62	515.92	313.51
6.00	1124.52	1094.84	991.99	512.95	313.31
7.00	1114.33	1082.71	975.69	510.30	313.15
8.00	1100.52	1067.52	958.09	507.34	312.97
9.00	1084.01	1050.08	939.42	503.71	312.75
10.00	1065.49	1030.92	919.94	499.32	312.49
11.00	1045.43	1010.47	899.85	494.10	312.17
12.00	1024.17	989.02	879.25	488.15	311.81
13.00	1001.95	966.78	857.79	481.47	311.40
14.00	978.91	943.83	831.99	474.12	310.95
15.00	955.10	920.14	715.13	466.05	310.45
16.00	930.63	895.92	643.25	457.52	309.92
17.00	905.60	871.34	610.36	448.86	309.38
18.00	880.04	845.84	586.07	440.28	308.84
19.00	853.55	812.75	565.27	431.86	308.31
20.00	822.67	700.42	546.21	423.63	307.80
21.00	726.40	636.27	528.35	415.60	307.29
22.00	645.62	600.10	511.53	407.84	306.80
23.00	605.54	572.58	495.81	400.39	306.33
24.00	577.29	550.12	481.63	393.55	305.90
25.00	562.91	538.06	473.69	389.68	305.66

ITERATION NO. 1000 TIME = 19.9978 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	0.93625	0.93993	0.95396	0.99351	0.99803
1.00	0.79558	0.80886	0.86306	0.97516	0.99083
2.00	0.66977	0.69393	0.78304	0.94954	0.97794
3.00	0.56098	0.59523	0.71665	0.91971	0.95976
4.00	0.47404	0.51625	0.66248	0.88790	0.93731
5.00	0.40776	0.45576	0.61894	0.85565	0.91176
6.00	0.35885	0.41081	0.58453	0.82397	0.88427
7.00	0.32377	0.37833	0.55786	0.79358	0.85584
8.00	0.29950	0.35574	0.53767	0.76491	0.82730
9.00	0.28372	0.34100	0.52288	0.73826	0.79933
10.00	0.27471	0.33262	0.51257	0.71379	0.77244
11.00	0.27129	0.32950	0.50599	0.69156	0.74698
12.00	0.27265	0.33089	0.50251	0.67160	0.72323
13.00	0.27829	0.33626	0.50167	0.65388	0.70135
14.00	0.28794	0.34532	0.50337	0.63839	0.68147
15.00	0.30147	0.35793	0.50808	0.62515	0.66364
16.00	0.31862	0.37337	0.51243	0.61384	0.64783
17.00	0.33882	0.39071	0.51576	0.60403	0.63388
18.00	0.36138	0.40924	0.51864	0.59548	0.62162
19.00	0.38562	0.42862	0.52148	0.58805	0.61086
20.00	0.41089	0.44854	0.52450	0.58167	0.60146
21.00	0.43581	0.46613	0.52759	0.57621	0.59328
22.00	0.45729	0.48072	0.53052	0.57158	0.58619
23.00	0.47433	0.49265	0.53313	0.56765	0.58009
24.00	0.48749	0.50211	0.53533	0.56440	0.57499
25.00	0.49413	0.50693	0.53642	0.56259	0.57218

BULK CONCENTRATION AT REACTOR EXIT = 0.550266

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	670.54	667.50	654.65	607.12	414.90
1.00	757.36	746.00	696.90	564.89	323.84
2.00	831.68	810.26	727.17	538.57	315.66
3.00	891.73	860.62	746.85	523.59	314.16
4.00	934.79	895.68	758.31	515.20	313.54
5.00	962.17	917.00	763.18	510.30	313.20
6.00	976.56	927.06	762.60	506.96	312.98
7.00	980.75	928.28	757.51	504.03	312.79
8.00	977.08	922.64	748.69	500.83	312.59
9.00	967.36	911.67	736.78	497.01	312.36
10.00	952.93	896.50	722.37	492.41	312.08
11.00	934.75	877.95	705.97	487.01	311.75
12.00	913.47	856.63	687.99	480.83	311.37
13.00	889.53	832.95	668.76	473.96	310.94
14.00	863.21	807.18	648.43	466.46	310.48
15.00	834.67	779.50	626.74	458.39	309.98
16.00	804.17	750.42	605.85	449.99	309.46
17.00	772.15	720.63	586.25	441.56	308.93
18.00	739.12	690.61	567.62	433.25	308.41
19.00	705.58	660.66	549.74	425.12	307.90
20.00	672.00	631.00	532.46	417.21	307.40
21.00	639.27	603.45	515.90	409.55	306.92
22.00	609.35	578.47	500.19	402.17	306.46
23.00	582.97	555.92	485.48	395.14	306.01
24.00	560.31	536.20	472.24	388.73	305.61
25.00	547.97	525.36	464.85	385.12	305.38

BULK TEMPERATURE AT REACTOR EXIT = 406.44

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.70276	0.71181	0.74669	0.98720	0.99805
1.00	0.48006	0.49696	0.62496	0.97441	0.99085
2.00	0.36113	0.39636	0.54977	0.94929	0.97795
3.00	0.26949	0.31059	0.50074	0.91958	0.95977
4.00	0.21247	0.25633	0.46677	0.88781	0.93731
5.00	0.17728	0.22265	0.44423	0.85557	0.91176
6.00	0.15594	0.20253	0.43070	0.82390	0.88426
7.00	0.14379	0.19176	0.42428	0.79351	0.85582
8.00	0.13813	0.18785	0.42349	0.76485	0.82728
9.00	0.13746	0.18936	0.42711	0.73820	0.79931
10.00	0.14096	0.19549	0.43408	0.71373	0.77241
11.00	0.14827	0.20579	0.44355	0.69151	0.74695
12.00	0.15932	0.22005	0.45484	0.67154	0.72320
13.00	0.17424	0.23817	0.46759	0.65383	0.70132
14.00	0.19330	0.26019	0.48226	0.63834	0.68143
15.00	0.21684	0.28617	0.50390	0.62510	0.66359
16.00	0.24499	0.31535	0.51065	0.61378	0.64778
17.00	0.27733	0.34637	0.51486	0.60397	0.63383
18.00	0.31291	0.37814	0.51815	0.59541	0.62156
19.00	0.35048	0.41042	0.52118	0.58798	0.61079
20.00	0.38898	0.44419	0.52431	0.58159	0.60138
21.00	0.42902	0.46455	0.52744	0.57613	0.59319
22.00	0.45535	0.47999	0.53038	0.57148	0.58610
23.00	0.47347	0.49225	0.53300	0.56755	0.58000
24.00	0.48702	0.50184	0.53519	0.56428	0.57488
25.00	0.49380	0.50672	0.53629	0.56248	0.57209

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	771.97	766.62	744.75	609.87	414.91
1.00	894.36	881.37	800.34	565.23	323.84
2.00	965.87	939.64	828.56	538.70	315.67
3.00	1018.46	984.39	840.74	523.67	314.17
4.00	1048.52	1008.70	843.43	515.26	313.55
5.00	1062.39	1018.36	839.17	510.36	313.21
6.00	1064.79	1017.63	829.52	507.02	312.99
7.00	1059.01	1009.41	815.62	504.08	312.80
8.00	1047.25	995.65	798.35	500.88	312.60
9.00	1030.96	977.61	778.44	497.06	312.36
10.00	1011.10	956.13	756.53	492.46	312.08
11.00	988.24	931.75	733.15	487.05	311.75
12.00	962.75	904.83	708.75	480.87	311.37
13.00	934.78	875.60	683.64	474.00	310.95
14.00	904.37	844.21	657.69	466.50	310.49
15.00	871.48	810.71	628.67	458.43	309.99
16.00	836.21	775.68	606.69	450.03	309.46
17.00	798.92	739.95	586.70	441.61	308.94
18.00	760.25	704.21	567.89	433.29	308.42
19.00	720.95	668.71	549.91	425.17	307.91
20.00	681.66	633.04	532.60	417.26	307.41
21.00	642.43	604.25	516.02	409.60	306.93
22.00	610.33	578.90	500.30	402.22	306.46
23.00	583.46	556.20	485.59	395.20	306.02
24.00	560.63	536.42	472.35	388.79	305.62
25.00	548.22	525.54	464.95	385.17	305.39

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.81633	0.99808
1.00	0.00000	0.00000	0.00000	0.96055	0.99077
2.00	0.00000	0.00000	0.00000	0.94425	0.97769
3.00	0.00000	0.00000	0.00000	0.91635	0.95928
4.00	0.00000	0.00000	0.00000	0.88502	0.93656
5.00	0.00000	0.00000	0.00000	0.85284	0.91074
6.00	0.00000	0.00000	0.00000	0.82112	0.88297
7.00	0.00000	0.00000	0.00000	0.79066	0.85428
8.00	0.00000	0.00000	0.00000	0.76192	0.82549
9.00	0.00000	0.00000	0.00000	0.73519	0.79727
10.00	0.00000	0.00000	0.00002	0.71065	0.77014
11.00	0.00000	0.00000	0.00013	0.68833	0.74445
12.00	0.00000	0.00000	0.00072	0.66824	0.72047
13.00	0.00000	0.00000	0.00394	0.65037	0.69836
14.00	0.00000	0.00000	0.02412	0.63469	0.67822
15.00	0.00000	0.00001	0.36918	0.62123	0.66014
16.00	0.00000	0.00008	0.46545	0.60971	0.64407
17.00	0.00003	0.00064	0.49184	0.59970	0.62987
18.00	0.00028	0.00450	0.50432	0.59094	0.61735
19.00	0.00225	0.03329	0.51156	0.58329	0.60634
20.00	0.01755	0.31730	0.51662	0.57666	0.59668
21.00	0.22327	0.42396	0.52061	0.57096	0.58824
22.00	0.40507	0.46014	0.52388	0.56607	0.58088
23.00	0.45071	0.47986	0.52656	0.56189	0.57452
24.00	0.47323	0.49238	0.52870	0.55839	0.56915
25.00	0.48249	0.49811	0.52973	0.55644	0.56620

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	1026.85	1024.61	1014.78	671.56	414.90
1.00	1069.07	1062.70	1028.21	570.33	323.84
2.00	1096.72	1083.35	1028.90	540.69	315.68
3.00	1116.29	1097.18	1023.03	525.07	314.19
4.00	1125.79	1101.93	1013.31	516.53	313.58
5.00	1126.95	1099.42	1000.83	511.60	313.25
6.00	1121.65	1091.41	986.23	508.26	313.03
7.00	1111.46	1079.28	969.97	505.31	312.84
8.00	1097.64	1064.09	952.35	502.09	312.65
9.00	1081.09	1046.59	933.67	498.25	312.42
10.00	1062.48	1027.31	914.18	493.61	312.14
11.00	1042.27	1006.66	894.08	488.18	311.81
12.00	1020.78	984.94	873.47	481.98	311.43
13.00	998.26	962.34	851.74	475.11	311.00
14.00	974.83	939.01	823.87	467.63	310.54
15.00	950.60	915.02	678.32	459.58	310.04
16.00	925.67	890.59	623.68	451.19	309.52
17.00	900.24	865.91	595.55	442.76	309.00
18.00	874.49	840.27	573.32	434.43	308.47
19.00	848.13	806.11	553.75	426.30	307.96
20.00	817.27	680.22	535.66	418.38	307.47
21.00	718.37	619.98	518.67	410.72	306.98
22.00	629.76	586.94	502.73	403.33	306.52
23.00	592.70	561.37	487.87	396.29	306.08
24.00	566.41	540.36	474.53	389.86	305.67
25.00	552.99	529.08	467.08	386.23	305.44

ITERATION NO. 1500 TIME = 29.9967 SEC.

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.93827	0.94226	0.95536	0.99376	0.99811
1.00	0.79931	0.81386	0.86922	0.97623	0.99123
2.00	0.67521	0.70070	0.79259	0.95176	0.97891
3.00	0.56747	0.60307	0.72764	0.92309	0.96151
4.00	0.48108	0.52465	0.67400	0.89232	0.93993
5.00	0.41506	0.46438	0.63062	0.86096	0.91527
6.00	0.36623	0.41949	0.59623	0.83007	0.88865
7.00	0.33117	0.38702	0.56951	0.80037	0.86105
8.00	0.30691	0.36443	0.54927	0.77232	0.83329
9.00	0.29118	0.34974	0.53442	0.74622	0.80604
10.00	0.28229	0.34147	0.52408	0.72224	0.77980
11.00	0.27908	0.33856	0.51747	0.70047	0.75494
12.00	0.28077	0.34027	0.51402	0.68093	0.73175
13.00	0.28692	0.34613	0.51335	0.66363	0.71040
14.00	0.29733	0.35596	0.51578	0.64864	0.69104
15.00	0.31193	0.36960	0.52131	0.63596	0.67375
16.00	0.33029	0.38597	0.52548	0.62511	0.65847
17.00	0.35174	0.40415	0.52883	0.61571	0.64504
18.00	0.37552	0.42353	0.53191	0.60758	0.63326
19.00	0.40107	0.44402	0.53511	0.60058	0.62299
20.00	0.42768	0.46482	0.53859	0.59465	0.61407
21.00	0.45349	0.48253	0.54211	0.58967	0.60639
22.00	0.47480	0.49724	0.54546	0.58553	0.59982
23.00	0.49174	0.50932	0.54849	0.58210	0.59424
24.00	0.50493	0.51898	0.55108	0.57933	0.58965
25.00	0.51170	0.52400	0.55248	0.57787	0.58721

BULK CONCENTRATION AT REACTOR EXIT = 0.565945

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	669.25	666.02	653.76	606.96	414.90
1.00	754.98	742.83	693.05	564.25	323.80
2.00	828.19	805.96	721.19	537.29	315.59
3.00	887.58	855.65	740.00	521.73	314.05
4.00	930.30	890.38	751.19	512.89	313.40
5.00	957.54	911.59	756.06	507.69	313.04
6.00	971.93	921.69	755.63	504.16	312.81
7.00	976.19	923.00	750.74	501.13	312.61
8.00	972.61	917.49	742.16	497.90	312.41
9.00	963.00	906.65	730.54	494.09	312.18
10.00	948.66	891.60	716.42	489.55	311.90
11.00	930.54	873.15	700.31	484.23	311.57
12.00	909.27	851.86	682.60	478.14	311.20
13.00	885.25	828.13	663.57	471.35	310.78
14.00	858.69	802.14	643.06	463.89	310.32
15.00	829.74	774.08	621.14	455.81	309.82
16.00	798.75	744.70	600.69	447.46	309.30
17.00	766.23	714.67	581.41	439.11	308.77
18.00	732.71	684.41	562.98	430.87	308.26
19.00	698.62	654.04	545.19	422.81	307.75
20.00	664.45	624.10	527.96	414.95	307.26
21.00	631.43	596.78	511.45	407.33	306.78
22.00	601.94	572.06	495.82	399.98	306.32
23.00	575.95	549.75	481.19	392.99	305.88
24.00	553.61	530.24	468.03	386.61	305.48
25.00	541.40	519.48	460.67	383.00	305.25

BULK TEMPERATURE AT REACTOR EXIT = 403.73

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.71198	0.72027	0.75059	0.98774	0.99813
1.00	0.47692	0.49543	0.64509	0.97550	0.99125
2.00	0.36715	0.40451	0.57066	0.95154	0.97893
3.00	0.27515	0.31832	0.51954	0.92298	0.96153
4.00	0.21771	0.26355	0.48415	0.89225	0.93994
5.00	0.18220	0.22949	0.46063	0.86091	0.91528
6.00	0.16065	0.20913	0.44636	0.83003	0.88866
7.00	0.14841	0.19827	0.43935	0.80033	0.86106
8.00	0.14278	0.19443	0.43805	0.77228	0.83329
9.00	0.14225	0.19615	0.44120	0.74619	0.80604
10.00	0.14601	0.20262	0.44776	0.72221	0.77979
11.00	0.15372	0.21344	0.45686	0.70045	0.75494
12.00	0.16534	0.22842	0.46791	0.68091	0.73175
13.00	0.18109	0.24754	0.48073	0.66361	0.71040
14.00	0.20136	0.27090	0.49697	0.64862	0.69103
15.00	0.22660	0.29848	0.51794	0.63594	0.67374
16.00	0.25672	0.32899	0.52395	0.62509	0.65846
17.00	0.29101	0.36110	0.52808	0.61570	0.64503
18.00	0.32835	0.39392	0.53153	0.60756	0.63325
19.00	0.36761	0.42847	0.53491	0.60057	0.62298
20.00	0.40817	0.46160	0.53849	0.59463	0.61406
21.00	0.44930	0.48132	0.54206	0.58966	0.60638
22.00	0.47337	0.49673	0.54542	0.58551	0.59980
23.00	0.49117	0.50910	0.54846	0.58208	0.59422
24.00	0.50468	0.51886	0.55106	0.57931	0.58963
25.00	0.51154	0.52393	0.55246	0.57786	0.58719

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	767.62	762.52	742.79	609.60	414.90
1.00	894.87	880.92	790.46	564.58	323.80
2.00	962.11	934.72	817.66	537.40	315.59
3.00	1014.66	979.44	830.47	521.79	314.06
4.00	1044.79	1003.89	833.74	512.93	313.41
5.00	1058.77	1013.71	829.97	507.72	313.05
6.00	1061.31	1013.14	820.79	504.19	312.81
7.00	1055.64	1005.06	807.34	501.16	312.62
8.00	1043.97	991.40	790.53	497.92	312.42
9.00	1027.75	973.43	771.08	494.12	312.18
10.00	1007.91	951.97	749.62	489.57	311.90
11.00	985.05	927.55	726.67	484.24	311.58
12.00	959.46	900.49	702.66	478.15	311.20
13.00	931.26	870.99	677.77	471.37	310.78
14.00	900.42	839.12	651.26	463.90	310.32
15.00	866.84	805.00	622.62	455.82	309.82
16.00	830.74	769.48	601.37	447.47	309.30
17.00	792.63	733.39	581.75	439.12	308.78
18.00	753.23	697.29	563.16	430.88	308.26
19.00	713.17	660.82	545.28	422.82	307.76
20.00	672.94	625.51	528.01	414.96	307.26
21.00	633.27	597.32	511.48	407.33	306.79
22.00	602.57	572.29	495.84	399.99	306.32
23.00	576.21	549.86	481.20	393.00	305.88
24.00	553.73	530.30	468.05	386.61	305.48
25.00	541.48	519.52	460.68	383.01	305.25

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.82803	0.99818
1.00	0.00000	0.00000	0.00000	0.96249	0.99128
2.00	0.00000	0.00000	0.00000	0.94744	0.97894
3.00	0.00000	0.00000	0.00000	0.92088	0.96149
4.00	0.00000	0.00000	0.00000	0.89079	0.93986
5.00	0.00000	0.00000	0.00000	0.85972	0.91516
6.00	0.00000	0.00000	0.00000	0.82899	0.88849
7.00	0.00000	0.00000	0.00000	0.79938	0.86085
8.00	0.00000	0.00000	0.00000	0.77141	0.83305
9.00	0.00000	0.00000	0.00001	0.74540	0.80575
10.00	0.00000	0.00000	0.00003	0.72150	0.77948
11.00	0.00000	0.00000	0.00017	0.69980	0.75460
12.00	0.00000	0.00000	0.00095	0.68032	0.73138
13.00	0.00000	0.00000	0.00537	0.66306	0.71000
14.00	0.00000	0.00000	0.04210	0.64809	0.69061
15.00	0.00000	0.00001	0.44825	0.63541	0.67330
16.00	0.00000	0.00010	0.49525	0.62456	0.65800
17.00	0.00004	0.00084	0.51435	0.61517	0.64454
18.00	0.00037	0.00630	0.52456	0.60702	0.63274
19.00	0.00321	0.06443	0.53120	0.60002	0.62245
20.00	0.03092	0.39651	0.53638	0.59407	0.61351
21.00	0.35948	0.45906	0.54072	0.58908	0.60581
22.00	0.44671	0.48755	0.54445	0.58492	0.59922
23.00	0.48067	0.50484	0.54766	0.58147	0.59362
24.00	0.49983	0.51658	0.55033	0.57869	0.58902
25.00	0.50830	0.52224	0.55175	0.57722	0.58656

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	1024.76	1022.62	1013.70	667.24	414.88
1.00	1068.42	1061.69	1023.64	569.28	323.79
2.00	1094.70	1080.82	1023.96	538.91	315.58
3.00	1114.06	1094.44	1018.22	522.57	314.05
4.00	1123.46	1099.12	1008.66	513.49	313.40
5.00	1124.63	1096.65	996.39	508.18	313.04
6.00	1119.38	1088.73	982.04	504.60	312.81
7.00	1109.29	1076.72	966.05	501.52	312.61
8.00	1095.58	1061.67	948.74	498.26	312.41
9.00	1079.16	1044.31	930.40	494.39	312.18
10.00	1060.67	1025.18	911.27	489.82	311.90
11.00	1040.58	1004.65	891.55	484.45	311.57
12.00	1019.18	982.99	871.23	478.32	311.20
13.00	996.66	960.39	849.34	471.52	310.78
14.00	973.14	936.95	815.47	464.04	310.32
15.00	948.67	912.77	647.83	455.94	309.82
16.00	923.44	888.22	611.74	447.59	309.30
17.00	897.69	863.44	586.69	439.22	308.78
18.00	871.62	837.20	565.65	430.98	308.26
19.00	844.70	792.23	546.58	422.91	307.76
20.00	809.11	649.03	528.72	415.05	307.26
21.00	665.73	605.35	511.89	407.42	306.78
22.00	612.20	575.58	496.12	400.07	306.32
23.00	579.98	551.36	481.40	393.07	305.88
24.00	555.45	531.08	468.22	386.68	305.48
25.00	542.60	520.06	460.84	383.07	305.25

ITERATION NO. 3351 TIME = 67.0172 SEC.

FINAL STEADY STATE CONDITIONS

NORMALIZED CONCENTRATION PROFILE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.93936	0.94278	0.95546	0.99379	0.99812
1.00	0.79453	0.80689	0.86927	0.97627	0.99124
2.00	0.67012	0.69553	0.79249	0.95178	0.97893
3.00	0.56315	0.59927	0.72731	0.92307	0.96152
4.00	0.47776	0.52188	0.67350	0.89225	0.93992
5.00	0.41260	0.46236	0.63005	0.86085	0.91525
6.00	0.36444	0.41801	0.59567	0.82993	0.88860
7.00	0.32986	0.38592	0.56901	0.80020	0.86098
8.00	0.30595	0.36360	0.54883	0.77215	0.83320
9.00	0.29047	0.34912	0.53406	0.74606	0.80595
10.00	0.28176	0.34100	0.52378	0.72210	0.77971
11.00	0.27869	0.33821	0.51724	0.70035	0.75487
12.00	0.28050	0.34003	0.51384	0.68084	0.73169
13.00	0.28675	0.34599	0.51324	0.66357	0.71037
14.00	0.29726	0.35592	0.51573	0.64862	0.69104
15.00	0.31196	0.36965	0.52132	0.63598	0.67378
16.00	0.33042	0.38609	0.52554	0.62517	0.65854
17.00	0.35195	0.40433	0.52895	0.61583	0.64515
18.00	0.37580	0.42377	0.53209	0.60774	0.63342
19.00	0.40140	0.44433	0.53534	0.60079	0.62320
20.00	0.42808	0.46516	0.53888	0.59491	0.61433
21.00	0.45396	0.48292	0.54245	0.58999	0.60670
22.00	0.47528	0.49767	0.54585	0.58590	0.60018
23.00	0.49226	0.50981	0.54893	0.58252	0.59466
24.00	0.50548	0.51951	0.55158	0.57981	0.59012
25.00	0.51229	0.52457	0.55302	0.57839	0.58772

BULK CONCENTRATION AT REACTOR EXIT = 0.566475

TEMPERATURE PROFILE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	668.58	665.70	653.70	606.94	414.89
1.00	758.00	747.20	693.03	564.23	323.80
2.00	831.39	809.19	721.27	537.28	315.59
3.00	890.27	858.00	740.21	521.74	314.05
4.00	932.34	892.08	751.51	512.94	313.41
5.00	959.03	912.82	756.41	507.76	313.05
6.00	973.00	922.57	755.96	504.25	312.81
7.00	976.95	923.65	751.04	501.22	312.62
8.00	973.16	917.97	742.41	497.98	312.42
9.00	963.39	907.00	730.73	494.17	312.18
10.00	948.94	891.85	716.57	489.61	311.90
11.00	930.73	873.32	700.42	484.27	311.57
12.00	909.39	851.97	682.68	478.17	311.20
13.00	885.31	828.17	663.61	471.37	310.78
14.00	858.69	802.13	643.06	463.89	310.32
15.00	829.68	774.01	621.11	455.79	309.82
16.00	798.64	744.60	600.64	447.44	309.30
17.00	766.07	714.53	581.33	439.07	308.77
18.00	732.52	684.25	562.89	430.83	308.26
19.00	698.41	653.85	545.08	422.76	307.75
20.00	664.20	623.90	527.83	414.89	307.26
21.00	631.16	596.58	511.32	407.26	306.78
22.00	601.68	571.85	495.68	399.91	306.31
23.00	575.70	549.54	481.04	392.92	305.87
24.00	553.37	530.02	467.88	386.53	305.47
25.00	541.15	519.26	460.51	382.92	305.24

BULK TEMPERATURE AT REACTOR EXIT = 403.63

NORMALIZED CONCENTRATION ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.71469	0.72177	0.75085	0.98793	0.99814
1.00	0.42889	0.42949	0.64674	0.97555	0.99126
2.00	0.36189	0.39887	0.57197	0.95157	0.97895
3.00	0.27154	0.31478	0.51969	0.92297	0.96154
4.00	0.21534	0.26128	0.48378	0.89219	0.93994
5.00	0.18061	0.22797	0.46010	0.86081	0.91526
6.00	0.15956	0.20807	0.44583	0.82990	0.88862
7.00	0.14763	0.19750	0.43888	0.80018	0.86099
8.00	0.14221	0.19385	0.43765	0.77213	0.83322
9.00	0.14182	0.19572	0.44087	0.74605	0.80596
10.00	0.14569	0.20231	0.44749	0.72209	0.77973
11.00	0.15348	0.21324	0.45665	0.70035	0.75489
12.00	0.16519	0.22833	0.46775	0.68084	0.73171
13.00	0.18103	0.24754	0.48062	0.66358	0.71039
14.00	0.20141	0.27101	0.49699	0.64863	0.69106
15.00	0.22676	0.29867	0.51796	0.63599	0.67380
16.00	0.25699	0.32924	0.52403	0.62519	0.65856
17.00	0.29137	0.36139	0.52823	0.61584	0.64517
18.00	0.32875	0.39424	0.53173	0.60775	0.63344
19.00	0.36804	0.42890	0.53517	0.60081	0.62321
20.00	0.40866	0.46198	0.53881	0.59493	0.61435
21.00	0.44981	0.48175	0.54243	0.59000	0.60672
22.00	0.47389	0.49720	0.54585	0.58591	0.60020
23.00	0.49172	0.50961	0.54894	0.58254	0.59468
24.00	0.50526	0.51943	0.55160	0.57983	0.59014
25.00	0.51215	0.52453	0.55304	0.57841	0.58774

TEMPERATURE ON CATALYST SURFACE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	766.25	761.78	742.66	609.51	414.89
1.00	916.33	910.41	789.77	564.56	323.80
2.00	965.39	938.15	817.13	537.39	315.59
3.00	1017.04	981.69	830.47	521.80	314.06
4.00	1046.43	1005.37	833.99	512.98	313.41
5.00	1059.89	1014.73	830.30	507.79	313.06
6.00	1062.08	1013.85	821.10	504.27	312.82
7.00	1056.18	1005.57	807.61	501.24	312.62
8.00	1044.35	991.77	790.75	498.00	312.42
9.00	1028.02	973.69	771.25	494.18	312.19
10.00	1008.10	952.15	749.74	489.63	311.91
11.00	985.18	927.66	726.77	484.28	311.58
12.00	959.53	900.53	702.72	478.18	311.21
13.00	931.27	870.98	677.79	471.38	310.79
14.00	900.37	839.05	651.22	463.90	310.32
15.00	866.73	804.88	622.58	455.80	309.83
16.00	830.57	769.32	601.31	447.44	309.30
17.00	792.42	733.21	581.66	439.08	308.78
18.00	752.98	697.10	563.05	430.83	308.27
19.00	712.92	660.56	545.17	422.77	307.76
20.00	672.66	625.30	527.88	414.90	307.26
21.00	632.98	597.10	511.34	407.26	306.78
22.00	602.30	572.06	495.69	399.92	306.32
23.00	575.95	549.63	481.05	392.92	305.88
24.00	553.48	530.07	467.88	386.53	305.48
25.00	541.22	519.29	460.52	382.93	305.25

NORMALIZED CONCENTRATION AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE	0.0	0.5	1.0	1.5	2.0
DISTANCE FROM ENTRANCE					
0.0	0.00000	0.00000	0.00000	0.83788	0.99819
1.00	0.00000	0.00000	0.00000	0.96264	0.99132
2.00	0.00000	0.00000	0.00000	0.94761	0.97901
3.00	0.00000	0.00000	0.00000	0.92107	0.96160
4.00	0.00000	0.00000	0.00000	0.89098	0.94000
5.00	0.00000	0.00000	0.00000	0.85991	0.91532
6.00	0.00000	0.00000	0.00000	0.82918	0.88868
7.00	0.00000	0.00000	0.00000	0.79959	0.86106
8.00	0.00000	0.00000	0.00000	0.77166	0.83329
9.00	0.00000	0.00000	0.00001	0.74568	0.80603
10.00	0.00000	0.00000	0.00003	0.72182	0.77980
11.00	0.00000	0.00000	0.00017	0.70018	0.75496
12.00	0.00000	0.00000	0.00096	0.68075	0.73179
13.00	0.00000	0.00000	0.00545	0.66353	0.71047
14.00	0.00000	0.00000	0.04462	0.64862	0.69113
15.00	0.00000	0.00001	0.45140	0.63602	0.67388
16.00	0.00000	0.00010	0.49661	0.62523	0.65864
17.00	0.00004	0.00085	0.51541	0.61590	0.64525
18.00	0.00037	0.00641	0.52554	0.60782	0.63352
19.00	0.00327	0.06898	0.53219	0.60088	0.62330
20.00	0.03212	0.40001	0.53740	0.59501	0.61443
21.00	0.36555	0.46079	0.54180	0.59009	0.60680
22.00	0.44877	0.48897	0.54559	0.58600	0.60028
23.00	0.48225	0.50620	0.54886	0.58262	0.59476
24.00	0.50129	0.51794	0.55159	0.57991	0.59023
25.00	0.50975	0.52362	0.55306	0.57849	0.58783

TEMPERATURE AT CATALYST CENTRE

DISTANCE FROM CENTER-LINE / DISTANCE FROM ENTRANCE	0.0	0.5	1.0	1.5	2.0
0.0	1024.18	1022.26	1013.62	663.65	414.88
1.00	1074.80	1070.44	1023.16	569.20	323.79
2.00	1095.95	1082.05	1023.53	538.80	315.58
3.00	1115.00	1095.25	1018.00	522.47	314.04
4.00	1124.11	1099.63	1008.55	513.39	313.39
5.00	1125.04	1096.96	996.32	508.09	313.03
6.00	1119.63	1088.90	981.97	504.51	312.80
7.00	1109.43	1076.81	965.97	501.43	312.61
8.00	1095.65	1061.70	948.66	498.16	312.40
9.00	1079.18	1044.29	930.33	494.29	312.17
10.00	1060.66	1025.14	911.20	489.71	311.89
11.00	1040.54	1004.59	891.48	484.33	311.56
12.00	1019.11	982.91	871.16	478.19	311.19
13.00	996.58	960.28	849.26	471.38	310.77
14.00	973.04	936.82	814.45	463.89	310.30
15.00	948.54	912.63	646.58	455.78	309.81
16.00	923.27	888.07	611.18	447.42	309.28
17.00	897.52	863.31	586.26	439.05	308.76
18.00	871.47	837.04	565.27	430.81	308.25
19.00	844.54	790.43	546.22	422.74	307.74
20.00	808.53	647.64	528.36	414.87	307.24
21.00	663.36	604.64	511.54	407.24	306.76
22.00	611.34	575.01	495.77	399.89	306.30
23.00	579.34	550.85	481.06	392.89	305.86
24.00	554.90	530.59	467.88	386.51	305.46
25.00	542.07	519.59	460.50	382.91	305.23

D-3

PROGRAM FOR INTERNAL RESISTANCE MODEL

SOURCE LISTING

```
C          ***** DEFINITION OF INPUT VARIABLES *****
C
C
C     NPI       FIRST TRANSIENT ITERATION TO BE PRINTED
C
C     NPO       THIS MANY ITERATIONS TO BE SKIPPED BETWEEN
C               EACH TRANSIENT PRINTOUT
C
C     NICO      LAST TRANSIENT ITERATION TO BE PRINTED
C
C     NI        CURRENT ITERATION NUMBER
C
C     KM        FLAG  (=0 IF NO INTERMEDIATE RESULTS ARE AVAIL-
C                     ABLE ON TAPE , =1 OTHERWISE)
C
C     NO        NUMBER OF COPIES OF RESULTS REQUIRED
C
C     TIME      TIME LEVEL AT END OF PREVIOUS TRANSIENT COMP-
C               UTATIONS
C
C     RRDIFF    RADIAL DIFFUSION COEFFICIENT
C
C     RADIFF    AXIAL DIFFUSION COEFFICIENT
C
C     RRCOND    RADIAL CONDUCTIVITY COEFFICIENT
C
C     RACOND    AXIAL CONDUCTIVITY COEFFICIENT
C
C     RHTCP     FLUID HEAT CAPACITY
C
C     RDEN      FLUID DENSITY
C
C     RPOR      REACTOR VOID FRACTION
C
C     RO        REACTOR RADIUS
C
C     SO        REACTOR LENGTH
C
C     TW        COOLING FLUID TEMPERATURE
C
C     BVEL      BULK FLUID LINEAR VELOCITY
C
C     SAPUV     SURFACE AREA OF CATALYST PER UNIT VOLUME
C
C     SMTC      MASS TRANSFER COEFFICIENT ACROSS CATALYST SUR-
C               FACE
C
C     SHTC      HEAT TRANSFER COEFFICIENT ACROSS CATALYST SUR-
C               FACE
C
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C     CDIFF    DIFFUSION COEFFICIENT WITHIN CATALYST
C
C     CCOND    THERMAL CONDUCTIVITY OF CATALYST
C
C     CHTCP    CATALYST HEAT CAPACITY
C
C     CDEN     CATALYST DENSITY
C
C     CPOR     CATALYST POROSITY
C
C     RC       CATALYST RADIUS
C
C     CO       INLET CONCENTRATION
C
C     TO       INLET TEMPERATURE
C
C     DC       STEP CHANGE IN INLET CONCENTRATION
C
C     DT       STEP CHANGE IN INLET TEMPERATURE
C
C     DELH     HEAT OF REACTION
C
C     WHTC     HEAT TRANSFER COEFFICIENT AT REACTOR WALL
C
C     EC       RELATIVE ERROR IN CONCENTRATION BETWEEN (N+1)
C              'TH AND N'TH ITERATIONS AT ASSUMED STEADY
C              -STATE
C
C     ET       ABSOLUTE ERROR IN TEMPERATURE BETWEEN (N+1)
C              'TH AND N'TH ITERATIONS AT ASSUMED STEADY
C              -STATE
C
C     ES       RELATIVE ERROR IN CONCENTRATION BETWEEN SUC-
C              CEEDING ITERATIONS AT NEWWTON-RAPHSON CONVER-
C              GENCE
C
C     EX       ABSOLUTE ERROR IN TEMPERATURE BETWEEN SUC-
C              CEEDING ITERATIONS AT NEWTON-RAPHSON CONVER-
C              GENCE
C
C     TM1      REACTOR TIME STEP FOR FIRST 100 ITERATIONS
C
C     TM2      REACTOR TIME STEP FOR SECOND 100 ITERATIONS
C
C     TM3      REACTOR TIME STEP FOR THIRD 100 ITERATIONS
C
C     TM4      REACTOR TIME STEP FOR ALL ITERATIONS AFTER 300
C
C     RAT1     RATIO OF CATALYST TIME STEP TO REACTOR TIME
C              STEP FOR FIRST 100 ITERATIONS
```

```
C
C       RAT2        RATIO OF CATALYST TIME STEP TO REACTOR TIME
C                   STEP FOR SECOND 100 ITERATIONS
C
C       RAT3        RATIO OF CATALYST TIME STEP TO REACTOR TIME
C                   STEP FOR THIRD 100 ITERATIONS
C
C       RAT4        RATIO OF CATALYST TIME STEP TO REACTOR TIME
C                   STEP FOR ALL ITERATIONS AFTER 300
C
C       M           NO. OF RADIAL GRID POINTS -1
C
C       N           NO. OF AXIAL GRID POINTS -1
C
C       L           NO. OF CATALYST GRID POINTS
C
C       RRE(I)      STATEMENT OF REACTION RATE EXPRESSION  (NOT
C                   MORE THAN 72 CHARACTERS)
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```
C      ***** PROGRAM FOR INTERNAL RESISTANCE MODEL *****
C
C                    ***** MAINLINE PROGRAM *****
C
C      THIS MAINLINE IS CONCERNED PRIMARILY WITH THE SUPER-
C      VISION OF THE DECISIONS REQUIRED AT VARIOUS STAGES IN
C      THE COMPUTATIONS
C
       COMMON T(260,25),C(260,25),X(25),S(25),XN(25),SN(25),
      1TS(260),CS(260),CONC(260),TEMP(260),CZNC(260),TZMP(260)
      2,TZ(260),CZ(260),R(25),RR(10),C1(260),C2(260),C3(260),
      3C4(260),C5(260),C6(260),C7(260),C8(260),C9(260),
      4T1(260),T2(260),T3(260),T4(260),T5(260),T6(260),
      5T7(260),T8(260),T9(260),A1(25),A2(25),A3(25),A4(25),
      6A5(25),A6(25),U1(25),U2(25),U3(25),U4(25),U5(25),U6(25)
      7,CCC(260),TCC(260),RL(100),CNORM(260),CSNORM(260),
      8CCNORM(260),CU(25)
       COMMON XS,SS,XSP,SSP,RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,
      1RDEN,RPOR,SAPUV,BVEL,SO,RO,TW,RTHETA,SMTC,SHTC,CDIFF,
      2CCOND,CDEN,CPOR,CHTCP,RC,DELH,WHTC,EC,ET,ES,EX,CO,TO,DR
      3,DX,CTHETA,WASP,DC,DT,ALPHA,BETA,GAMMA,ZETA,PHI,SIGMA,
      4SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,ST3,ST4,ST5,ST6,TIME,
      5STS,TM1,TM2,TM3,TM4,RAT1,RAT2,RAT3,RAT4
       COMMON L,M,N,MN,MP,NP,LL,IN,NI,NC,JG,LR,NPI,NPO,NICO,KM
      1,NO
       DIMENSION QP(10)
       IN=0
       CALL INIT
       CON=CO
   70  CALL COEFF
C
C      CALCULATION OF THE REACTOR CROSS SECTIONAL AREA REP-
C      RESENTED BY EACH RADIAL GRID
C
       QP(1)=3.14159*(DR/2.)**2.
       DO 613 I=2,M
       QP(I)=3.14159*((RR(I)+DR/2.)**2.-(RR(I)-DR/2.)**2.)
  613  CONTINUE
       QP(MP)=3.14159*(RO**2.-(RO-DR/2.)**2.)
       KFSS=0
       NPT=NPI
       JG=1
   10  CONTINUE
C
C      CHANGES TO PROGRAM VARIABLES REQUIRED IF CATALYST TIME
C      STEP IS CHANGED AT ITERATION NUMBER 100 , 200 OR 300
C
       IF (NI.EQ.100) GO TO 813
       IF (NI.EQ.200) GO TO 814
       IF (NI.EQ.300) GO TO 815
```

```
      GO TO 17
  813 RTHETA=TM2
      STS=RAT2
      CTHETA=STS*RTHETA
      CALL COEFF
      CALL CACOEF
      WASP=RTHETA*(STS+1.5)
      GO TO 17
  814 RTHETA=TM3
      STS=RAT3
      CTHETA=STS*RTHETA
      CALL COEFF
      CALL CACOEF
      WASP=RTHETA*(STS+1.5)
      GO TO 17
  815 RTHETA=TM4
      STS=RAT4
      CTHETA=STS*RTHETA
      CALL COEFF
      CALL CACOEF
      WASP=RTHETA*(STS+1.5)
   17 CALL RETI
      JG=JG*(-1)
      TIME=TIME+RTHETA
      NI=NI+1
      IF (WASP.LT.RTHETA) GO TO 116
      GO TO 20
  116 CONTINUE
C
C     COMPARE SOLUTION AT (N+1)'TH ITERATION WITH SOLUTION
C     AT N'TH ITERATION
C
      DO 40 I=1,MN
      IF (ABS((CZNC(I)-CONC(I))/CZNC(I)).GT.EC) GO TO 20
      IF (ABS(TZMP(I)-TEMP(I)).GT.ET) GO TO 20
      IF (ABS((CS(I)-CZ(I))/CS(I)).GT.EC) GO TO 20
      IF (ABS(TS(I)-TZ(I)).GT.ET) GO TO 20
   40 CONTINUE
      KFSS=1
      GO TO 9
   20 DO 50 I=1,MN
      CZ(I)=CS(I)
      TZ(I)=TS(I)
      CCC(I)=C(I,L)
      TCC(I)=T(I,L)
      CONC(I)=CZNC(I)
   50 TEMP(I)=TZMP(I)
      DO 211 I=1,MN
      CNORM(I)=CONC(I)/CON
      CSNORM(I)=CS(I)/CON
```

```
      CCNORM(I)=C(I,L)/CON
      IF (CCNORM(I).GT.0.) GO TO 211
      CCNORM(I)=0.
  211 CONTINUE
      WASP=WASP+RTHETA
      IF (NI.NE.NPT) GO TO 10
      NPT=NPT+NPO
    9 CONTINUE
      DO 11 JW=1,NO
      IF (KFSS.NE.1) GO TO 61
      IF (IN.EQ.0) GO TO 18
      GO TO 19
C
C     PRINT OUT INTERMEDIATE RESULTS
C
   61 WRITE (6,235) NI,TIME
  235 FORMAT (1H1////' ',18X,'ITERATION NO.',I6,5X,'TIME = '
     1,F10.4,' SEC.'/'-',26X,'NORMALIZED CONCENTRATION PROF'
     2,'ILE')
      GO TO 21
C
C     PRINT OUT INITIAL STEADY STATE CONDITIONS
C
   18 WRITE (6,240) DC,DT
  240 FORMAT (1H1////' ',18X                          /'0',12X,'IN'
     1,'ITIAL STEADY STATE CONDITIONS PRECEDING STEP CHANGE'
     2,'S OF'/'0',12X,F10.7,5X,'GM-MOLES/C.C. IN INLET CONC'
     3,'ENTRATION'/'0',12X, F8.2,7X,'DEGREES KELVIN  IN INL'
     4,'ET TEMPERATURE'/'-',18X,'NORMALIZED CONCENTRATION P'
     5,'ROFILE')
      GO TO 21
C
C     PRINT OUT FINAL STEADY STATE CONDITIONS
C
   19 WRITE (6,245) NI,TIME
  245 FORMAT (1H1////' ',18X,'ITERATION NO.',I6,5X,'TIME = '
     1,F10.4,' SEC.'/'0',12X,'FINAL STEADY STATE CONDITIONS'
     2/'-',26X,'NORMALIZED CONCENTRATION PROFILE')
   21 CONTINUE
C
C     CALCULATE BULK CONCENTRATION AND TEMPERATURE AT REACTOR
C     EXIT
C
      LMN=MN-MP
      BCE=0.
      BTE=0.
      DO 614 I=1,MP
      NML=I+LMN
      BCE=BCE+QP(I)*CONC(NML)
      BTE=BTE+QP(I)*TEMP(NML)
```

```
 614 CONTINUE
     BCE=BCE/((3.14159*(RO**2.))*CON)
     BTE=BTE/(3.14159*(RO**2.))
     WRITE (6,200) (RR(I),I=1,MP)
 200 FORMAT ('-',12X,'DISTANCE FROM',5(F6.1,4X)/' ',12X,'C'
    1,'ENTER-LINE'/'0',12X,'DISTANCE FROM'/' ',12X,'ENTRAN'
    2,'CE'/' ',12X)
     K=1
     KK=MP
     DO 250 I=1,NP,2
     WRITE (6,204) RL(I),(CNORM(J),J=K,KK)
 204 FORMAT (' ', 9X,F10.2,3X,5F10.5)
     K=K+2*MP
     KK=KK+2*MP
 250 CONTINUE
     WRITE (6,615) BCE
 615 FORMAT ('-',12X,'BULK CONCENTRATION AT REACTOR EXIT = '
    1,F10.6)
     WRITE (6,230)
 230 FORMAT (1H1////' ',26X,'          TEMPERATURE PROFILE')
     WRITE (6,200) (RR(I),I=1,MP)
     K=1
     KK=MP
     DO 705 I=1,NP,2
     WRITE (6,207) RL(I),(TEMP(J),J=K,KK)
 207 FORMAT (' ',9X,F10.2,5X,5(F8.2,2X))
     K=K+2*MP
     KK=KK+2*MP
 705 CONTINUE
     WRITE (6,616) BTE
 616 FORMAT ('-',12X,'BULK TEMPERATURE AT REACTOR EXIT = ',
    1F10.2)
     WRITE (6,714)
 714 FORMAT (1H1////' ',20X,'NORMALIZED CONCENTRATION ON C'
    1,'ATALYST SURFACE')
     WRITE (6,200) (RR(I),I=1,MP)
     K=1
     KK=MP
     DO 715 I=1,NP,2
     WRITE (6,204) RL(I),(CSNORM(J),J=K,KK)
     K=K+2*MP
     KK=KK+2*MP
 715 CONTINUE
     WRITE (6,724)
 724 FORMAT (1H1////' ',28X,'TEMPERATURE ON CATALYST SURFA'
    1,'CE')
     WRITE (6,200) (RR(I),I=1,MP)
     K=1
     KK=MP
     DO 725 I=1,NP,2
```

```
      WRITE (6,207) RL(I),(TS(J),J=K,KK)
      K=K+2*MP
      KK=KK+2*MP
  725 CONTINUE
      WRITE (6,734)
  734 FORMAT (1H1////' ',20X,'NORMALIZED CONCENTRATION AT C'
     1,'ATALYST CENTRE')
      WRITE (6,200) (RR(I),I=1,MP)
      K=1
      KK=MP
      DO 735 I=1,NP,2
      WRITE (6,204) RL(I),(CCNORM(J),J=K,KK)
      K=K+2*MP
      KK=KK+2*MP
  735 CONTINUE
      WRITE (6,744)
  744 FORMAT (1H1////' ',28X,'TEMPERATURE AT CATALYST CENTR'
     1,'E')
      WRITE (6,200) (RR(I),I=1,MP)
      K=1
      KK=MP
      DO 745 I=1,NP,2
      WRITE (6,207) RL(I),(TCC(J),J=K,KK)
      K=K+2*MP
      KK=KK+2*MP
  745 CONTINUE
      WRITE (6,44)
   44 FORMAT (1H1////' ',15X,'INTERNAL PROFILE OF CATALYST '
     1,'IN CENTRE OF REACTOR'/'-',12X,2X,'RADIUS',5X,'NORMA'
     2,'LIZED CONCENTRATION',5X,'TEMPERATURE'/'-',10X)
      WRITE (6,55) RC,CSNORM(126),TS(126)
   55 FORMAT (' ',12X,F8.3,11X,F10.5,15X,F8.2)
      DO 29 I=1,L
      CU(I)=C(126,I)/CON
      IF (CU(I).GE.0.) GO TO 29
      CU(I)=0.
   29 WRITE (6,55) R(I),CU(I),T(126,I)
   11 CONTINUE
      IF (KFSS.EQ.1) GO TO 30
      IF (NI.NE.NICO) GO TO 555
  765 CONTINUE
C
C     STORE INTERMEDIATE RESULTS ON TAPE 2
C
      REWIND 2
      WRITE (2) C,T,CS,TS,CONC,TEMP,STS,RTHETA,CTHETA,WASP,IN
      ENDFILE 2
      BACKSPACE 2
      REWIND 2
      STOP
```

```
  555 CONTINUE
      GO TO 10
   30 IF (IN.EQ.1) GO TO 60
C
C     AN INITIAL STEADY STATE CONDITION HAS BEEN FOUND.
C     THE FOLLOWING PROGRAM VARIABLES ARE NOW DEFINED PREPAR-
C     ATORY TO BEGINNING THE TRANSIENT COMPUTATIONS.
C
      IN=1
      RTHETA=TM1
      STS=RAT1
      CTHETA=STS*RTHETA
      WASP=RTHETA*(STS+1.5)
      GO TO 765
   60 CONTINUE
      STOP
      END
```

```
C                ***** SUBROUTINE INIT *****
C
      SUBROUTINE INIT
C
C     THIS SUBROUTINE SERVES THE FOLLOWING PURPOSES.
C     1) READS IN THE SYSTEM PARAMETERS
C     2) WRITES OUT THESE PARAMETERS
C     3) INITIALIZES THE DEPENDENT VARIABLES
C     4) READS IN PREVIOUS INTERMEDIATE RESULTS FROM A TAPE
C        IF REQUIRED
C     5) IMPLEMENTS THE STEP CHANGE IN THE INLET CONDITIONS
C
      COMMON T(260,25),C(260,25),X(25),S(25),XN(25),SN(25),
     1TS(260),CS(260),CONC(260),TEMP(260),CZNC(260),TZMP(260)
     2,TZ(260),CZ(260),R(25),RR(10),C1(260),C2(260),C3(260),
     3C4(260),C5(260),C6(260),C7(260),C8(260),C9(260),
     4T1(260),T2(260),T3(260),T4(260),T5(260),T6(260),
     5T7(260),T8(260),T9(260),A1(25),A2(25),A3(25),A4(25),
     6A5(25),A6(25),U1(25),U2(25),U3(25),U4(25),U5(25),U6(25)
     7,CCC(260),TCC(260),RL(100),CNORM(260),CSNORM(260),
     8CCNORM(260),CU(25)
      COMMON XS,SS,XSP,SSP,RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,
     1RDEN,RPOR,SAPUV,BVEL,SO,RO,TW,RTHETA,SMTC,SHTC,CDIFF,
     2CCOND,CDEN,CPOR,CHTCP,RC,DELH,WHTC,EC,ET,ES,EX,CO,TO,DR
     3,DX,CTHETA,WASP,DC,DT,ALPHA,BETA,GAMMA,ZETA,PHI,SIGMA,
     4SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,ST3,ST4,ST5,ST6,TIME,
     5STS,TM1,TM2,TM3,TM4,RAT1,RAT2,RAT3,RAT4
      COMMON L,M,N,MN,MP,NP,LL,IN,NI,NC,JG,LR,NPI,NPO,NICO,KM
     1,NO
      DIMENSION RRE(20)
C
C     READ IN THE INPUT PARAMETERS
C
      READ (5,44) NPI,NPO,NICO,NI,KM,NO,TIME
   44 FORMAT (1X,6I6,F12.6)
      READ (5,10) RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,RDEN,
     1RPOR,RO,SO,TW,BVEL,SAPUV,SMTC,SHTC,CDIFF,CCOND,CHTCP,
     2CDEN,CPOR,RC,CO,TO,DC,DT,DELH,WHTC,EC,ET,ES,EX,TM1,TM2,
     3TM3,TM4,RAT1,RAT2,RAT3,RAT4
   10 FORMAT (1X,4E16.8)
      READ (5,50) M,N,L
   50 FORMAT (1X,3I6)
      READ (5,901) (RRE(I),I=1,20)
  901 FORMAT (20A4)
      MP=M+1
      NP=N+1
      MN=MP*NP
C
C     WRITE OUT THE REACTOR PARAMETERS
C
```

```
      WRITE (6,900) SO,RO,RRDIFF,RADIFF,RHTCP,RDEN,RPOR,TW
      WRITE (6,905) BVEL,CO,TO,SAPUV
      WRITE (6,910) SMTC,SHTC,WHTC,RC,CDIFF,CCOND,CHTCP,CDEN
      WRITE (6,915) CPOR,DELH,MP,NP
      WRITE (6,902) (RRE(I),I=1,20)
  900 FORMAT (1H1////' ',12X,'PHYSICAL,THERMODYNAMIC AND KI'
     1,'NETIC DATA'/'-',12X,'ALL UNITS ARE IN CM.,SEC.,CAL.'
     2,',GM.-MOLES,DEGREES KELVIN'/'-',12X,'REACTOR LENGTH',
     326X,F16.6/'0',12X,'REACTOR RADIUS',26X,F16.6/'0',12X,
     4'RADIAL DIFFUSION COEFFICIENT',12X,F16.6/'0',12X,'AXI'
     5,'AL DIFFUSION COEFFICIENT',13X,F16.6/'0',12X,'FLUID '
     6,'HEAT CAPACITY',21X,F16.6/'0',12X,'FLUID DENSITY',27X
     7,F16.6/'0',12X,'REACTOR VOID FRACTION',19X,F16.6/'0',
     812X,'COOLING FLUID TEMPERATURE',15X,F16.6)
  905 FORMAT ('0',12X,'BULK FLUID LINEAR VELOCITY',14X,
     1F16.6/'0',12X,'INLET REACTANT CONCENTRATION',12X,F16.6
     2/'0',12X,'INLET FLUID TEMPERATURE',17X,F16.6/'0',12X,
     3'CATALYST SURFACE AREA PER UNIT VOLUME',3X,F16.6)
  910 FORMAT ('0',12X,'MASS TRANSFER COEFF AT CATALYST SURF'
     1,'ACE',1X,F16.6/'0',12X,'HEAT TRANSFER COEFF AT CATAL'
     2,'YST SURFACE',1X,F16.6/'0',12X,'HEAT TRANSFER COEFF '
     3,'AT REACTOR WALL',5X,F16.6/'0',12X,'CATALYST PARTICL'
     4,'E RADIUS',16X,F16.6/'0',12X,'DIFFUSION COEFF IN CAT'
     5,'ALYST',13X,F16.6/'0',12X,'CATALYST THERMAL CONDUCTI'
     6,'VITY',11X,F16.6/'0',12X,'CATALYST HEAT CAPACITY',18X
     7,F16.6/'0',12X,'CATALYST DENSITY',24X,F16.6)
  915 FORMAT ('0',12X,'CATALYST VOID FRACTION',18X,F16.6/'0'
     1,12X,'HEAT OF REACTION',24X,F16.6/'0',12X,'NO. OF RAD'
     2,'IAL POINTS',21X,I8/'0',12X,'NO. OF AXIAL POINTS',
     322X,I8)
  902 FORMAT ('0',12X,'RATE OF REACTION = ',20A4)
      IF (KM.EQ.1) GO TO 545
C
C     INITIALIZE THE INDEPENDENT VARIABLES TO THE INLET CON-
C     DITIONS
C
      RTHETA=TM1
      STS=RAT1
      CTHETA=STS*RTHETA
      WASP=RTHETA*(STS+1.5)
      DO 33 I=1,300
      CZ(I)=0.
      TZ(I)=0.
      CZNC(I)=0.
      CCC(I)=0.
      TCC(I)=0.
      TZMP(I)=0.
      TEMP(I)=0.
   33 CONC(I)=0.
      DO 30 I=1,MN
```

```
      CZ(I)=CO
      TZ(I)=TO
      CONC(I)=CO
      TEMP(I)=TO
      CS(I)=CO
      TS(I)=TO
      CCC(I)=CO
      TCC(I)=TO
      DO 40 J=1,L
      C(I,J)=CO
   40 T(I,J)=TO
   30 CONTINUE
      CALL SSCAT
      RETURN
  545 CONTINUE
C
C     READ IN THE PREVIOUS INTERMEDIATE RESULTS
C
      REWIND 1
      READ (1) C,T,CS,TS,CONC,TEMP,STS,RTHETA,CTHETA,WASP,IN
      REWIND 1
      IF (IN.EQ.0) GO TO 666
C
C     APPLY THE STEP CHANGE TO INLET CONDITIONS
C
      CO=CO+DC
      TO=TO+DT
  666 CONTINUE
      CALL CACOEF
      RETURN
      END
```

```
C                ***** SUBROUTINE COEFF *****
C
      SUBROUTINE COEFF
C
C     THIS SUBROUTINE CALCULATES THE COEFFICIENTS OF THE EQ-
C     UATIONS DESCRIBING HEAT AND MASS TRANSFER IN THE EX-
C     TERNAL FIELD OF THE REACTOR
C
      COMMON T(260,25),C(260,25),X(25),S(25),XN(25),SN(25),
     1TS(260),CS(260),CONC(260),TEMP(260),CZNC(260),TZMP(260)
     2,TZ(260),CZ(260),R(25),RR(10),C1(260),C2(260),C3(260),
     3C4(260),C5(260),C6(260),C7(260),C8(260),C9(260),
     4T1(260),T2(260),T3(260),T4(260),T5(260),T6(260),
     5T7(260),T8(260),T9(260),A1(25),A2(25),A3(25),A4(25),
     6A5(25),A6(25),U1(25),U2(25),U3(25),U4(25),U5(25),U6(25)
     7,CCC(260),TCC(260),RL(100),CNORM(260),CSNORM(260),
     8CCNORM(260),CU(25)
      COMMON XS,SS,XSP,SSP,RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,
     1RDEN,RPOR,SAPUV,BVEL,SO,RO,TW,RTHETA,SMTC,SHTC,CDIFF,
     2CCOND,CDEN,CPOR,CHTCP,RC,DELH,WHTC,EC,ET,ES,EX,CO,TO,DR
     3,DX,CTHETA,WASP,DC,DT,ALPHA,BETA,GAMMA,ZETA,PHI,SIGMA,
     4SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,ST3,ST4,ST5,ST6,TIME,
     5STS,TM1,TM2,TM3,TM4,RAT1,RAT2,RAT3,RAT4
      COMMON L,M,N,MN,MP,NP,LL,IN,NI,NC,JG,LR,NPI,NPO,NICO,KM
     1,NO
      DR=RO/M
      DX=SO/N
      RL(1)=0.
      DO 707 I=2,NP
      RL(I)=RL(I-1)+DX
  707 CONTINUE
      RR(1)=0.
      DO 7 I=2,MP
    7 RR(I)=RR(I-1)+DR
      DO 100 I=1,MN
      LR=I+1-(((I-1)/(M+1))*(M+1)+1)
      IF (I.EQ.1) GO TO 10
      IF (I.EQ.MP) GO TO 20
      IF (I.LT.MP) GO TO 30
      IF (I.EQ.MN) GO TO 40
      IF (I.EQ.(MN-M)) GO TO 50
      IF (I.GT.(MN-M)) GO TO 60
      IF (LR.EQ.1) GO TO 70
      IF (LR.EQ.MP) GO TO 80
      SA=3.14159*((RR(LR)+DR/2.)**2-(RR(LR)-DR/2.)**2)*RPOR
      AO=2.*3.14159*DX*(RR(LR)+DR/2.)*RPOR
      AI=2.*3.14159*DX*(RR(LR)-DR/2.)*RPOR
      CDEP=SA*DX*SAPUV*SMTC/(2.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
```

```
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(2.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=0.
      GO TO 100
   10 AO=RPOR*3.14159*DR*DX/2.
      SA=3.14159*RPOR*(DR**2)/4.
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=0.
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)-CDEP-BVEL*SA
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=BVEL*SA*CO
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
      T1(I)=0.
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)-TDEP-BVEL*SA*RHTCP*RDEN
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=BVEL*SA*RHTCP*RDEN*TO
      GO TO 100
   30 AI=RPOR*3.14159*(RR(LR)-DR/2.)*DX
      AO=RPOR*3.14159*(RR(LR)+DR/2.)*DX
      SA=RPOR*3.14159*((RR(LR)+DR/2.)**2-(RR(LR)-DR/2.)**2)
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=0.
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP-BVEL*SA
      C5(I)=RRDIFF*AO/DR
```

```
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=BVEL*SA*CO
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
      T1(I)=0.
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP-BVEL*SA*RHTCP*RDEN
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=BVEL*SA*RHTCP*RDEN*TO
      GO TO 100
   20 SA=RPOR*3.14159*(RO**2-(RO-DR/2.)**2)
      AO=RPOR*3.14159*DX*RO
      AI=RPOR*3.14159*DX*(RO-DR/2.)
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=0.
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP-BVEL*SA
      C5(I)=0.
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=BVEL*SA*CO
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
      T1(I)=0.
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP-BVEL*SA*RHTCP*RDEN
      T5(I)=0.
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP-AO*WHTC
      T7(I)=TDEP
      T8(I)=BVEL*SA*RHTCP*RDEN*TO    +AO*WHTC*TW
      GO TO 100
   70 SA=RPOR*3.14159*(DR**2)/4.
      AO=RPOR*3.14159*DR*DX
      CDEP=SA*DX*SAPUV*SMTC/(2.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=RRDIFF*AO/DR
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
```

```
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(2.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=RRCOND*AO/DR
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=0.
      GO TO 100
   80 SA=RPOR*3.14159*(RO*DR-(DR**2)/4.)
      AO=RPOR*2.*3.14159*DX*RO
      AI=RPOR*2.*3.14159*(RO-DR/2.)*DX
      CDEP=SA*DX*SAPUV*SMTC/(2.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=0.
      C6(I)=RADIFF*SA/DX
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(2.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=0.
      T6(I)=RACOND*SA/DX
      T4(I)=-T5(I)-T6(I)-TDEP-AO*WHTC
      T7(I)=TDEP
      T8(I)=AO*WHTC*TW
      GO TO 100
   50 SA=RPOR*3.14159*(DR**2)/4.
      AO=RPOR*3.14159*DR*DX/2.
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=0.
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=RRDIFF*AO/DR
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
```

```
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=0.
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=RRCOND*AO/DR
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=0.
      GO TO 100
   60 SA=RPOR*3.14159*((RR(LR)+DR/2.)**2-(RR(LR)-DR/2.)**2)
      AO=RPOR*3.14159*DX*(RR(LR)+DR/2.)
      AI=RPOR*3.14159*DX*(RR(LR)-DR/2.)
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=RRDIFF*AO/DR
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=RRCOND*AO/DR
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)-TDEP
      T7(I)=TDEP
      T8(I)=0.
      GO TO 100
   40 SA=RPOR*3.14159*(RO*DR-(DR**2)/4.)
      AO=RPOR*3.14159*DX*RO
      AI=RPOR*3.14159*DX*(RO-DR/2.)
      CDEP=SA*DX*SAPUV*SMTC/(4.*RPOR)
      C9(I)=SA*DX/RTHETA
      C1(I)=RADIFF*SA/DX+BVEL*SA
      C2(I)=RRDIFF*AI/DR
      C3(I)=-C1(I)-C2(I)-CDEP
      C5(I)=0.
      C6(I)=0.
      C4(I)=-C5(I)-C6(I)-CDEP
      C7(I)=CDEP
      C8(I)=0.
      TDEP=SA*DX*SAPUV*SHTC/(4.*RPOR)
      T9(I)=SA*DX*RHTCP*RDEN/RTHETA
      T1(I)=RACOND*SA/DX+BVEL*SA*RHTCP*RDEN
      T2(I)=RRCOND*AI/DR
```

```
      T3(I)=-T1(I)-T2(I)-TDEP
      T5(I)=0.
      T6(I)=0.
      T4(I)=-T5(I)-T6(I)-TDEP-AO*WHTC
      T7(I)=TDEP
      T8(I)=AO*WHTC*TW
  100 CONTINUE
      RETURN
      END
```

```
C                ***** SUBROUTINE SSCAT *****
C
      SUBROUTINE SSCAT
C
C     THIS SUBROUTINE CALCULATES THE STEADY-STATE CONCENTRA-
C     TION AND TEMPERATURE PROFILES WITHIN A CATALYST PARTI-
C     CLE UNDER CONSTANT BOUNDARY CONDITIONS OF CO AND TO .
C     THESE PROFILES THEN SERVE AS A CONVENIENT INITIAL GUESS
C     FOR THE CATALYST PARTICLES IN THE REACTOR . IT ALSO
C     CALCULATES THE COEFFICIENTS OF THE EQUATIONS DESCRIBING
C     HEAT AND MASS TRANSFER ACROSS THE CATALYST SURFACE
C
      COMMON T(260,25),C(260,25),X(25),S(25),XN(25),SN(25),
     1TS(260),CS(260),CONC(260),TEMP(260),CZNC(260),TZMP(260)
     2,TZ(260),CZ(260),R(25),RR(10),C1(260),C2(260),C3(260),
     3C4(260),C5(260),C6(260),C7(260),C8(260),C9(260),
     4T1(260),T2(260),T3(260),T4(260),T5(260),T6(260),
     5T7(260),T8(260),T9(260),A1(25),A2(25),A3(25),A4(25),
     6A5(25),A6(25),U1(25),U2(25),U3(25),U4(25),U5(25),U6(25)
     7,CCC(260),TCC(260),RL(100),CNORM(260),CSNORM(260),
     8CCNORM(260),CU(25)
      COMMON XS,SS,XSP,SSP,RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,
     1RDEN,RPOR,SAPUV,BVEL,SO,RO,TW,RTHETA,SMTC,SHTC,CDIFF,
     2CCOND,CDEN,CPOR,CHTCP,RC,DELH,WHTC,EC,ET,ES,EX,CO,TO,DR
     3,DX,CTHETA,WASP,DC,DT,ALPHA,BETA,GAMMA,ZETA,PHI,SIGMA,
     4SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,ST3,ST4,ST5,ST6,TIME,
     5STS,TM1,TM2,TM3,TM4,RAT1,RAT2,RAT3,RAT4
      COMMON L,M,N,MN,MP,NP,LL,IN,NI,NC,JG,LR,NPI,NPO,NICO,KM
     1,NO
      DIMENSION SA1(35),SA2(35),SA3(35),SA4(35),SA5(35),SU1(
     135),SU2(35),SU3(35),SU4(35),SU5(35)
C
C     THE FOLLOWING STATEMENTS DEFINE THE RATE OF REACTION
C     EXPRESSION AND ITS DERIVATIVE WITH RESPECT TO CONCEN-
C     TRATION
C
      F(Q,Z)=(1.0E+07)*EXP(-12000./Z)*Q
      FD(Q,Z,W)=(1.0E+07)*(EXP(-12000./Z))*(1.+Q*12000./(Z**
     12)*W)
      CALL CACOEF
      OM=1.75
      DO 321 I=1,L
      SA1(I)=A1(I)
      SU1(I)=U1(I)
      SA4(I)=A4(I)
      SU4(I)=U4(I)
      SA5(I)=A5(I)
      SU5(I)=U5(I)
      SA2(I)=-(A1(I)+A4(I))/OM
      SU2(I)=-(U1(I)+U4(I))/OM
```

```
      SA3(I)=-(A1(I)+A4(I))*(OM-1.)/OM
      SU3(I)=-(U1(I)+U4(I))*(OM-1.)/OM
  321 CONTINUE
      ZC1=SC1
      ZT1=ST1
      ZC4=SC4
      ZT4=ST4
      ZC5=SC5
      ZT5=ST5
      ZC2=-(SC1+SC4)/OM
      ZT2=-(ST1+ST4)/OM
      ZC3=-(SC1+SC4)*(OM-1.)/OM
      ZT3=-(ST1+ST4)*(OM-1.)/OM
      NC=1
      SS=CS(NC)
      XS=TS(NC)
      SSN=SS
C
C     NEWTON RAPHSON ITERATION FOR EACH EQUATION AT SURFACE
C     GRID POINT
C
   17 FUN=ZC1*CONC(NC)+ZC2*SS+ZC3*CS(NC)+ZC4*C(NC,1)+ZC5*F(
     1SS,XS)
      DER=-ZC2-ZC5*FD(SS,XS,((ZT5/ZC5)*(ZC2/ZT2)))
      SS=SS+FUN/DER
      XS=-(ZT1*TEMP(NC)+ZT3*TS(NC)+ZT4*T(NC,1)-(ZT5/ZC5)*(ZC1
     1 *CONC(NC)+ZC2*SS+ZC3*CS(NC)+ZC4*C(NC,1)))/ZT2
      IF (ABS((SS-SSN)/SS).GT.ES) GO TO 16
      GO TO 13
   16 SSN=SS
      GO TO 17
   13 DO 10 I=1,L
      IF (I.EQ.1) GO TO 404
      IF (NI.GT.0) GO TO 404
      S(I)=S(I-1)
      X(I)=X(I-1)
      SN(I)=S(I)
      GO TO 110
  404 S(I)=C(NC,I)
      X(I)=T(NC,I)
      SN(I)=S(I)
C
C     NEWTON RAPHSON ITERATION FOR EQUATIONS AT INTERIOR GRID
C     POINTS OF CATALYST
C
  110 IF (I.EQ.1) GO TO 20
      IF (I.EQ.L) GO TO 30
      FUN=SA1(I)*S(I-1)+SA2(I)*S(I)+SA3(I)*C(NC,I)+SA4(I)*C(
     1NC,I+1)+SA5(I)*F(S(I),X(I))
      GO TO 40
```

```
   20 FUN=SA1(I)*SS     +SA2(I)*S(I)+SA3(I)*C(NC,I)+SA4(I)*C(
     1NC,2)+SA5(I)*F(S(I),X(I))
      GO TO 40
   30 FUN=SA1(L)*S(LL)+SA2(L)*S(L)+SA3(L)*C(NC,L)+SA5(L)*F(S
     1(L),X(L))
   40 DER=-SA2(I)-SA5(I)*FD(S(I),X(I),((SU5(I)/SA5(I))*(SA2(
     1 I)/SU2(I))))
      S(I)=S(I)+FUN/DER
      IF (I.EQ.1) GO TO 60
      IF (I.EQ.L) GO TO 70
      X(I)=-(SU1(I)*X(I-1)+SU3(I)*T(NC,I)+SU4(I)*T(NC,I+1)-(
     1SU5(I)/SA5(I))*(SA1(I)*S(I-1)+SA2(I)*S(I)+SA3(I)*C(NC,
     2I)+SA4(I)*C(NC,I+1)))/SU2(I)
      GO TO 80
   60 X(1)=-(SU1(1)*XS     +SU3(1)*T(NC,1)+SU4(I)*T(NC,2)-(
     1SU5(I)/SA5(I))*(SA1(1)*SS+SA2(1)*S(1)+SA3(1)*C(NC,1)+
     2SA4(1)*C(NC,2)))/SU2(1)
      GO TO 80
   70 X(L)=-(SU1(L)*X(LL)+SU3(L)*T(NC,L)-(SU5(L)/SA5(L))*(
     1SA1(L)*S(LL)+SA2(L)*S(L)+SA3(L)*C(NC,L)))/SU2(L)
   80 CONTINUE
      IF (ABS((S(I)-SN(I))/S(I)).GT.ES) GO TO 90
      GO TO 10
   90 SN(I)=S(I)
      GO TO 110
   10 CONTINUE
      DO 21 I=1,L
      IF (ABS((S(I)-C(NC,I))/S(I)).GT.ES) GO TO 31
      IF (ABS(X(I)-T(NC,I)).GT.EX) GO TO 31
   21 CONTINUE
      GO TO 51
   31 DO 41 I=1,L
      C(NC,I)=S(I)
      T(NC,I)=X(I)
   41 CONTINUE
      CS(NC)=SS
      TS(NC)=XS
      GO TO 17
   51 CONTINUE
C
C     INITIALIZATION OF PROFILES WITHIN THE CATALYST PARTI-
C     CLES IN THE REACTOR AT THE STEADY-STATE VALUES CALCUL-
C     ATED ABOVE
C
      DO 61 I=1,MN
      DO 71 J=1,L
      C(I,J)=S(J)
   71 T(I,J)=X(J)
      CS(I)=SS
      TS(I)=XS
```

```
61 CONTINUE
   RETURN
   END
```

```
C                ***** SUBROUTINE RETI *****
C
      SUBROUTINE RETI
C
C     THIS SUBROUTINE CALCULATES THE EXTERNAL FIELD CONCEN-
C     TRATIONS AND TEMPERATURES AT EACH REACTOR GRID POINT
C     IN TERMS OF THE CONCENTRATION AND TEMPERATURE ON THE
C     SURFACE OF THE CATALYST AT THESE GRID POINTS
C
      COMMON T(260,25),C(260,25),X(25),S(25),XN(25),SN(25),
     1TS(260),CS(260),CONC(260),TEMP(260),CZNC(260),TZMP(260)
     2,TZ(260),CZ(260),R(25),RR(10),C1(260),C2(260),C3(260),
     3C4(260),C5(260),C6(260),C7(260),C8(260),C9(260),
     4T1(260),T2(260),T3(260),T4(260),T5(260),T6(260),
     5T7(260),T8(260),T9(260),A1(25),A2(25),A3(25),A4(25),
     6A5(25),A6(25),U1(25),U2(25),U3(25),U4(25),U5(25),U6(25)
     7,CCC(260),TCC(260),RL(100),CNORM(260),CSNORM(260),
     8CCNORM(260),CU(25)
      COMMON XS,SS,XSP,SSP,RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,
     1RDEN,RPOR,SAPUV,BVEL,SO,RO,TW,RTHETA,SMTC,SHTC,CDIFF,
     2CCOND,CDEN,CPOR,CHTCP,RC,DELH,WHTC,EC,ET,ES,EX,CO,TO,DR
     3,DX,CTHETA,WASP,DC,DT,ALPHA,BETA,GAMMA,ZETA,PHI,SIGMA,
     4SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,ST3,ST4,ST5,ST6,TIME,
     5STS,TM1,TM2,TM3,TM4,RAT1,RAT2,RAT3,RAT4
      COMMON L,M,N,MN,MP,NP,LL,IN,NI,NC,JG,LR,NPI,NPO,NICO,KM
     1,NO
      IF (JG.EQ.(-1)) GO TO 300
C
C     FORWARD SWEEP OF THE ADEP
C
      DO 100 I=1,MN
      NC=I
      IMMP=I-MP
      IPMP=I+MP
      LR=I+1-(((I-1)/(M+1))*(M+1)+1)
      SS=CS(I)
      XS=TS(I)
   28 IF (I.EQ.1) GO TO 10
      IF (I.LE.MP) GO TO 20
      ALPHA=C4(I)*CONC(I)+C5(I)*CONC(I+1)+C6(I)*CONC(IPMP)+C
     17(I)*CS(I)+C8(I)+C2(I)*CZNC(I-1)+C1(I)*CZNC(IMMP)+C9(
     2I)*CONC(I)
      BETA=T4(I)*TEMP(I)+T5(I)*TEMP(I+1)+T6(I)*TEMP(IPMP)+T7
     1(I)*TS(I)+T8(I)+T2(I)*TZMP(I-1)+T1(I)*TZMP(IMMP)+T9(I)
     2*TEMP(I)
      CALL SURF
      GO TO 38
   10 ALPHA=C4(I)*CONC(I)+C5(I)*CONC(I+1)+C6(I)*CONC(IPMP)+C
     17(I)*CS(I)+C8(I)+C9(I)*CONC(I)
      BETA=T4(I)*TEMP(I)+T5(I)*TEMP(I+1)+T6(I)*TEMP(IPMP)+T7
```

```
     1(I)*TS(I)+T8(I)+T9(I)*TEMP(I)
      CALL SURF
      GO TO 38
   20 ALPHA=C4(I)*CONC(I)+C5(I)*CONC(I+1)+C6(I)*CONC(IPMP)+C
     17(I)*CS(I)+C8(I)+C2(I)*CZNC(I-1)+C9(I)*CONC(I)
      BETA=T4(I)*TEMP(I)+T5(I)*TEMP(I+1)+T6(I)*TEMP(IPMP)+T7
     1(I)*TS(I)+T8(I)+T2(I)*TZMP(I-1)+T9(I)*TEMP(I)
      CALL SURF
   38 CZNC(I)=(-ALPHA-C7(I)*SS)/(C3(I)-C9(I))
      TZMP(I)=(-BETA-T7(I)*XS)/(T3(I)-T9(I))
   18 CS(NC)=SS
      TS(NC)=XS
      IF (WASP.LT.(2.*CTHETA)) GO TO 211
      CALL CATPRO
      IF (I.NE.MN) GO TO 211
      WASP=0.5*RTHETA
  211 CONTINUE
  100 CONTINUE
      RETURN
  300 CONTINUE
C
C     REVERSE SWEEP OF THE ADEP
C
      DO 200 K=1,MN
      I=MN+1-K
      NC=I
      IF (WASP.GT.(2.*RTHETA)) GO TO 311
      CALL CATPRO
  311 CONTINUE
      CALL SURF
      IMMP=I-MP
      IPMP=I+MP
      IF (I.EQ.1) GO TO 110
      IF (I.LE.MP) GO TO 120
      CZNC(I)=-(C1(I)*CONC(IMMP)+C2(I)*CONC(I-1)+C3(I)*CONC(
     1I)+C5(I)*CZNC(I+1)+C6(I)*CZNC(IPMP)+C7(I)*(CS(I)+SS)+
     2C8(I)+C9(I)*CONC(I))/(C4(I)-C9(I))
      TZMP(I)=-(T1(I)*TEMP(IMMP)+T2(I)*TEMP(I-1)+T3(I)*TEMP(
     1I)+T5(I)*TZMP(I+1)+T6(I)*TZMP(IPMP)+T7(I)*(TS(I)+XS)+
     2T8(I)+T9(I)*TEMP(I))/(T4(I)-T9(I))
      GO TO 138
  110 CZNC(I)=-(C3(I)*CONC(I)+C5(I)*CZNC(I+1)+C6(I)*CZNC(IPM
     1P)+C7(I)*(CS(I)+SS)+C8(I)+C9(I)*CONC(I))/(C4(I)-C9(I))
      TZMP(I)=-(T3(I)*TEMP(I)+T5(I)*TZMP(I+1)+T6(I)*TZMP(IPM
     1P)+T7(I)*(TS(I)+XS)+T8(I)+T9(I)*TEMP(I))/(T4(I)-T9(I))
      GO TO 138
  120 CZNC(I)=-(C2(I)*CONC(I-1)+C3(I)*CONC(I)+C5(I)*CZNC(I+1
     1)+C6(I)*CZNC(IPMP)+C7(I)*(CS(I)+SS)+C8(I)+C9(I)*CONC(
     2I))/(C4(I)-C9(I))
      TZMP(I)=-(T2(I)*TEMP(I-1)+T3(I)*TEMP(I)+T5(I)*TZMP(I+1
```

```
     1)+T6(I)*TZMP(IPMP)+T7(I)*(TS(I)+XS)+T8(I)+T9(I)*TEMP(I
     2))/(T4(I)-T9(I))
138  CONTINUE
     CS(NC)=SS
     TS(NC)=XS
200  CONTINUE
     RETURN
     END
```

```
C                ***** SUBROUTINE SURF *****
C
      SUBROUTINE SURF
C
C     THIS SUBROUTINE CALCULATES THE CONCENTRATION AND TEMP-
C     ERATURE ON THE SURFACE OF THE CATALYST AT EACH GRID
C     POINT IN THE REACTOR AT EVERY ITERATION OR TIME STEP
C
      COMMON T(260,25),C(260,25),X(25),S(25),XN(25),SN(25),
     1TS(260),CS(260),CONC(260),TEMP(260),CZNC(260),TZMP(260)
     2,TZ(260),CZ(260),R(25),RR(10),C1(260),C2(260),C3(260),
     3C4(260),C5(260),C6(260),C7(260),C8(260),C9(260),
     4T1(260),T2(260),T3(260),T4(260),T5(260),T6(260),
     5T7(260),T8(260),T9(260),A1(25),A2(25),A3(25),A4(25),
     6A5(25),A6(25),U1(25),U2(25),U3(25),U4(25),U5(25),U6(25)
     7,CCC(260),TCC(260),RL(100),CNORM(260),CSNORM(260),
     8CCNORM(260),CU(25)
      COMMON XS,SS,XSP,SSP,RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,
     1RDEN,RPOR,SAPUV,BVEL,SO,RO,TW,RTHETA,SMTC,SHTC,CDIFF,
     2CCOND,CDEN,CPOR,CHTCP,RC,DELH,WHTC,EC,ET,ES,EX,CO,TO,DR
     3,DX,CTHETA,WASP,DC,DT,ALPHA,BETA,GAMMA,ZETA,PHI,SIGMA,
     4SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,ST3,ST4,ST5,ST6,TIME,
     5STS,TM1,TM2,TM3,TM4,RAT1,RAT2,RAT3,RAT4
      COMMON L,M,N,MN,MP,NP,LL,IN,NI,NC,JG,LR,NPI,NPO,NICO,KM
     1,NO
C
C     THE FOLLOWING STATEMENTS DEFINE THE RATE OF REACTION
C     EXPRESSION AND ITS DERIVATIVE WITH RESPECT TO CONCEN-
C     TRATION
C
      F(Q,Z)=(1.0E+07)*EXP(-12000./Z)*Q
      FD(Q,Z,W)=(1.0E+07)*(EXP(-12000./Z))*(1.+Q*12000./(Z**
     12)*W)
      IF (JG.EQ.(-1)) GO TO 300
C
C     FORWARD SWEEP OF THE ADEP
C
      PHI=-SC1*C7(NC)/(C3(NC)-C9(NC))+SC2-SC6
      GAMMA=-SC1*ALPHA/(C3(NC)-C9(NC))+((SC3+SC6)*CS(NC)+SC4
     1*C(NC,1))
      ZETA=-ST1*T7(NC)/(T3(NC)-T9(NC))+ST2-ST6
      SIGMA=-ST1*BETA/(T3(NC)-T9(NC))+((ST3+ST6)*TS(NC)+ST4*
     1T(NC,1))
C
C     NEWTON RAPHSON ITERATION
C
   15 FUN=PHI*SS+GAMMA+SC5*F(SS,XS)
      DER=-PHI-SC5*FD(SS,XS,((ST5/SC5)*(PHI/ZETA)))
   29 CONTINUE
      SSP=SS
```

```
      XSP=XS
      SS=SSP+FUN/DER
      XS=(-SIGMA+(ST5/SC5)*(PHI*SS+GAMMA))/ZETA
      IF (ABS(XS-XSP).GT.EX) GO TO 15
      IF (ABS((SS-SSP)/SS).GT.ES) GO TO 15
   19 RETURN
  300 CONTINUE
C
C     REVERSE SWEEP OF THE ADEP
C
      SUM=SC1*CONC(NC)+(SC2+SC6)*CS(NC)+SC4*C(NC,1)
      TUM=ST1*TEMP(NC)+(ST2+ST6)*TS(NC)+ST4*T(NC,1)
      DUM=(ST5/SC5)*((SC3-SC6)/(ST3-ST6))
      SS=CS(NC)
      XS=TS(NC)
C
C     NEWTON RAPHSON ITERATION
C
  315 FUN=SUM+(SC3-SC6)*SS+SC5*F(SS,XS)
      DER=-SC3+SC6-SC5*FD(SS,XS,DUM)
      XSP=XS
      SSP=SS
      SS=SSP+FUN/DER
      XS=-(TUM-(ST5/SC5)*(SUM+(SC3-SC6)*SS))/(ST3-ST6)
      IF (ABS((SS-SSP)/SS).GT.ES) GO TO 315
      IF (ABS(XS-XSP).GT.EX) GO TO 315
  567 CONTINUE
      RETURN
      END
```

```
C                ***** SUBROUTINE CATPRO *****
C
      SUBROUTINE CATPRO
C
C     THIS SUBROUTINE CALCULATES THE CONCENTRATION AND TEMP-
C     ERATURE PROFILES WITHIN THE CATALYST AT EACH GRID
C     POINT IN THE REACTOR AT EVERY ITERATION OR TIME STEP
C
      COMMON T(260,25),C(260,25),X(25),S(25),XN(25),SN(25),
     1TS(260),CS(260),CONC(260),TEMP(260),CZNC(260),TZMP(260)
     2,TZ(260),CZ(260),R(25),RR(10),C1(260),C2(260),C3(260),
     3C4(260),C5(260),C6(260),C7(260),C8(260),C9(260),
     4T1(260),T2(260),T3(260),T4(260),T5(260),T6(260),
     5T7(260),T8(260),T9(260),A1(25),A2(25),A3(25),A4(25),
     6A5(25),A6(25),U1(25),U2(25),U3(25),U4(25),U5(25),U6(25)
     7,CCC(260),TCC(260),RL(100),CNORM(260),CSNORM(260),
     8CCNORM(260),CU(25)
      COMMON XS,SS,XSP,SSP,RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,
     1RDEN,RPOR,SAPUV,BVEL,SO,RO,TW,RTHETA,SMTC,SHTC,CDIFF,
     2CCOND,CDEN,CPOR,CHTCP,RC,DELH,WHTC,EC,ET,ES,EX,CO,TO,DR
     3,DX,CTHETA,WASP,DC,DT,ALPHA,BETA,GAMMA,ZETA,PHI,SIGMA,
     4SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,ST3,ST4,ST5,ST6,TIME,
     5STS,TM1,TM2,TM3,TM4,RAT1,RAT2,RAT3,RAT4
      COMMON L,M,N,MN,MP,NP,LL,IN,NI,NC,JG,LR,NPI,NPO,NICO,KM
     1,NO
C
C     THE FOLLOWING STATEMENTS DEFINE THE RATE OF REACTION
C     EXPRESSION AND ITS DERIVATIVE WITH RESPECT TO CONCEN-
C     TRATION
C
      F(Q,Z)=(1.0E+07)*EXP(-12000./Z)*Q
      FD(Q,Z,W)=(1.0E+07)*(EXP(-12000./Z))*(1.+Q*12000./(Z**
     12)*W)
      IF (JG.EQ.(-1)) GO TO 300
C
C     FORWARD SWEEP OF THE ADEP
C
      SUM   =A1(1)*CS(NC)+(A3(1)+A6(1))*C(NC,1)+A4(1)*C(NC,2)
      TUM   =U1(1)*TS(NC)+(U3(1)+U6(1))*T(NC,1)+U4(1)*T(NC,2)
      DUM=(U5(1)/A5(1))*((A2(1)-A6(1))/(U2(1)-U6(1)))
   13 DO 10 I=1,L
      S(I)=0.
      X(I)=T(NC,I)
      SN(I)=S(I)
C
C     NEWTON RAPHSON ITERATION
C
  110 FUN=SUM   +(A2(I)-A6(I))*S(I)+A5(I)*F(S(I),X(I))
   40 DER=-A2(I)+A6(I)-A5(I)*FD(S(I),X(I),DUM)
      S(I)=S(I)+FUN/DER
```

```
      X(I)=-(TUM-(U5(I)/A5(I))*(SUM+(A2(I)-A6(I))*S(I)))/(U2
     1(I)-U6(I))
      IF (ABS((S(I)-SN(I))/S(I)).GT.ES) GO TO 90
      IF (I.EQ.LL) GO TO 16
      IF (I.EQ.L) GO TO 10
      K=I+1
      SUM   =A1(K)*S(K-1)+(A3(K)+A6(K))*C(NC,K)+A4(K)*C(NC,
     1K+1)
      TUM   =U1(K)*X(K-1)+(U3(K)+U6(K))*T(NC,K)+U4(K)*T(NC,
     1K+1)
      DUM=(U5(K)/A5(K))*((A2(K)-A6(K))/(U2(K)-U6(K)))
      GO TO 10
   16 SUM   =A1(L)*S(LL)+(A3(L)+A6(L))*C(NC,L)
      TUM   =U1(L)*X(LL)+(U3(L)+U6(L))*T(NC,L)
      DUM=(U5(L)/A5(L))*((A2(L)-A6(L))/(U2(L)-U6(L)))
      GO TO 10
   90 SN(I)=S(I)
      GO TO 110
   10 CONTINUE
      DO 373 I=1,L
      C(NC,I)=S(I)
  373 T(NC,I)=X(I)
      RETURN
C
C     REVERSE SWEEP OF THE ADEP
C
  300 CONTINUE
      SUM   =A1(L)*C(NC,LL)+(A2(L)+A6(L))*C(NC,L)
      TUM   =U1(L)*T(NC,LL)+(U2(L)+U6(L))*T(NC,L)
      DUM=(U5(L)/A5(L))*((A3(L)-A6(L))/(U3(L)-U6(L)))
      DO 310 K=1,L
      IF (K.NE.L) GO TO 600
      I=L+1-K
      S(I)=0.
      X(I)=T(NC,I)
      SN(I)=S(I)
      GO TO 311
  600 CONTINUE
      I=L+1-K
      S(I)=0.
      X(I)=T(NC,I)
      SN(I)=S(I)
C
C     NEWTON RAPHSON ITERATION
C
  311 FUN=SUM   +(A3(I)-A6(I))*S(I)+A5(I)*F(S(I),X(I))
  340 DER=-A3(I)+A6(I)-A5(I)*FD(S(I),X(I),DUM)
      S(I)=S(I)+FUN/DER
      X(I)=-(TUM   -(U5(I)/A5(I))*(SUM   +(A3(I)-A6(I))*S(I)
     1))/(U3(I)-U6(I))
```

```
380 CONTINUE
    IF (ABS((S(I)-SN(I))/S(I)).GT.ES) GO TO 390
    IF (K.EQ.LL) GO TO 316
    IF (K.EQ.L) GO TO 310
    J=I-1
    SUM   =A1(J)*C(NC,J-1)+(A2(J)+A6(J))*C(NC,J)+A4(J)*S(J
   1+1)
    TUM   =U1(J)*T(NC,J-1)+(U2(J)+U6(J))*T(NC,J)+U4(J)*X(J
   1+1)
    DUM=(U5(J)/A5(J))*((A3(J)-A6(J))/(U3(J)-U6(J)))
    GO TO 310
316 SUM   =A1(1)*CS(NC)+(A2(1)+A6(1))*C(NC,1)+A4(1)*S(2)
    TUM   =U1(1)*TS(NC)+(U2(1)+U6(1))*T(NC,1)+U4(1)*X(2)
    DUM=(U5(1)/A5(1))*((A3(1)-A6(1))/(U3(1)-U6(1)))
    GO TO 310
390 SN(I)=S(I)
    GO TO 311
310 CONTINUE
    DO 302 I=1,L
    C(NC,I)=S(I)
    T(NC,I)=X(I)
302 CONTINUE
    RETURN
    END
```

```
C                ***** SUBROUTINE CACOEF *****
C
      SUBROUTINE CACOEF
C
C     THIS SUBROUTINE CALCULATES THE COEFFICIENTS OF THE EQ-
C     UATIONS DESCRIBING HEAT AND MASS TRANSFER WITHIN THE
C     CATALYST PARTICLES
C
      COMMON T(260,25),C(260,25),X(25),S(25),XN(25),SN(25),
     1TS(260),CS(260),CONC(260),TEMP(260),CZNC(260),TZMP(260)
     2,TZ(260),CZ(260),R(25),RR(10),C1(260),C2(260),C3(260),
     3C4(260),C5(260),C6(260),C7(260),C8(260),C9(260),
     4T1(260),T2(260),T3(260),T4(260),T5(260),T6(260),
     5T7(260),T8(260),T9(260),A1(25),A2(25),A3(25),A4(25),
     6A5(25),A6(25),U1(25),U2(25),U3(25),U4(25),U5(25),U6(25)
     7,CCC(260),TCC(260),RL(100),CNORM(260),CSNORM(260),
     8CCNORM(260),CU(25)
      COMMON XS,SS,XSP,SSP,RRDIFF,RADIFF,RRCOND,RACOND,RHTCP,
     1RDEN,RPOR,SAPUV,BVEL,SO,RO,TW,RTHETA,SMTC,SHTC,CDIFF,
     2CCOND,CDEN,CPOR,CHTCP,RC,DELH,WHTC,EC,ET,ES,EX,CO,TO,DR
     3,DX,CTHETA,WASP,DC,DT,ALPHA,BETA,GAMMA,ZETA,PHI,SIGMA,
     4SC1,SC2,SC3,SC4,SC5,SC6,ST1,ST2,ST3,ST4,ST5,ST6,TIME,
     5STS,TM1,TM2,TM3,TM4,RAT1,RAT2,RAT3,RAT4
      COMMON L,M,N,MN,MP,NP,LL,IN,NI,NC,JG,LR,NPI,NPO,NICO,KM
     1,NO
      SL=L
      LL=L-1
      R(L)=0.
      DO 60 I=1,LL
      RP=I
      R(I)=((SL-RP)/SL)**(1./3.)*RC
   60 CONTINUE
      CCAP=((RC**3)/3.-((RC+R(1))**3)/24.)
      SC1=SMTC*RC**2
      SC2=-SC1
      SC4=(CDIFF/4.)*((RC+R(1))**2)/(RC-R(1))
      SC3=-SC4
      SC5=-CCAP
      SC6=CCAP*CPOR/RTHETA
      ST1=SHTC*RC**2
      ST2=-ST1
      ST4=(CCOND/4.)*((RC+R(1))**2)/(RC-R(1))
      ST3=-ST4
      ST5=-CCAP*DELH
      ST6=CCAP*CHTCP*CDEN/RTHETA
      A5(1)=-(1./24.)*((R(1)+RC)**3-(R(2)+R(1))**3)
      DO 30 I=2,LL
   30 A5(I)=-(1./24.)*(((R(I)+R(I-1))**3)-(R(I)+R(I+1))**3)
      A5(L)=-(1./24.)*(R(LL)**3)
      A1(1)=((CDIFF/4.)*(R(1)+RC)**2)/(RC-R(1))
```

```
      A4(1)=((CDIFF/4.)*(R(1)+R(2))**2)/(R(1)-R(2))
      A2(1)=-A1(1)
      A3(1)=-A4(1)
      A6(1)=-A5(1)*CPOR/CTHETA
      U1(1)=((CCOND/4.)*(R(1)+RC)**2)/(RC-R(1))
      U4(1)=((CCOND/4.)*(R(1)+R(2))**2)/(R(1)-R(2))
      U2(1)=-U1(1)
      U3(1)=-U4(1)
      U5(1)=A5(1)*DELH
      U6(1)=-A5(1)*CDEN*CHTCP/CTHETA
      DO 40 I=2,LL
      A1(I)=((CDIFF/4.)*(R(I)+R(I-1))**2)/(R(I-1)-R(I))
      A4(I)=((CDIFF/4.)*(R(I)+R(I+1))**2)/(R(I)-R(I+1))
      A2(I)=-A1(I)
      A3(I)=-A4(I)
      A6(I)=-A5(I)*CPOR/CTHETA
      U1(I)=((CCOND/4.)*(R(I)+R(I-1))**2)/(R(I-1)-R(I))
      U4(I)=((CCOND/4.)*(R(I)+R(I+1))**2)/(R(I)-R(I+1))
      U2(I)=-U1(I)
      U3(I)=-U4(I)
      U6(I)=-A5(I)*CDEN*CHTCP/CTHETA
   40 U5(I)=A5(I)*DELH
      A1(L)=(CDIFF/4.)*R(LL)
      A4(L)=0.
      A2(L)=-A1(L)
      A3(L)=0.
      A6(L)=-A5(L)*CPOR/CTHETA
      U1(L)=(CCOND/4.)*R(LL)
      U4(L)=0.
      U2(L)=-U1(L)
      U3(L)=0.
      U6(L)=-A5(L)*CDEN*CHTCP/CTHETA
      U5(L)=DELH*A5(L)
      RETURN
      END
```