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MASTER

PHYSICS OF REACTOR SAFETY

Quarterly Report

July—September 1980

OF MICROFILM
COVER

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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PHYSICS OF REACTOR SAFETY

Quarterly Report
July-September 1980

ABSTRACT

This Quarterly progress report summarizes work done during the months of July-September 1980 in Argonne National Laboratory's Applied Physics and Components Technology Divisions for the Division of Reactor Safety Research of the U.S. Nuclear Regulatory Commission. The work in the Applied Physics Division includes reports on reactor safety modeling and assessment by members of the Reactor Safety Appraisals Section. Work on reactor core thermal-hydraulics is performed in ANL's Components Technology Division, emphasizing 3-dimensional code development for LMFBR accidents under natural convection conditions. An executive summary is provided including a statement of the findings and recommendations of the report.

<u>FIN No.</u>	<u>Title</u>
A2015	Reactor Safety Modeling and Assessment
A2045	3-D Time-dependent Code Development

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EXECUTIVE SUMMARY

BIFLO has been significantly improved to achieve faster running times following the inception of boiling through the development and incorporation of a new implicit formulation of the two-phase thermohydrodynamics equations permitting the use of time step sizes an order of magnitude larger than were possible with the old explicit scheme. On the basis of one-dimensional calculations, this new methodology appears to have the potential to achieve the running speeds which we believe are required for whole-core accident analysis applications. BIFLO has also been improved to provide a better description of thermohydrodynamic motions in coarse mesh applications where the void fraction varies by large amounts between adjacent numerical grid cells.

An effort has been initiated to use pre-release versions of the COMMIX-2 computer code during its development process as a part of BIFLO benchmarking. Access to the code has been obtained; array dimensions have been adjusted and input data have been prepared for a 19-pin bundle geometry problem. Attempts to execute the code have uncovered several coding problems which are being resolved in close cooperation with the code developers in the Components Technology Division of ANL.

The computer programs used to produce plots of the data from the magnetic tape records of the 19-pin tests performed in the THORS Facility at Oak Ridge National Laboratory have undergone further modifications to aid in interpretation of the transient boiling tests.

In the development work of the COMMIX codes, all efforts this quarter were devoted to the two-phase COMMIX-2 code. The following two problems were analyzed using the homogeneous-equilibrium formulations incorporated in COMMIX-2.

- (i) German Seven Pin Hexagonal Fuel Assembly: This analysis considered flow rundown transient in a test section with seven electrically heated rods arranged in a hexagonal array.
- (ii) 31-Pin Fuel Assembly: This analysis considered the boiling test (Test 20, Run #104) with bundle 3C in the LMFBR THORS facility. The bundle has 31 electrically heated pins. The initial and final steady state conditions were predicted with COMMIX-2.

The results of COMMIX-2, for these two problems were compared with the experimental data and were found to be in good agreement. Simultaneously, efforts were also devoted to (i) developing the thermal structure model; (ii) incorporating symmetry boundary condition, pressure boundary condition, heat transfer model, wire wrap model, and alternative rebalancing scheme; (iii) cleaning up the code; and, (iv) preparing the user's manual.

In the area of BODYFIT code development, two major changes were implemented in the code. The semi-implicit time differencing scheme in the fuel pin model was changed to a fully-implicit scheme. This change permitted use of larger time step sizes. The second modification was the inclusion of a constant term in the pressure correction equations. This was done in such a way as to obtain an effective pressure correction with a large time step for steady state analysis. Considerable amounts of effort were devoted to cleaning up the code and making it more user oriented.

I. REACTOR SAFETY MODELING AND ASSESSMENT

(A2015)

A. BIFLO Development (J. J. Sienicki)

BIFLO has been significantly improved to generally achieve faster running times following the inception of boiling and to provide a better description of thermohydrodynamic motions in coarse mesh applications where the void fraction varies by large amounts between adjacent numerical grid cells. The faster running times have been obtained through the development and incorporation of a new implicit formulation of the two-phase thermohydrodynamics equations permitting the use of time step sizes an order of magnitude larger than were possible with the old explicit scheme. On the basis of one-dimensional calculations, this new methodology appears to have the potential to achieve the running speeds which we believe are required for whole-core accident analysis applications. As well as reducing running times, our methodology employs a new finite difference formulation of the two-phase momentum equations which better represents two-phase pressure drops in coarse mesh calculations. The single-phase portions of BIFLO have also been improved by replacing the previous calculation of single-phase pressures and velocities which assumed a radially uniform pressure field by one modeling radial single-phase pressure gradients and pressure driven radial single-phase flow. This provides a better description of the diversion of bypass flow around the two-phase voiding region. These improvements together with our early calculational experience with them are described below.

Previously, BIFLO calculated two-phase thermohydrodynamic motions following the inception of boiling with a numerical scheme in which the convection of mass, enthalpy and momentum was formulated explicitly. The use of such an explicit scheme entails the use of computational time steps satisfying a Courant stability restriction based upon the material velocities (i.e. $\frac{U \delta t}{\delta z} < 1$). In practice, for calculations involving high void fractions (e.g. $\alpha \gtrsim 0.9$), it was found to be necessary to employ time steps a factor of five or more smaller than the basic stability limit. Thus, the use of an explicit description of convection led to unacceptably long computational running times for the calculation of sodium boiling/voiding phenomena having a duration of the order of seconds. To remove the necessity of using such severely limited time step sizes and achieve faster running times, we have developed a new implicit formulation of the two-phase thermohydrodynamics equations which overcomes the Courant (explicit) stability restriction.

To illustrate the new methodology, we consider a one-dimensional example. In two-phase regions, BIFLO assumes that sodium liquid and vapor remain in thermodynamic equilibrium at saturation. Thus, the two-phase pressure P is assumed to be equal to the saturation vapor pressure which can be expressed as a function of a single thermodynamic variable such as the common liquid-vapor temperature T . Similarly, the thermodynamic densities and specific enthalpies for the liquid and vapor phases may be expressed as functions of a single thermodynamic variable such as T or P . We assume mass and enthalpy equations for the two-phase mixture given by

$$\frac{\partial}{\partial t}(\rho_l VF_l + \rho_v VF_v) + \frac{\partial}{\partial z}(\rho_l VF_l V_l + \rho_v VF_v V_v) = 0, \quad (1)$$

$$\frac{\partial}{\partial t}(\rho_l VF_l e_l + \rho_v VF_v e_v) + \frac{\partial}{\partial z}(\rho_l VF_l e_l V_l + \rho_v VF_v e_v V_v) = Q \quad (2)$$

where

t = time,

z = space coordinate,

l = denotes liquid,

v = denotes vapor,

ρ = thermodynamic density,

VF = volume fraction,

e = specific enthalpy,

V = velocity,

Q = source term accounting for heat transfer from fuel pins and the hexcan.

BIFLO solves distinct liquid and vapor momentum equations to model the effects of liquid-vapor slip. However, for the purposes of illustration, it is sufficient here to consider a case where no-slip homogeneous flow is assumed. We thus assume a single momentum equation for the two-phase mixture

$$\bar{\rho} \frac{\partial V}{\partial t} + \bar{\rho} V \frac{\partial V}{\partial z} + \frac{2F\bar{\rho}|V|V}{D} + \bar{\rho}g = -\frac{\partial P}{\partial z} \quad (3)$$

where

$\bar{\rho} = \rho_l VF_l + \rho_v VF_v$ = smeared density of two-phase mixture,

F = two-phase friction factor,

D = hydraulic diameter,

g = gravity,

P = pressure.

In formulating Eqs. 1-3 numerically, we assume a staggered mesh on which P , ρ , VF , e are defined at numerical grid cell centers and U is defined at cell edges. We difference the mass and enthalpy equations as

$$\begin{aligned} & \frac{(\rho_l VF_l + \rho_v VF_v)_j^{n+1} - (\rho_l VF_l + \rho_v VF_v)_j^n}{\delta t} \\ & + \frac{1}{\delta z_j} \left\{ \left[f_{j+1/2}^{n+1} (\rho_l VF_l + \rho_v VF_v)_j^{n+1} + \tilde{f}_{j+1/2}^{n+1} (\rho_l VF_l + \rho_v VF_v)_{j+1}^{n+1} \right] V_{j+1/2}^{n+1} \right. \\ & \left. - \left[f_{j-1/2}^{n+1} (\rho_l VF_l + \rho_v VF_v)_{j-1}^{n+1} + \tilde{f}_{j-1/2}^{n+1} (\rho_l VF_l + \rho_v VF_v)_j^{n+1} \right] V_{j-1/2}^{n+1} \right\} = 0, \quad (4) \end{aligned}$$

$$\begin{aligned}
& \frac{(\rho_L^{VF} e_L + \rho_V^{VF} e_V)_j^{n+1} - (\rho_L^{VF} e_L + \rho_V^{VF} e_V)_j^n}{\delta t} \\
& + \frac{1}{\delta z_j} \left\{ \left[f_{j+1/2}^{n+1} (\rho_L^{VF} e_L + \rho_V^{VF} e_V)_j^{n+1} + \tilde{f}_{j+1/2}^{n+1} (\rho_L^{VF} e_L + \rho_V^{VF} e_V)_{j+1}^{n+1} \right] v_{j+1/2}^{n+1} \right. \\
& \left. - \left[f_{j-1/2}^{n+1} (\rho_L^{VF} e_L + \rho_V^{VF} e_V)_{j-1}^{n+1} + \tilde{f}_{j-1/2}^{n+1} (\rho_L^{VF} e_L + \rho_V^{VF} e_V)_j^{n+1} \right] v_{j-1/2}^{n+1} \right\} \\
& = Q(T_j^{n+1}) \tag{5}
\end{aligned}$$

where

$n+1$ = denotes the end of the current time step,

n = denotes the beginning of the current time step,

j = denotes the center of cell j ,

$j-1/2$ = denotes the lower edge of cell j ,

$$f_{j-1/2} = \begin{cases} 1, & \text{if } v_{j-1/2} > 0 \\ 0, & \text{if } v_{j-1/2} < 0, \end{cases}$$

$$\tilde{f}_{j-1/2} = 1 - f_{j-1/2}.$$

The terms modeling mass and enthalpy convection in Eqs. 4-5 are formulated using a donor cell differencing prescription. Formulating the densities, volume fractions, enthalpies and velocities in these terms all implicitly at the end of the current time step overcomes the Courant stability restriction which would have been incurred had these terms been formulated explicitly (i.e. at the beginning of the time step). It should be noted that the heat transfer source term is assumed to be a function of the end of time step temperature. In sodium thermohydrodynamics calculations, such a functional dependence is dictated by a necessity to couple the fluid dynamics calculation implicitly to calculations of thermal conditions within the fuel pins and hexcan.

We difference the momentum equation as

$$\begin{aligned}
& \frac{1}{\delta t} \left[(\bar{\rho}_{j-1}^n \bar{X}_{j-1/2} Y_{j-1/2}^{n+1} + \bar{\rho}_j^n \tilde{X}_{j-1/2} \tilde{Y}_{j-1/2}^{n+1}) v_{j-1/2}^{n+1} \right. \\
& \left. - (\bar{\rho}_{j-1}^n \bar{X}_{j-1/2} Y_{j-1/2}^n + \bar{\rho}_j^n \tilde{X}_{j-1/2} \tilde{Y}_{j-1/2}^n) v_{j-1/2}^n \right] \\
& + f_{j-1/2}^{n+1} \left(\bar{\rho}_{j-1}^n \bar{X}_{j-1/2} Y_{j-1/2}^{n+1} + \bar{\rho}_j^n \tilde{X}_{j-1/2} \tilde{Y}_{j-1/2}^{n+1} \frac{\tilde{Y}_{j-1/2}^{n+1}}{Y_{j-1/2}^{n+1}} \right) v_{j-1/2}^{n+1}
\end{aligned}$$

$$\begin{aligned}
& \times \frac{1}{\delta z_{j-1}} (Y_{j-1/2}^{n+1} V_{j-1/2}^{n+1} - \tilde{Y}_{j-3/2}^{n+1} V_{j-3/2}^{n+1}) \\
& + \tilde{f}_{j-1/2}^{n+1} \left(\bar{\rho}_{j-1}^{n+1} X_{j-1/2} Y_{j-1/2}^{n+1} \frac{Y_{j-1/2}^{n+1}}{\tilde{Y}_{j-1/2}^{n+1}} + \bar{\rho}_j^{n+1} \tilde{X}_{j-1/2} \tilde{Y}_{j-1/2}^{n+1} \right) V_{j-1/2}^{n+1} \\
& \times \frac{1}{\delta z_j} (Y_{j+1/2}^{n+1} V_{j+1/2}^{n+1} - \tilde{Y}_{j-1/2}^{n+1} V_{j-1/2}^{n+1}) \\
& + \left(\frac{2F_{j-1}^{n+1} \bar{\rho}_{j-1}^{n+1} X_{j-1/2} Y_{j-1/2}^{n+1} Y_{j-1/2}^{n+1}}{D_{j-1}} + \frac{2F_j^{n+1} \bar{\rho}_j^{n+1} \tilde{X}_{j-1/2} \tilde{Y}_{j-1/2}^{n+1} \tilde{Y}_{j-1/2}^{n+1}}{D_j} \right) |V_{j-1/2}^{n+1}| V_{j-1/2}^{n+1} \\
& + (\bar{\rho}_{j-1}^{n+1} X_{j-1/2} + \bar{\rho}_j^{n+1} \tilde{X}_{j-1/2}) g \\
& = - \frac{P_j^{n+1} - P_{j-1}^{n+1}}{\delta z_{j-1/2}} \quad (6)
\end{aligned}$$

where

$$X_{j-1/2} = \frac{\delta z_{j-1}}{\delta z_{j-1} + \delta z_j},$$

$$\tilde{X}_{j-1/2} = 1 - X_{j-1/2},$$

$$\delta z_{j-1/2} = \frac{1}{2}(\delta z_{j-1} + \delta z_j).$$

Equation 6 has been formulated by considering the pressure drop between the centers of cells $j-1$ and j to be the sum of individual pressure drops within cells $j-1$ and j . The factor $X_{j-1/2}$ is just the portion of the distance between the centers of cell $j-1$ and cell j which lies in cell $j-1$. $Y_{j-1/2}$, $\tilde{Y}_{j-1/2}$ are "coarse mesh velocity scaling factors" having the following significance. In calculations, cells $j-1$ and j may develop very different void fractions. For example, cell $j-1$ might represent a two-phase mixture at near single-phase density while cell j models high void fraction annular flow conditions. If we model the total mass flux as being equal on both sides of cell edge $j-1/2$, then the velocities on the two sides of $j-1/2$ will be different. The scale factors $Y_{j-1/2}$, $\tilde{Y}_{j-1/2}$ are defined so that $Y_{j-1/2} V_{j-1/2}$ is the velocity between cell center $j-1$ and cell edge $j-1/2$ while $\tilde{Y}_{j-1/2} V_{j-1/2}$ is the velocity between cell edge $j-1/2$ and cell center j . We assume that the mass flux is the same on both sides of cell edge $j-1/2$ so that

$$\bar{\rho}_{j-1} Y_{j-1/2} V_{j-1/2} = \bar{\rho}_j \tilde{Y}_{j-1/2} V_{j-1/2}.$$

Considering two different velocities for each cell edge results in a better representation of the two-phase pressure drop in situations where the void fraction varies by large amounts between adjacent cells. This is a significant improvement in the formulation of the momentum equations on a staggered mesh and is far superior to other formulations which assume that a single velocity can be assumed between adjacent cell centers for all combinations of flow conditions within those two cells.

In implementing a two velocity scheme, one could bookkeep two velocities at each cell edge (i.e. define two distinct arrays). However, in carrying out the solution of Eqs. 4-6, it is desirable to reference only one of those velocities. We have chosen to work with only one velocity $V_{j-1/2}$ which we assume to be the velocity on the donor (i.e. upwind) side of the cell edge. This choice eliminates the need of introducing the scale factors into Eqs. 4-5. Thus, in our present example, the scale factors are given by

$$Y_{j-1/2} = f_{j-1/2} + \tilde{f}_{j-1/2} \frac{\bar{\rho}_j}{\bar{\rho}_{j-1}}, \quad (7)$$

$$\tilde{Y}_{j-1/2} = \tilde{f}_{j-1/2} + f_{j-1/2} \frac{\bar{\rho}_{j-1}}{\bar{\rho}_j}. \quad (8)$$

In our approach, it is necessary to test for sign changes in $V_{j-1/2}$ and whenever such a sign change occurs, rescale $V_{j-1/2}$ accordingly.

We note here in passing that in BIFLO, where slip flow is modeled with separate liquid and vapor momentum equations, scale factors are defined for both the liquid and vapor velocities and the generalization of Eqs. 7-8 is

$$Y_{l,j-1/2} = f_{l,j-1/2} + \tilde{f}_{l,j-1/2} R_{j-1/2},$$

$$Y_{v,j-1/2} = f_{v,j-1/2} + \tilde{f}_{v,j-1/2} R_{j-1/2},$$

$$\tilde{Y}_{l,j-1/2} = \tilde{f}_{l,j-1/2} + f_{l,j-1/2} \frac{1}{R_{j-1/2}},$$

$$\tilde{Y}_{v,j-1/2} = \tilde{f}_{v,j-1/2} + f_{v,j-1/2} \frac{1}{R_{j-1/2}},$$

where

$$R_{j-1/2} = \frac{(\rho_l V F_l)_j + (\rho_v V F_v)_j |\sigma|}{(\rho_l V F_l)_{j-1} + (\rho_v V F_v)_{j-1} |\sigma|},$$

$$\sigma = \frac{Y_{v,j-1/2} V_{v,j-1/2}}{Y_{l,j-1/2} V_{l,j-1/2}} = \text{slip ratio.}$$

In Eq. 6, the velocities at adjacent cell edges are formulated at the end of the current time step permitting a stable solution to be obtained with the use of time steps exceeding the Courant restriction.

We now consider the solution of Eqs. 4-6. At each cell center, we choose the independent variables to be the pressure P^{n+1} and the liquid volume fraction VF_ℓ^{n+1} . Recalling that P is the saturation vapor pressure, the variables ρ_ℓ^{n+1} , e_ℓ^{n+1} , ρ_v^{n+1} , e_v^{n+1} , T^{n+1} may be expressed as functions of P^{n+1} . The vapor volume fraction is eliminated via the equation

$$VF_v^{n+1} = 1 - VF_\ell^{n+1}.$$

For our one-dimensional example, we assume the existence of a single two-phase region bounded by columns of single-phase liquid above and below. For the two-phase portion of the overall calculation, we assume that the velocities at cell edges corresponding to the two-phase/single-phase interfaces may be treated as known boundary conditions. If N is the number of two-phase cells, then Eqs. 4-6 constitute a set of coupled nonlinear equations for N pressures, N volume fractions and $N-1$ velocities. We solve this system of equations with a Newton iteration. For our present example, the matrix of derivatives is a block tridiagonal matrix in which each block has dimension three. If separate liquid and vapor momentum equations to model slip flow had been assumed, then the dimension of each block would be four.

To assess the potential to achieve faster running times within BIFLO through the use of implicit methods, an implicit formulation of the two-phase thermohydrodynamics equations of the type described above (but modeling liquid-vapor slip) was programmed into BIFLO and applied to a one-dimensional (i.e. one channel) subassembly voiding problem. It was found that a significant reduction in running time following boiling inception (the preboiling portions of BIFLO were already highly implicit and very fast running) of a factor between five and eight could be obtained. For example, for the particular problem considered in which a real time interval of about two seconds was required to completely void the fission gas plenum following boiling initiation, the old explicit scheme using 0.1 ms time steps required more than twenty minutes of central processor time (on an IBM 3033). In contrast, for the implicit scheme with 1.0 ms time steps (corresponding to a factor of one to two times the Courant limit), the running time was less than four minutes. Further increases of the time step were hampered by the calculation of large changes in either the vapor velocity (e.g. > 10%) or temperature (several Kelvins) over the course of one time step or by a degradation of accuracy. On the basis of our one-dimensional calculations, the new implicit methodology which we have developed appears to have the potential to achieve the running speeds that we believe are required for whole-core accident applications (~ 1 min CPU/1 s real time) although further improvement and optimization are desirable.

In general, the application of an implicit numerical formulation such as we have described above must be made with care because it is possible to generate a derivative matrix which is ill conditioned (i.e. singular to working precision) or even exactly singular. For example, if one applies

Eqs. 4-5 to a problem where for all numerical cells, Q is zero, VF_v is zero, $U_l = U_v$ and T is spatially uniform, then Eqs. 4-5 are multiples of one another and the derivative matrix will be singular. In our calculations, we found that estimates of a condition number for the derivative matrix increase during the calculation from values of the order 10^5 to values of the order of 10^8 as more cells undergo voiding and convective effects tend to equilibrate temperatures within the two-phase region. However, for our calculations, which are performed with sixteen digit/double precision IBM hardware, poor conditioning has not been a problem and the Newton method usually converges in just a few iterations (e.g. two to five).

Originally, it was our intent to hold the derivative matrix constant during the Newton iteration thereby effecting a further reduction in computational running time. It was found that for low void fractions ($\alpha \leq 0.95$), the solution could be obtained in this manner. However, for higher void fractions, numerical difficulties which are probably a result of the particular heat transfer flow regime modeling assumed in BIFLO were encountered with this approach. For high void fractions ($\alpha > 0.95$), the current BIFLO modeling attempts to describe the dryout of a liquid sodium film. The heat transfer coefficient between cladding and coolant is thus decreased continuously from a large value appropriate for a thin liquid film to a much smaller value characteristic of a dispersed two-phase mixture. We have found that for void fractions close to the value assumed to demarcate the all dispersed regime, the iteration with the derivative matrix held constant sometimes converges very slowly, frequently failing to converge or diverging. When the derivative matrix is updated during each iteration step, the convergence behavior is very much improved and although slow convergence is still sometimes obtained, it is far less severe than in the previous case. It is therefore our current practice to update the derivative matrix during the Newton iteration.

Because our initial investigations into implicit methods have considered one-dimensional calculations, BIFLO currently assumes an implicit coupling between adjacent two-phase cells only in the axial direction. The radial transfer of mass, enthalpy and momentum between two-phase cells is still formulated explicitly. We shall attempt to perform two channel calculations with an explicit or semi-implicit radial coupling between two-phase cells as this degree of coupling may prove to be adequate for the case of only two channels and extending the current methodology to more than one dimension will increase the bandwidth of the elimination problem defined by the Newton iteration resulting in a degradation of running time.

Previously, BIFLO assumed that the pressure field was radially uniform in single-phase regions. While this is usually an excellent assumption before boiling inception, it is inaccurate after boiling begins because it forces the flow diversion around a two-phase cell to occur entirely within the axial levels immediately adjacent to that cell. However, when it is adequate, the assumption of a radially uniform pressure eliminates the need to determine an implicit multidimensional pressure field and can contribute significantly to the computational efficiency per time step, especially as the number of channels increases. With our incorporation of a large time step/implicit methodology for the two-phase portions of the overall calculation, the efficiency requirements for the single-phase portions become less stringent. Accordingly, we have replaced the old single-phase calculation with one which models single-phase radial pressure gradients and pressure driven single-phase radial flow.

We shall illustrate the calculation of single-phase pressures and velocities with an example in which the interconnected channels represent concentric coolant rings. Within the single-phase regions, we assume incompressible flow and write for each mesh cell the mass conservation equation

$$\begin{aligned}
 & \langle \rho A \rangle_{j-1/2,k}^n v_{j-1/2,k}^{n+1} - \langle \rho A \rangle_{j+1/2,k}^n v_{j+1/2,k}^{n+1} \\
 & + S_{k-1,k} \langle \rho \rangle_{j,k-1/2}^n U_{j,k-1/2}^{n+1} - S_{k,k+1} \langle \rho \rangle_{j,k+1/2}^n U_{j,k+1/2}^{n+1} \\
 & + S_{k,k+1} (w_{\ell,j,k+k+1}^n - w_{\ell,j,k+1+k}^n) + S_{k-1,k} (w_{\ell,j,k+k-1}^n - w_{\ell,j,k-1+k}^n) = 0 \quad (9)
 \end{aligned}$$

where

k = channel index,

A_k = area for axial flow in channel k ,

$S_{k-1,k}$ = area for radial flow between channels $k-1$ and k .

ρ = liquid thermodynamic density,

U = radial velocity,

$$\langle \rho A \rangle_{j-1/2,k} = \begin{cases} (\rho A)_{j-1,k}, & \text{if } v_{j-1/2,k} > 0 \\ (\rho A)_{j,k}, & \text{if } v_{j-1/2,k} < 0. \end{cases}$$

$w_{\ell,j,k+k+1}^n$ = explicitly calculated source term modeling the sweeping crossflow induced by wire-wrap spacers directed from channel k to channel $k+1$.

The mass fluxes in Eq. 9 are formulated using a donor cell prescription. The crossflow term is modeled as

$$w_{\ell,j,k+k+1}^n = \frac{1}{2} C_{\text{sweep}} \left| \langle \rho \rangle_{j-1/2,k}^n v_{j-1/2,k}^n + \langle \rho \rangle_{j+1/2,k}^n v_{j+1/2,k}^n \right|$$

where C_{sweep} is an input constant dependent upon bundle geometry (for a bundle possessing FFTF/CRBR geometry, we take $C_{\text{sweep}} = 0.023$). Thus, the magnitude of the transverse sweeping crossflow is a fraction C_{sweep} of the magnitude of the axial flow.

We assume the axial and radial single-phase momentum equations

$$\rho \frac{\partial v}{\partial t} + \frac{\partial}{\partial z} \left(\frac{1}{2} \rho v^2 \right) + \frac{1}{2} (\rho v)^2 \frac{\partial}{\partial z} \left(\frac{1}{\rho} \right) + \frac{2F\rho |v| v}{D} + \rho g = - \frac{\partial P}{\partial z}, \quad (10)$$

$$\rho \frac{\partial U}{\partial t} + \frac{2F\rho |U| U}{D} = - \frac{\partial P}{\partial r} \quad (11)$$

where

F = friction factor,

D = hydraulic diameter,

P = single-phase pressure.

In Eq. 10, we have neglected cross convective terms modeling the radial transfer of axial momentum while all convective terms have been ignored in Eq. 11. The effects of radial momentum convection within the momentum equations are probably bounded by uncertainties in the modeling of radial frictional effects within wire-wrapped pin bundles.

Equation 10 is differenced as

$$\begin{aligned}
 & (\rho_{j-1,k}^n \bar{X}_{j-1/2}^n \bar{Y}_{j-1/2,k}^n + \rho_{j,k}^n \tilde{X}_{j-1/2}^n \tilde{Y}_{j-1/2,k}^n) \frac{v_{j-1/2,k}^{n+1} - v_{j-1/2,k}^n}{\delta t} \\
 & + \frac{1}{2} \frac{1}{\delta z_{j-1/2}} (\rho_{j,k}^n v_{j,k}^n v_{j,k}^n - \rho_{j-1,k}^n v_{j-1,k}^n v_{j-1,k}^n) \\
 & + \frac{1}{2} (\rho_{j-1,k}^n \bar{X}_{j-1/2}^n \bar{Y}_{j-1/2,k}^n + \rho_{j,k}^n \tilde{X}_{j-1/2}^n \tilde{Y}_{j-1/2,k}^n)^2 v_{j-1/2,k}^n \\
 & \times v_{j-1/2,k}^{n+1} \frac{1}{\delta z_{j-1/2}} \left(\frac{1}{\rho_{j,k}^n} - \frac{1}{\rho_{j-1,k}^n} \right) \\
 & + \left(\frac{2F_{j-1,k}^n \rho_{j-1,k}^n \bar{X}_{j-1/2}^n \bar{Y}_{j-1/2,k}^n \bar{Y}_{j-1/2,k}^n}{D_{j-1,k}} \right. \\
 & \left. + \frac{2F_{j,k}^n \rho_{j,k}^n \tilde{X}_{j-1/2}^n \tilde{Y}_{j-1/2,k}^n \tilde{Y}_{j-1/2,k}^n}{D_{j,k}} \right) |v_{j-1/2,k}^n| v_{j-1/2,k}^{n+1} \\
 & + (\rho_{j-1,k}^n \bar{X}_{j-1/2}^n + \rho_{j,k}^n \tilde{X}_{j-1/2}^n) g = - \frac{P_{j,k}^{n+1} - P_{j-1,k}^{n+1}}{\delta z_{j-1/2}} \quad (12)
 \end{aligned}$$

where

$$v_{j,k} = \frac{1}{2} (\tilde{Y}_{j-1/2,k} v_{j-1/2,k} + \bar{Y}_{j+1/2,k} v_{j+1/2,k}).$$

In Eq. 10, the convective term

$$\rho v \frac{\partial v}{\partial z}$$

has been replaced by the equivalent expression

$$\frac{\partial}{\partial z} \left(\frac{1}{2} \rho v^2 \right) + \frac{1}{2} (\rho v)^2 \frac{\partial}{\partial z} \left(\frac{1}{\rho} \right) \quad (13)$$

which has been finite differenced in Eq. 12 using a space centered differencing prescription. The use of Eq. 13 (central differenced) in Eq. 12 is preferred because it provides a better representation of Bernoulli flow in coarse mesh situations where the velocity varies by large amounts between adjacent cell edges. In Eq. 12, the derivative of $\frac{1}{2} \rho V^2$ is formulated explicitly. In our calculations, the velocities in single-phase regions following boiling inception have usually remained below the Courant limit even when the two-phase velocities have not so that the use of an explicit formulation for this particular term has been adequate thus far. According to the folklore of numerical fluid dynamics, explicit central differencing is supposed to result in numerical instability. However, we have experienced no such difficulty with the use of Eq. 12 in our calculations. Perhaps the decomposition defined by Eq. 13 or the particular numerical formulation used for the second term in Eq. 13 has something to do with the avoidance of an instability. Before boiling initiation, it is usually an excellent approximation to replace

$$\frac{\partial}{\partial z} \left(\frac{1}{2} \rho V^2 \right)$$

by

$$\frac{1}{2} (\rho V)^2 \frac{\partial}{\partial z} \left(\frac{1}{\rho} \right)$$

This is because prior to the onset of boiling, the pressure field within the bundle has been found to be very nearly one dimensional. Radial pressure gradients and radial pressure driven velocities are small (eg. < 1 cm/s). Consequently, the axial mass flux (ρV) within each channel is essentially constant and making the aforementioned replacement is permissible. We therefore make this replacement in Eq. 12 thereby avoiding entirely an explicit stability restriction before the initiation of boiling. Although we have included velocity scale factors in Eq. 12, the additional precision gained through the consideration of different velocities on two sides of a cell edge separating two single-phase cells is probably minor.

Equation 12 has been linearized in terms of the end of time step liquid velocity $v_{\ell, j-1/2, k}^{n+1}$. From Eq. 12, we directly obtain the forward elimination constants $a_{\ell, j-1/2, k}$, $b_{\ell, j-1/2, k}$ in the equation

$$v_{\ell, j-1/2, k}^{n+1} = a_{\ell, j-1/2, k} + b_{\ell, j-1/2, k} (p_{j, k}^{n+1} - p_{j-1, k}^{n+1}) \quad (14)$$

expressing the end of time step velocity as a linear function of the pressure drop between cells $j-1$ and j . Similar to Eqs. 12 and 14, the radial single-phase momentum equation is differenced in a linearized fashion to obtain an equation

$$v_{\ell, j, k-1/2}^{n+1} = a_{\ell, j, k-1/2} + b_{\ell, j, k-1/2} (p_{j, k}^{n+1} - p_{j, k-1}^{n+1}). \quad (15)$$

Substituting Eqs. 14-15 into Eq. 9 yields a Poisson like equation for the single-phase pressure field which is solved by elimination. The single-phase velocities are then calculated by back substitution into Eqs. 14-15.

In our example, we have written the mass equation Eq. 9 for a single-phase cell embedded within the single-phase region. For a single-phase cell adjacent to a two-phase cell, the mass flux at the single-phase/two-phase interface is replaced by a two-phase mass flux. For example, if cell $j-1, k$ is two-phase, then the mass flux at $j-1/2, k$ is assumed to be

$$\langle \rho_{\ell}^{VF} A \rangle_{\ell, j-1/2, k}^n v_{\ell, j-1/2, k}^{n+1} + \langle \rho_v^{VF} A \rangle_{v, j-1/2, k}^n v_{v, j-1/2, k}^{n+1}$$

For the two-phase velocities at the interface, the two-phase momentum equations are differenced with the axial convective terms formulated explicitly. A forward elimination similar to Eqs. 14-15 is performed to express the liquid and vapor velocities as a linear function of the local pressure drop. In the resulting equation for the single-phase pressure field, the pressures on the two-phase side of the single-phase/two-phase interface are assumed to be the saturation vapor pressures at the beginning of the current time step. In this manner, the conditions in the two-phase region serve as boundary conditions for the single-phase pressure field.

After the single-phase pressures have been determined, the velocities on two-phase/single-phase interfaces are determined by back substitution of the single-phase pressures and the beginning of time step two-phase saturation pressures. These velocities are then used as boundary conditions for the implicit two-phase calculation. The resulting loose coupling between the velocities on the interface and the highly implicit calculation of two-phase thermohydrodynamic motions is not known to have caused any numerical problems in the calculations that we have performed thus far. This is a highly advantageous circumstance because it allows us to divide the overall calculation into separate calculations within the two-phase and single-phase regions which are loosely coupled together. Such a division significantly reduces the computational running time.

B. BIFLO Benchmarking Activities (P. L. Garner)

1. COMMIX-2 Code Usage

The COMMIX-2 code is being developed within the Components Technology (CT) Division of ANL to model two-phase thermalhydraulics in three dimensions. The code, when sufficiently developed, will provide a detailed calculation of sodium boiling situations to which BIFLO calculations may be compared for benchmarking purposes. Discussions with the code developers in CT have indicated that the code has probably reached the point of usefulness for our purposes; therefore, an effort has been initiated to use pre-release versions of COMMIX-2 during its continuing development process.

The procedures for accessing COMMIX-2, an input guide, and a sample set of input (for a 7-pin bundle problem) have been obtained. The access procedures (which are in the form of EXECs on the CMS timesharing computer system at ANL) have been reviewed and modified to fit our needs. The array dimensions have been increased to accommodate a 19-pin bundle problem. (The re-dimensioning process has been generalized in the form of an EXEC on CMS and given to the code developers for their future use.) Input data to describe the 19-pin THORS Bundle 6A conditions has been prepared.

Numerous difficulties were encountered while trying to run the 19-pin problem on COMMIX-2. Most of the problems were related to a lack of generality in some of the bookkeeping procedures within the code. Briefly, a 19-pin problem requires a grid system in which an axial level is represented by 10 cells for each of the two perpendicular directions within the plane. Superposition of the 10x10 Cartesian grid onto a 19-pin hexagonal bundle shows that 8 (out of 100) cells lie entirely outside the hexcan walls and are, thus, not used in the calculation; quantities associated with these cells were, however, being referenced in several portions of the coding. (The problem does not arise in a 7-pin problem since all 36 cells of the 6x6 planar grid lie at least partially within the hexcan.) The portions of the coding referencing the cells outside of the computational grid have been identified in close cooperation with the code developers and modifications have been suggested. Incorporation of these modifications did allow the 19-pin calculation to proceed through the initial stages of convergence to steady state.

The code developers were going through a cleanup operation near the end of the fiscal year to eliminate unused variables, realign storage, and modify the input. Further use of COMMIX-2 in the BIFLO benchmarking effort has been deferred until early in the next fiscal year at which time the majority of this cleanup activity will be completed.

2. THORS Bundle-6A Tests

The data obtained in the 19-pin bundle geometry in the THORS facility at Oak Ridge National Laboratory (ORNL) are being analyzed as a part of the BIFLO benchmarking effort. The data from several steady-state non-boiling tests are aiding in bundle characterization prior to analysis of the transient tests which proceeded into dryout. The computer code obtained from ORNL to plot radial temperature profiles using the test data from magnetic tape has been modified to work on the computers at ANL. Both plotting programs obtained from ORNL have now been modified to display the test results in SI units to facilitate comparisons with the results of computer code (e.g. BIFLO and COMMIX) calculations of these tests.

C. Pressure in the Molten Fuel Cavity Due to the Fission Gas Not Released Out of Grains Up to the Time of Melting (Kalimullah, H. H. Hummel and P. A. Pizzica)

Introduction: The NEFIG model^{1,2} shows that during fast transient heating of irradiated fuel typical of an LOF-TOP a large fraction of the retained fission gas is not released out of grains before fuel melting. When the fuel approaches melting this unreleased gas is mostly in the form of very small highly pressurized bubbles inside the grains, a negligible fraction being in the form of dissolved gas atoms. Before fuel melting the unreleased gas is assumed not to exert its pressure on the cladding. After melting, the constraint posed by the solid fuel grains is removed and the fission gas not released up to the time of melting (now in the form of bubbles in the molten fuel cavity) can exert pressure on the cavity and solid-fuel interface. These highly pressurized bubbles will expand to reach an equilibrium radius such that the internal gas pressure equals the sum of the external restraint pressure acting on the molten fuel (equal to the pressure on the cavity and solid-fuel interface) and the surface tension forces. This pressure equilibration process is assumed to be instantaneous for the molten fuel. The effect of bubble surface tension constraint on cavity pressure has been incorporated in the SAS3D/EPIC code.

Characterization of Fission Gas Bubbles in the Molten Fuel Cavity

If the bubble velocity in the molten fuel of gas not released from the fuel grains before melting is assumed to be provided only by buoyancy forces it is found that coalescence can be neglected for the millisecond time scale of an LOF-TOP event. Therefore, it is assumed that the bubble concentration remains that for bubbles still within the fuel grains at the time of melting. We currently calculate this concentration for each mesh cell from the NEFIG model, which assumes a single average bubble size. It is assumed that bubbles released from the grains prior to fuel melting, with the release fraction also calculated by NEFIG, are available to pressurize the clad but have coalesced to sufficiently large size that surface tension constraint can be neglected for them. This gas will then be at the molten fuel cavity hydrostatic pressure P_o , while with the assumption of equilibrium the gas in bubbles still within the grains at the time of fuel melting will be at pressure P_g related to P_o by

$$P_o = P_g - \frac{2\gamma}{r_b}, \quad (16)$$

where γ is the molten fuel surface tension and r_b is the equilibrium bubble radius in the molten fuel. This size depends on the available void space as well as on the bubble concentration.

Molten Fuel Cavity Pressure Calculation in the SAS3D-EPIC Code: In this analysis solid fuel implies melt fraction less than or equal to an adjustable value β_s and molten fuel implies melt fraction greater than β_s . A value of 0.5 for β_s has been coded in the FORTRAN source. Below this melt fraction the fuel is assumed to be rigid, and above this melt fraction the fuel is assumed to become fluid without any granular structure. The total number of gas atoms released out of grains before melting N_s , the total number of gas atoms contained in bubbles inside the cavity N_b , and the total number of bubbles in the cavity B are given by

$$N_s = \sum_{ij} C_{oij} V_{ij} F_{mij}, \quad (17)$$

$$N_b = \sum_{ij} C_{oij} V_{ij} (1 - F_{mij}), \quad (18)$$

$$B = \sum_{ij} C_{bm,ij} V_{ij} (1 - F_{mij}), \quad (19)$$

where

ij = Fuel mesh cell radial and axial indices,

V_{ij} = Volume of fuel mesh cell, i.e., the volume upon which gas concentration input data is based, cm^3 ,

C_{oij} = Total initial fission gas atoms/ cm^3 of fuel mesh cell ij ,

F_{mij} = NEFIG-model computed fission gas release fraction at β_s melt fraction in mesh cell ij .

$C_{bm,ij}$ = NEFIG-model computed bubble concentration (representing total initial gas) at β_s melt fraction in mesh cell ij .

The summation in Eqs. 17-19 is over all the mesh cells in the cavity. Using the Van der Waals equation the gas pressure inside a bubble is given by

$$P_g = \frac{N_b kT}{V_b - bN_b} - 27 P_c \left(\frac{bN_b}{V_b} \right)^2 \quad (20)$$

where

k = Boltzmann constant, 1.38×10^{-16} erg/K-molecule,

T = Average fuel temperature in the cavity, K,

V_b = Volume of all bubbles in the cavity, cm^3 ,

b = Van der Waals constant for fission gas, 63.55×10^{-24} $\text{cm}^3/\text{molecule}$,

P_c = Critical pressure for fission gas, 57.9×10^6 dynes/ cm^2 .

The bubble radius is obtained from

$$r_b = \left(\frac{3V_b}{4\pi B} \right)^{1/3} \quad (21)$$

The pressure due to the gas released from the fuel grains before melting, for which no surface tension constraint is assumed, is given by

$$P_o = \frac{N_s kT}{V_g - V_b - bN_s} - 27 P_c \left(\frac{bN_s}{V_g - V_b} \right)^2 \quad (22)$$

where V_g is the total gas volume in the cavity and $(V_g - V_b)$ is the volume of gas released before melting. For given values of N_b , N_s , B , T and V_g , the volume of all bubbles in the cavity V_b is determined from Eq. 16.

Substituting the values of P_g , r_b and P_o from Eqs. 20-22 into Eq. 16, the following nonlinear algebraic equation for V_b is obtained:

$$\frac{N_b kT}{V_b - bN_b} - 27 P_c \left(\frac{bN_b}{V_b} \right)^2 - 2\gamma \left(\frac{4\pi B}{3V_b} \right)^{1/3} - \frac{N_s kT}{V_g - V_b - bN_s} + 27 P_c \left(\frac{bN_s}{V_g - V_b} \right)^2 = 0 \quad (23)$$

Equation 23 is solved iteratively for V_b and then the pressure P_o acting on the cavity and solid-fuel interface is evaluated using Eq. 22.

Typical Results for Surface Tension Constraint

In these cases no release from the fuel grains prior to melting was assumed. The total fission gas concentration, obtained from fuels characterization calculations, was assumed to be 1.1×10^{20} atoms/cc, and the liquid fuel surface tension was taken to be 450 dynes/cm. The bubble concentration from NEFIG was 1.3×10^{14} bubbles/cc. Available void fractions were assumed based

on SAS/EPIC calculations. For a void fraction of 0.20, at the melting temperature of 3033 K a bubble radius r_b of 7.2×10^{-6} cm was obtained with corresponding P_o and P_g equal to 112 atm and 237 atm respectively. For a void fraction of 0.15, $r_b = 6.6 \times 10^{-6}$ cm, $P_o = 181$ atm, and $P_g = 319$ atm. These hydrostatic pressures are in the range that will produce clad failure under LOF-TOP conditions. The amount of delay in failure time produced by the surface tension constraint is evidently dependent to a considerable extent on the void fraction available at the time of melting.

D. Gap Conductance Bounds for HEDL P-20 Phase-III Test Pins Using the HGBOUNDS Code (Kalimullah)

Introduction: Fuel-cladding gap conductance is an important parameter required in the thermal analysis of a fuel pin but involves large uncertainties. A computer code HGBOUNDS described in Ref. 3, was developed earlier using the Baker's calibrated model⁴ to estimate the lower and upper bounds of fuel-cladding gap conductance of a mixed-oxide fuel pin at a steady-state power. The model is based on the concepts proposed by Ross and Stoute,⁵ and has recently been calibrated to HEDL P-19⁶ and P-20^{7,8} power-to-melt tests, and is believed to be the most realistic gap conductance and temperature prediction model currently available for mixed-oxide fuel pins. The earlier computer codes GAPCON⁹ and SIEX¹⁰ for estimating gap conductance are also based on the concepts of Ross and Stoute but not based on the present model, and compute an estimate of gap conductance without its error bounds.

The HGBOUNDS code translates the uncertainties of the calibrated gap conductance model and some of the input data into an uncertainty range for the gap conductance. The purpose of the present analysis is to check the code against the HEDL P-20 phase-III test and to see the size of the uncertainties in gap conductance and in fuel pellet inner surface temperature.

There have been made two additions to the earlier version of the code described in Ref. 3: (1) The additional pressure in pin plenum caused by the sorbed gases and water vapor in the fabricated fuel pellets (which is significant for fresh pin jump distance calculation) has been accounted, (2) An option has been added to evaluate fuel-cladding interface pressure using Eq. 17 of Ref. 5, the equation used in the calibration of the gap conductance model, and this is the option used in the present calculation. The other option for the interface pressure is that all values between a minimum value of zero and a maximum value which would load the cladding to yield stress are assumed (for obtaining the gap conductance bounds) when the hot radial gap is computed to be negative.

In the present calculation, the uncertainty in gap conductance given by its lower and upper bounds arise from the following two sources: (1) All the experimental (i.e. the tests used in the calibration of the model) and modeling uncertainties (i.e. the uncertainties in all the material property correlations, in the correlation for cold post-irradiation gap, in the calculation of hot gap from the cold post-irradiation gap, in the calculation of fuel-cladding solid-to-solid interface pressure, etc.); (2) Uncertainty in the ratio, fission gas in plenum/total fission gas generated.

Analysis and Results: Most of the input data have been obtained from measurements on sibling and test pins. The HEDL P-20 phase-III test consisted of 19 encapsulated fuel pins out of which two with xenon tag in the fill gas are not included in the present analysis because the HGBOUNDS code assumes a pure helium fill gas; and two mixed gap pins and a high burnup pin are also not included in the present analysis because of the lack of some required input data. The remaining 14 pins are included in the present calculation. Six of these fuel pins experienced fuel melting limited in the radial direction and only over a part of the fuel pin length. The two axial extents of melting (the farthest distance fuel melting is observed from the axial peak power position, one below and the other above the peak power position) are actually located where incipient fuel melting occurred (the fuel inner surface temperature is 3033 K equal to the fuel melting temperature in the model). For each of these six pins, calculations have been done for two locations, the bottom and the top axial extents of melting. The other 8 pins did not experience any fuel melting. For these pins, gap conductance bounds have been computed at only one axial location, a small distance above the peak power position, and the fuel inner surface temperature is believed to be the highest at this location.

For the six partially melted fuel pins at each axial extent of melting, the fuel inner surface temperature observed in the test, i.e. the fuel melting temperature lies between the two bounds of pellet inner surface temperature computed by the code. The upper bound of pellet inner surface temperature corresponds to the lower bound of gap conductance, and vice-versa. The difference between the two computed bounds of fuel inner surface temperature (160 K to 280 K) is mostly due to the uncertainty of the temperature drop across the fuel-cladding gap, only a small part (up to 40 K) being due to the temperature-dependence of fuel thermal conductivity. The value of gap conductance obtained from the SIEX-M1 code (Table VIII of Ref. 4) lies between the two bounds of gap conductance obtained in the present analysis.

For all the unmelted fuel pins except two low fabricated gap pins, the upper bound of the fuel pellet inner surface temperature obtained from the code is less than the fuel melting temperature; and this is in good agreement with the test observations. For the two low fabricated gap pins, the lower bound of the fuel inner surface temperature is less than the fuel melting temperature, and the upper bound is greater than the melting temperature, and no clear agreement or disagreement can be concluded.

In a typical case of gap conductance estimation for a fuel pin other than the test pins, the measured values of a number of input quantities (which are available for the test pins) may not be available, e.g. the pellet central void radius, columnar grain region radius and columnar fuel density may not have been measured. The use of estimated values of these input quantities with their associated uncertainties in the HGBOUNDS code should further increase the uncertainties of gap conductance and fuel pellet inner surface temperature. Since the code has not been checked against any experimental data above a peak burnup of 11 MWd/KgM, it may not be reliable above this burnup.

A comprehensive topical report on the up-to-date model of the code and the details of the present calculation is under preparation.

II. THREE-DIMENSIONAL CODE DEVELOPMENT FOR CORE THERMAL-HYDRAULIC ANALYSIS OF LMFBR ACCIDENTS UNDER NATURAL CONVECTION CONDITIONS

A2045

A. Introduction

The objective of this program is to develop computer programs (COMMIX and BODYFIT) which can be used for either single-phase or two-phase thermal-hydraulic analysis of reactor components under normal and off-normal operating conditions. The governing equations of conservation of mass, momentum, and energy are solved as a boundary value problem in space and initial value problem in time.

COMMIX is a three-dimensional, transient, compressible flow computer code for reactor thermal-hydraulic analysis. It is a component code and uses a porous medium formulation. The concept of volume porosity, surface permeability, and distributed resistance and heat source (or sink) is employed in the COMMIX Code for quasi-continuum (or rod-bundle) thermal-hydraulic analysis. It provides a greater range of applicability and an improved accuracy than subchannel analysis. By setting volume porosity and surface permeability equal to unity, and resistance equal to zero, the COMMIX code can equally handle continuum problems (reactor inlet or outlet plenum, etc.).

BODYFIT is a three-dimensional, transient, compressible flow computer code for reactor rod bundle thermal-hydraulic analysis. This is also a component code, and it uses a boundary-fitted coordinate transformation. The complex rod bundle geometry is transformed into either rectangular or cylindrical coordinates with uniform mesh. Thus, the physical boundaries, including each rod, coincide with computational grids. This allows the Navier-Stokes equations, together with the boundary conditions, to be represented accurately in the finite-difference formulation. Thus, the region in the immediate vicinity of solid surfaces, which is generally dominant in determining the character of the flow, can be accurately resolved.

During this quarter all efforts were devoted to the development of COMMIX-2 (3-D, two-phase) computer code and BODYFIT-1 code.

B. COMMIX-2, Two-Phase Code Development (H. M. Domanus, C. C. Miao, W. T. Sha and V. L. Shah)

During this quarter, the following two problems were analyzed using the homogeneous model in COMMIX-2.

1. German Seven-Pin Hexagonal Fuel Assembly [1]

Problem Description

In this test, liquid sodium having a temperature of 553°C enters the hexagonal test section, with a uniform velocity of 2.15 m/sec. The test section has seven electrically heated rods arranged in a hexagonal array as shown in Fig. 1. At time $t = 0$, the inlet velocity begins the transient wherein the flow rate is decreased to 30% of its initial value in 10 seconds

(see Fig. 2). Results have been obtained up to a transient time of 9.75 seconds.

Results

The variation of the exit coolant temperature and the central cladding surface temperature at the end of the heated section are compared with the experimental measurements in Figs. 3 and 4. The axial distribution of the void fraction along the central axis is shown in Fig. 5. The spread of the boiling region is shown in Fig. 6. We can see from these figures that the COMMIX-2 predictions with the homogeneous model are in close agreement with the measurements.

2. 31-Pin Fuel Assembly

Problem Description

This is the analysis of the boiling test (Test 20; Run #104) with bundle 3C in the Liquid Metal Fast Breeder Reactor (LMFBR) Thermal-Hydraulic Out of Reactor Safety (THORS) facility. Bundle 3C has 19 pins in the center, arranged in a hexagonal array and 12 pins in the surrounding annular region. All pins are electrically heated to simulate fuel pins. The heating section is 533 mm long and has a blockage plate at axial position $Z = 381$ mm. The flow transient is shown in Fig. 7.

Results

Results have been obtained with COMMIX-2 using homogeneous model for initial and final steady state conditions. Figures 8 - 11 show the comparisons of axial and cross-sectional temperature distributions for initial steady state condition. Figures 12 and 13 show the comparison of axial temperature distribution and the spread of the boiling region respectively for the final steady state condition. We can see that the COMMIX-2 predictions are in close agreement with the measurements.

Other Development Work

- (1) A generalized thermal structure model has been formulated and incorporated in COMMIX-2. With this generalized thermal structure model, it is now possible to resolve the effects of thermal inertia of a structure (fuel rod, duct wall, wire wrap, etc.) on coolant response to flow transients. Generality has been extended to permit a structure made up of any number of composite materials.
- (2) A symmetry boundary condition has been added in the code. With this modification, it is now possible to analyze only a section of the geometry, resulting in a great saving of computer storage and computer running time.
- (3) An option, along with the necessary modifications and changes, has been added to permit pressure boundary condition. This option has been tested and found to operate satisfactorily for a steady state case. Efforts are now underway to test it for a transient case.

- (4) The formulations of heat transfer coefficient model and wire wrap model have been completed. These models have been incorporated in the code. The next step will be to test these models.
- (5) The convergence criterion check has been implemented in the subroutine for solution of the pressure equation. With this check implementation, the reiteration of the pressure equation is stopped as soon as the convergence criterion is satisfied. This prevents unnecessary computation.
- (6) An alternative rebalancing scheme has been formulated and implemented in the code.
- (7) An alternate, less implicit method for evaluation of velocities from the momentum equation has been formulated and implemented in the code. This procedure requires less computer storage. Some preliminary results with this procedure gave the same results as those with more implicit procedure. Further tests are continued in this direction.
- (8) Efforts were devoted to cleaning up the code and in preparation of a users manual.

C. Development of BODYFIT-1FE (B. C-J. Chen and W. T. Sha)

During this quarter, major effort was concentrated on the writing of the BODYFIT-1FE document, which is in the stage of being typed and edited.

Two significant improvements of the code were also implemented during the quarter. One deals with the fuel pin model, the other with the pressure correction. The semi-implicit time differencing scheme used in the fuel pin model was changed to the fully-implicit scheme. This change allows the use of a large time step in the fuel temperature calculation. However, this change necessitates an iterative calculational procedure between the fuel pin temperature and coolant temperature calculations.

The second modification is the inclusion of a constant term A in the $1/\Delta t$ term of the pressure correction formula as

$$\Delta P = \beta \Delta R \left(A + \frac{1}{\Delta t} \right),$$

where ΔP is the cell pressure correction, ΔR is the cell residue mass, β is the geometric proportional constant, Δt is the dimensionless time step used in the transient calculation defined by

$$\Delta t = \frac{\Delta \bar{t} \, v_{in}}{D_e}$$

where v_{in} is the inlet velocity, D_e is the hydraulic diameter of the assembly and $\Delta \bar{t}$ is the dimensional time step. In the case of small Δt , A term is dominated by the $1/\Delta t$ term. Only when the large Δt is used, A term becomes important. This treatment gives a very effective pressure correction scheme when a very large Δt is used to obtain a steady state solution.

With the above two modifications, constraint on the size of the time step used for the calculation is eliminated. Therefore, one can use a large Δt to simulate a transient process and reduce the computation time tremendously. Other modifications to improve the computational efficiencies are described as follows.

Some of the three dimensional arrays were changed to two dimensional arrays by renumbering the computational cells. For example the fuel pin temperature array, TCL (N,K, NP, NQ), was changed to TCL (N, K, NPQ) array, where N is the index for the radial node of the fuel pin, K is the index for the axial node of the fuel pin, NP is the index for the pin number, and NQ is the index for the fuel pin quadrant. The last two indices were combined to form NPQ index, which identifies the fuel pin quadrant consecutively for all the fuel pins. This combination eliminates a lot of unnecessary storage spaces occupied by non-computational cells for rod bundles having symmetric boundary conditions. In the case of hexagonal rod bundle with one-twelfth symmetry, the computer storage saving is almost 30%.

Capability to utilize quarter and half symmetry in square rod bundle was also incorporated in the code. The functional form of the sodium property subroutines were also modified to be the same as those of the water property subroutines so that both water and sodium can be used as coolant for simulation of rod bundle experiments.

Flow charts of main subroutines were prepared. Few sample problems were also tested for inclusion in the documentation of the code.

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Fig. 1. (A) Axial
(B) Transverse Partitioning
of Model 7-Pin Bundle

TEST 7-2/16, FLOW TRANSIENT

Fig. 2. Flow Rundown
Transient for
Test 7-2/16

Fig. 3. Comparison of Exit Coolant Temperature
With the Experimental Data

Fig. 4. Comparison of the Central Cladding Surface Temperature at the End of the Heated Section With the Experimental Data

Fig. 5. Axial Distribution of the Void Fraction Along the Central Axis

SIMULATION OF GERMAN SEVEN PIN FUEL ASSEMBLY TEST

Fig. 6. Comparison of Boiling Region

Fig. 7. Variation of Inlet Flow, Inlet Pressure and Total Bundle Power With Time for THORS Bundle 3C-Test 20, Run 104

Fig. 8. Comparison of the Axial Temperature Distribution

T_c	Experiment	COMMIX-2
3	721	721
15	670	672
19	669	659
38	670	672
94	620	632

Fig. 9. Temperature Distribution at $z = 432$ (mm) from the Start of Heated Section

T_c	Experiment	COMMIX-2
11	742	730
16	694	683
26	672	680
39	680	696
90	646	656

Fig. 10. Temperature Distribution at $z = 438$ (mm) from the Start of Heated Section

T_c	Experiment	COMMIX-2
10	758	764
12	760	761
56	676	669
59	666	670
74	666	674
76	762	673
91	693	711
147	694	706
149	694	678

Fig. 11. Temperature Distribution at End of Heated Section

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Fig. 12. Comparison of Axial Temperature Distribution
(Distance Between Two Stations = 25.4 mm)

Fig. 13. Comparison of Boiling Region in THORS Bundle 3C

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