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PHYSICS OF REACTOR SAFETY

Quarterly Report
July – September 1984

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS
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PHYSICS OF REACTOR SAFETY

Quarterly Report
July—September 1984

Applied Physics Division
Components Technology Division

November 1984

Previous reports in this series

ANL-83-11 (III)	July—September 1983
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PHYSICS OF REACTOR SAFETY

Quarterly Report
July-September 1984

ABSTRACT

This Quarterly progress report summarizes work done during the months of July-September 1984 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.

FIN No.	Title
A2015	Reactor Safety Modeling and Assessment
A2045	3-D Time-Dependent Code Development

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Executive Summary

A series of parameter studies of slow TOP accidents in oxide-fueled LMFBR's is underway in preparation for final documentation of our studies in this area. This work has been slowed by the necessity for correcting several bugs in PLUTO2. We found that in previous calculations heat transfer rates in the annular flow regime were too high relative to those in the particulate regime. This situation has now been corrected.

There has recently been concern that the fuel ejection in a LOF-TOP pin failure into a partially voided channel was greater in SAS/EPIC than is physically possible because of inertial constraints. This could lead to too high a rate of positive reactivity feedback from fuel motion. A physical constraint on fuel ejection has now been programmed into SAS/EPIC. Some reduction in peak power and energy deposition was noted as a result, but this was not large compared to the effects of other uncertainties in the calculation.

In the area of single-phase COMMIX development, the following three major efforts were made this quarter.

- Free Surface Boundary Option: The development of free surface boundary option has been continued. We are now testing the procedure that has been implemented.

- The implementation of the "Automatic Time-Step Control Option" has been completed.

- Cleaning, preparation of user instruction, and testing of sample problems were continued as part of the efforts leading to the documentation of COMMIX-1B.

In the area of two-phase COMMIX development, the efforts were continued to:

- simulate German Seven-Pin test,

- debug the separated phase model, and

- document up to date development of COMMIX-2.

Furthermore, an attempt was made to see if the momentum flux formulation of Padilla and Rowe reduces the computer running time. We found that it does not in the case of COMMIX-2 computer code.

I. REACTOR SAFETY MODELING AND ASSESSMENT

(A2015)

A. TOP Studies with SAS4A/PLUTO2 (H. H. Hummel and P. A. Pizzica)

In preparation for final documentation of our studies of slow TOP accidents in oxide-fueled LMFBR's, performed in support of CRBR licensing, it seemed desirable to perform additional parameter studies with the PLUTO2 code to fill in gaps in our understanding of such events and also to obtain complete consistency in various parametric variations. These studies are now underway. A 10 ¢/s TOP in the CRBR is assumed with a centerline failure location as in the previous work. This work has been showed by the discovery of several bugs in PLUTO2 which have now been corrected.

A review of parameter studies performed to date has led to the conclusion that fuel-coolant heat transfer in the annular flow regime in these calculations when liquid Na is still present has been too high relative to that in the particulate flow regime. The most reasonable assumption about this heat transfer is that it is about the same per unit fuel surface area in the two flow regimes, so that the total heat transfer declines according to the decrease in surface area when a transition occurs from particulate to annular flow. However, we now realize that the heat transfer coefficient we have been using in the annular flow regime to express the thermal resistance in the fuel, an input variable, is too high relative to that used in the particulate flow regime. This coefficient has been reevaluated. This is not too important if no liquid sodium is present because of the low heat transfer coefficient for sodium vapor. However, even though no liquid sodium film is permitted on fuel or clad in the annular flow regime, the forms of the equations for heat transfer from fuel or clad to sodium together with recommended input parameter choices still permitted rather high heat transfer rates to liquid droplets suspended in vapor which seem physically unreasonable. We have revised input parameter choices for heat transfer in the annular flow region to correct this situation.

The problem of too high heat transfer rate in the annular flow regime was not evident in the L8 analysis because this was an LOF-TOP simulation in which voiding was more advanced, so that liquid sodium did not remain in the annular flow regime to as great an extent as in the current calculations.

B. Fuel Ejection in SAS3D/EPIC (P. A. Pizzica)

Recently there has been a concern that SAS3D/EPIC has not been treating fuel ejection properly. The problem stems from the fact that EPIC assumes that the pressure in the pin cavity ejection cell and that in the adjacent coolant channel cell can be equilibrated in one time step. This may not in fact be physically possible because of inertial considerations. Indeed, preliminary hand calculations confirmed that only a fraction of the fuel presumed to move the distance between the pin cavity and the coolant channel (in order for pressure equilibration to occur) could actually be moved in the timestep used in the calculation.

This effect would be most noticeable in an LOF-TOP pin failure when fuel is being ejected into a partially voided channel. If the channel is mostly voided in front of a pin ejection cell in EPIC, the pin cell must eject a large fraction of its fuel practically instantaneously in order to equilibrate pressure with the channel. Of course, inertial constraints place a lower limit on the time in which this can occur. The rapidity of fuel ejection in LOF-TOP conditions has a significant bearing on reactivity feedback immediately after failure, which is the most crucial part of the fuel motion reactivity calculation for an LOF-TOP event.

Therefore, it was decided to program into EPIC a real physical constraint based only on inertia to prevent a certain amount of fuel each time step from being ejected. When this was done with a particular test case (the WAC LOF for the irradiated core), a reduction in peak power of 28% and a reduction in energy deposition at the time of peak power (as a difference with the energy deposition at the time of first pin failure) of 15% resulted. Although this is a noticeable difference it is much less than differences caused when certain poorly understood parameters in the calculation such as failure location and failure length are varied. Therefore this inaccuracy in SAS3D/EPIC's LOF-TOP calculations is a small part of the total variation in results obtained during parametric variations already presented. It is, however, a real physical effect and should be included in the calculation even if other constraints on fuel ejection such as the interaction of molten fuel with the solid fuel annulus and the cladding during ejection are not included since they cannot be calculated with any degree of confidence.

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, especially under natural circulation. The governing equations of conservation of mass, momentum, and energy are solved as a boundary value problem in space and as an 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 to permit analysis of a reactor component/multicomponent system, such as fuel assembly/assemblies, plenum, piping system, etc., or any combination of these components. The concept of volume porosity, surface permeability, and distributed resistance and heat source (or sink) is employed in the COMMIX code for quasi-continuum thermal-hydraulic analysis. It provides a much 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.).

B. COMMIX-1A, COMMIX-1B, Single-Phase Code Development (F. F. Chen, H. N. Chi, H. M. Domanus, R. C. Schmitt, W. T. Sha, V. L. Shah, and W. T. Sha)

B.1 Free Surface Boundary Option

As described in the last quarterly report, the insertion of the free surface term in the continuity equation may transform it into a free-surface equation. The same concept can be applied to the momentum equation. The x-direction momentum equation can be written as

$$\frac{\Delta}{\Delta t}\left(\beta_v r_v \rho u\right) + \frac{\Delta\left(\beta_x r_x \rho u^2\right)}{\Delta x} + \frac{\Delta\left(\beta_y r_y \rho v u\right)}{\Delta y} + \frac{\Delta\left(\beta_z r_z \rho w u\right)}{\Delta z}$$

$$= -\beta_v r_v \frac{\Delta(P)}{\Delta x} + \beta_v r_v \rho g_x - \beta_v r_v R_x$$

$$+ \frac{\Delta\left(\beta_x r_x \tau_{xx}\right)}{\Delta x} + \frac{\Delta\left(\beta_y r_y \tau_{xy}\right)}{\Delta y} + \frac{\Delta\left(\beta_z r_z Z_{xz}\right)}{\Delta \lambda}$$

By introducing a device called the Flexible Momentum Control Volume (FMCV) approach shown in Fig. 1, the continuity-momentum-pressure cycle in the modeling of free surface can be greatly simplified in the computation. An example is shown in Fig. 2. The free surface locations are shown in the

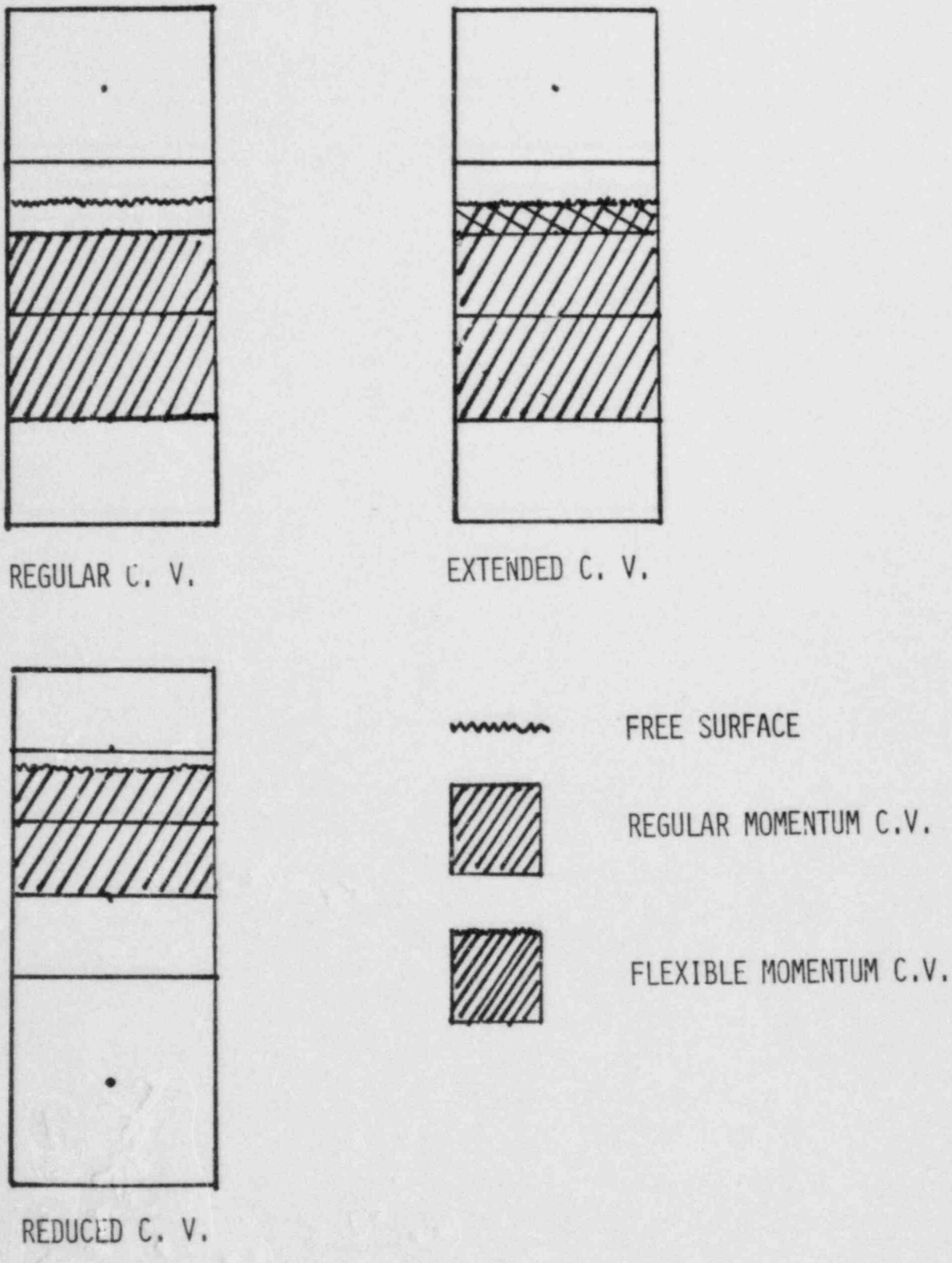

Fig. 1. Flexible Momentum Control Volume

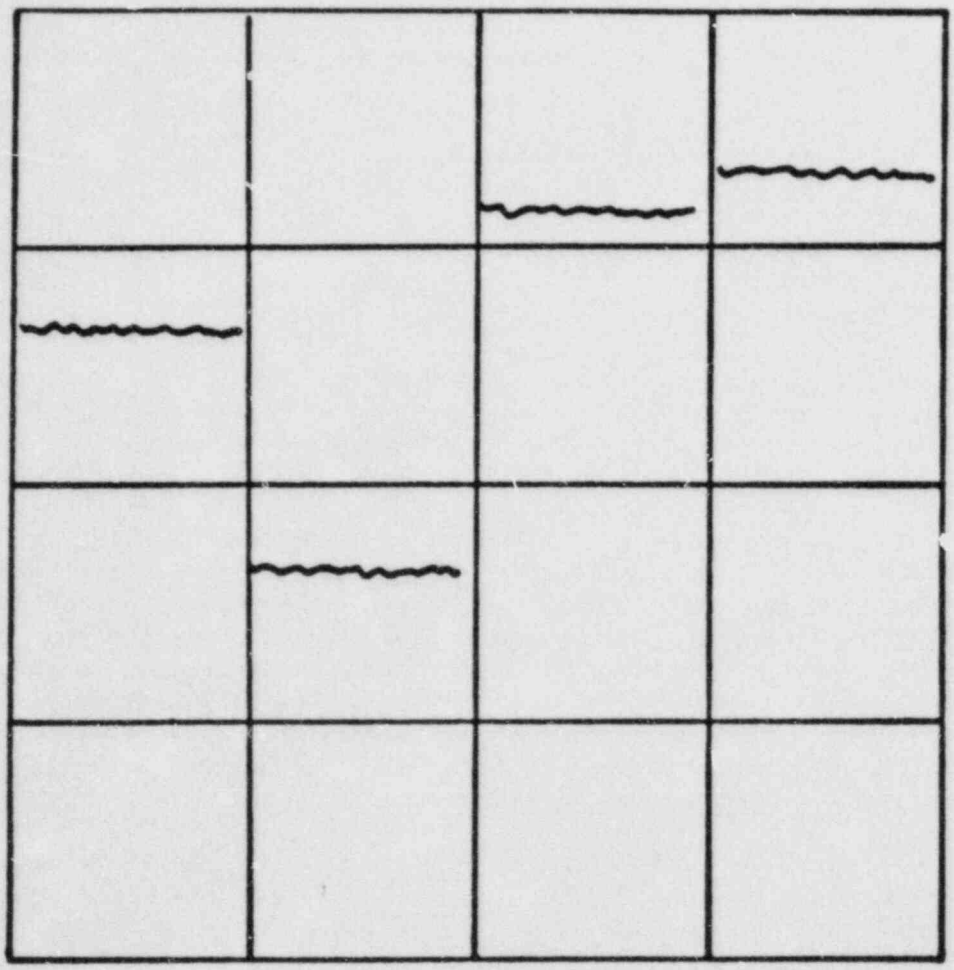

Fig. 2. Location of Free Surface in COMMIX Geometry

COMMIX geometry. By applying the FMCV approach, the computational configuration can be reduced to a single-phase system with a pressure boundary as shown in Fig. 3. The free surface pressures are defined. Pressure in the cells without free surface are to be solved.

A self-correcting process has been developed, such that the final resulting solution of the free-surface permeability vector $[\beta_l]$ satisfies the contraint

$$\beta_l \in [0, 1] \text{ for all } i = 1, \ldots. n.$$

This procedure has been implemented in the code. We are now testing this procedure with several simple problems.

B.2 Automatic Time Step Control

To reduce the cpu time in the computation, several approaches have been proposed. In the previous monthly report, we mentioned the use of an efficient solver, such as the Conjugate Gradient Method. The latest approach is the use of automatic time step control to reduce the computational time.

Previously, there are two types of time step control in the COMMIX code: a fixed time step as specified by the user, or the multiplier of courant time. Because courant time is based on the transport of convective flux, the time step size generally varies in the first 10-20 time steps, then levels off for the rest of the computation. Therefore, the advantage of using a very large time step near the steady state to save computational time is very small. An alternative approach of automatic time step control has been proposed and implemented in the COMMIX code. The algorithm of our automatic time step control is listed in the following:

1. Compute the maximum change for the sets of crucial variables, i.e., pressure and enthalpies.

$$DPMAX = MAX \left| \left(P_i^{n+1} - \rho_i^n \right) / P_i \right|$$

$$DHMAX = MAX \left| \left(H_i^{n+1} - H_i^n \right) / H_i^n \right|$$

$$DELMAX = MAX(DPMAX, DHMAX)$$

2. According to the user input variables, EPSMIN and EPSMAX,

   a. double the time step size if DELMAX < EPSMIN for 5 successive time steps,

   b. immediately halve the time step size if DELMAX > EPSMAX.

3. The values of EPSMIN and EPSMAX have to be empirically determined by the user. Based on our experience, the values of 0.50 for EPSMIN and 0.10 for EPSMAX are recommended.

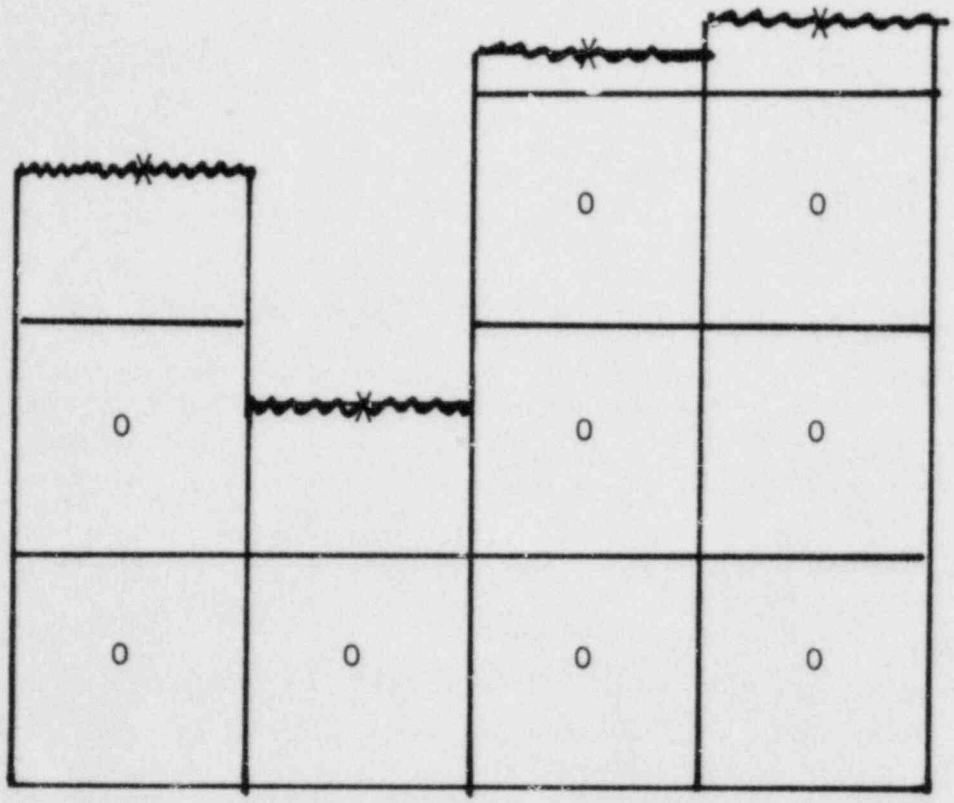

Fig. 3. Resulting Configuration for Pressure Computation

Three problems were tested with the automatic time step option: an isothermal duct flow, an isothermal tubulent pipe flow, and a thermal mixing problem with volume-weighted skew-upwind differencing. Comparisons of no. of time steps used and cpu time are listed below:

Test Problem	No. of Time Steps Used		cpu Time	
	Fixed Δt	Automatic Δt	Fixed Δt	Automatic Δt
Isothermal duct flow	32	24	7:59 s	7:47 s
Turbulent pipe flow	73	73	33:41 s	32:16 s
Thermal mixing	24	21	3:07 s	2.88 s

Although the savings of cpu time seems not very impressive (approximately 5%), at least the results are encouraging (cpu time did reduce) when the present automatic time step control is used. More extensive research on this subject such as the values of EPSMIN and EPSMAX will continue.

B.3 Documentation of COMMIX-1B

In the process of documentation and release of COMMIX-1B, we have started the following efforts

(i) cleaning of the code,

(ii) preparation of input and user instructions, and

(iii) rerunning the several sample problems to ensure no errors have been introduced.

C. DEVELOPMENT OF COMMIX-2 (H. N. Chi, T. H. Chien, H. M. Domanus, C. C. Miao, and W. T. Sha)

C.1 New Momentum Flux Formulation

Motivated by the paper by Padilla and Rowe[1], the momentum flux formulation used in COMMIX-2 was changed. The old and new formulations are explained below.

Consider the steady one-dimensional momentum equation with zero gravity and equal area given by

$$\frac{d}{dx}(Fu) + \frac{dP}{dx} = 0 \qquad (1)$$

where

$F = \rho u$ = constant.

Equation 1 may be integrated between the points 0 and 2 as shown in Fig. 4 as

$$\int_0^2 \frac{d}{dx}(Fu)\,dx + \int_0^2 \frac{dP}{dx}\,dx = \bar{F}_2 \langle u_2 \rangle - \bar{F}_1 \langle u_1 \rangle + P_2 - P_0 = 0 \qquad (2)$$

The brackets denote that donor celling is being applied based on the sign of $\bar{F}$.

The old formulation for the fluxes $\bar{F}_1$ and $\bar{F}_2$ defined at the edges of the dotted momentum cell shown in Fig. 4 are given by

$$\bar{F}_1 = \frac{1}{2}(F_1 + F_0)$$

$$\bar{F}_2 = \frac{1}{2}(F_0 + F_2)$$

where

$$F_0 = \langle \rho_0 \rangle u_0$$

$$F_1 = \langle \rho_1 \rangle u_1$$

and

$$F_2 = \langle \rho_2 \rangle u_2 .$$

For $u > 0$, $\langle u_1 \rangle = u_1$, $\langle u_2 \rangle = u_0$; $\langle \rho_0 \rangle = \rho_0$, $\langle \rho_1 \rangle = \rho_1$, and $\langle \rho_2 \rangle = \rho_2$. Equation 2 then becomes, solving for $-(P_2 - P_0)$,

$$-\Delta P_{acc} = -(P_2 - P_0) = \frac{1}{2}(\rho_0 u_0 + \rho_2 u_2)\,u_0 - \frac{1}{2}(\rho_1 u_1 + \rho_0 u_0)\,u_1 . \qquad (3)$$

At steady state, $\rho_0 u_0 = \rho_1 u_1 = \rho_2 u_2 = \rho u$ = constant, and therefore Equation 3 may be expressed as

$$-(P_2 - P_0) = (\rho u)(u_0 - u_1) = (\rho u)\left(\frac{\rho u}{\rho_0} - \frac{\rho u}{\rho_1}\right)$$

or

$$-(P_2 - P_0) = (\rho u)^2 \left(\frac{1}{\rho_0} - \frac{1}{\rho_1}\right) = -\Delta P_{acc} . \qquad (4)$$

Equation 4 shows that the acceleration pressure drop does not occur where the density change occurs. If ρ_2 is much less than either ρ_0 or ρ_1, then the largest pressure drop does not occur between points 0 and 2, but is shifted a full node further downstream.

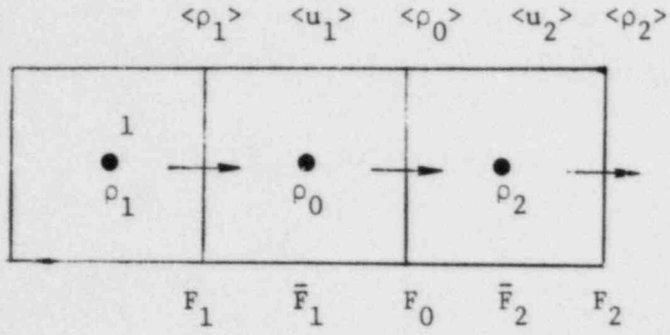

Fig. 4. COMMIX-2 Nodalization Scheme

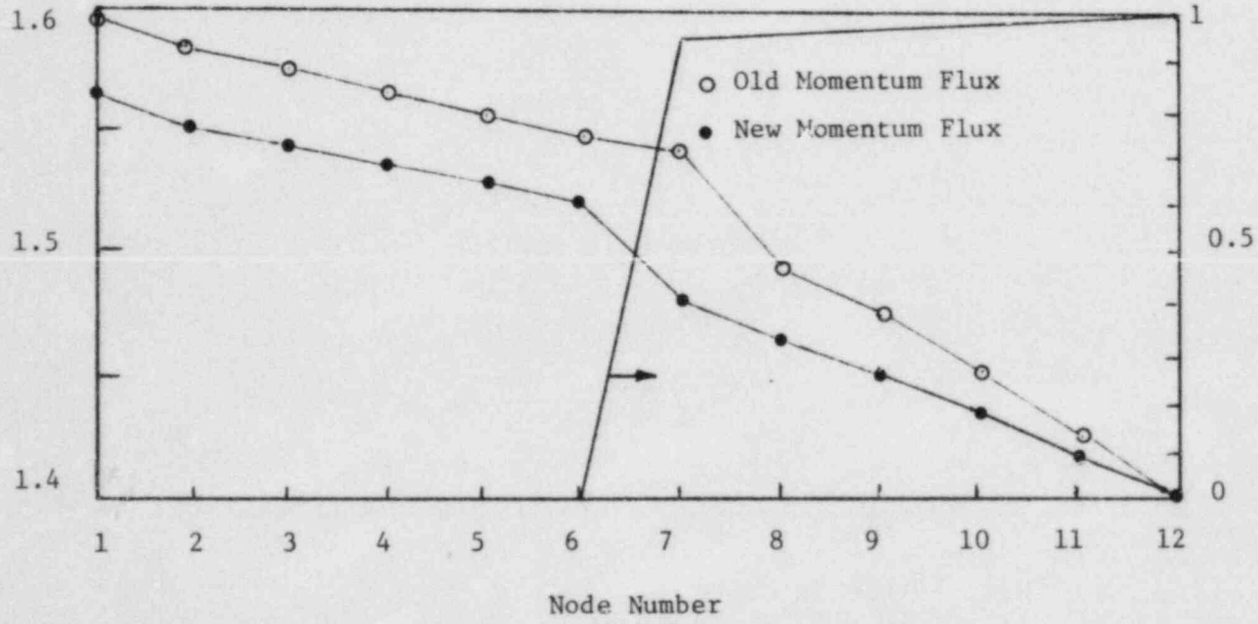

Fig. 5. Comparison of Old and New Momentum Flux Formulation

The modifications made in COMMIX-1A are

$$\langle u_1 \rangle = \langle \rho_1 \rangle u_1 / \rho_0 = \begin{cases} \langle \rho_1 \rangle u_1/\rho_0, & \bar{F}_1 > 0 \\ \langle \rho_0 \rangle u_0/\rho_0, & \bar{F}_1 < 0 \end{cases}$$

and

$$\langle u_2 \rangle = \langle \rho_2 \rangle u_2 / \rho_2 = \begin{cases} \langle \rho_0 \rangle u_0/\rho_2, & \bar{F}_2 > 0 \\ \langle \rho_2 \rangle u_2/\rho_2, & \bar{F}_2 < 0 \end{cases} .$$

$\bar{F}_1$ and $\bar{F}_2$ are unchanged in their formulation.

For $u > 0$, we obtain

$$-(P_2 - P_0) = (\rho u)^2 \left(\frac{1}{\rho_2} - \frac{1}{\rho_0}\right). \qquad (5)$$

Now the pressure drop occurs where the density changes.

A sample problem was run to test the new formulation. It is a one-dimensional representation of a 19-pin electrically heated steady-state test performed on the CFNa loop at Grenoble, France[2]. The conditions of the simulations are

Inlet: Temperature = 400°C

Velocity = 0.413 m/s

Outlet: Pressure = 1.4×10^5 Pa

The total power is 4.25×10^4 W. Twelve nodes were used. The first node is adiabatic and the middle six have a volumetric heat source of 4.17×10^8 W/m^3.

The results are shown in Fig. 2 for the case of slip ratio = 1.0. The upper pressure profile (denoted by circles) is computed with the unmodified momentum flux. This pressure profile shows that the largest pressure drop occurs between nodes 7 and 8, which is shifted downstream of where the density changes the most (between nodes 6 and 7). The void fraction, α_g, changes from 0 to 0.94 and the density changes from 740 to 47 kg/m^3. The lower pressure profile is computed using the new momentum flux formulation. This time, the largest pressure drop occurs where the density changes the most. Although Padilla and Rowe found their execution time reduced by 50%, we found the opposite. The number of time steps needed to converge the solution to a relative error of 10^{-6} increased from 58 to 84. Further investigations are underway.

C.2 German Seven-Pin Test 7-2/16

Calculation of the 7-2/16 Experiment of the KNS series run at KfK, has been initiated with inlet boundary conditions for pressure (instead of velocity). The input data has been changed accordingly. Some program modifications necessary for dealing correctly with the new boundary conditions have been made and a correct steady-state solution has been obtained. The transient calculations are being carried out.

C.3 Separated Phase Model

Debugging of the Separated Phases Model. This activity has been continued. Difficulties were encountered at the beginning of boiling inception due to the treatment of the compressibility terms $\partial\rho/\partial p = 1/c^2$ for the two phases separately. These difficulties have been overcome by continuing the two terms in the Poisson equations for pressure.

So far all subroutines of the SPM model have been checked in these cases: (a) single-phase, both 1D and 3D, up to boiling inception; (b) in the two-phase flow, only 1D. One second of problem time has been computed without numerical problems.

However, the completion of the SPM model deserves a series of model implementations. A list has been prepared.

C.4 Documentation of COMMIX-2

A complete report about the physical modeling and the numerical methods used in the program is now in preparation. Both the slip model and the model of separated phases are documented. The writing of the report has been completed. It is now being typed.

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13. ABSTRACT (200 words or less)

This quarterly progress report summarizes work done during the months of July-September 1984 in Argonne National Laboratory's Applied Physics and Components Technology Divisions for the Division of Reactor Safety Research in 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 at 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.

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