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Fractional Step Methods for Thermohydraulic Calculation*

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A method of fractional steps is used to extend a semi-implicit finite-difference technique for multidimensional two-phase flow calculations. This extension permits time step size to be chosen independent of convection velocities in one space direction, and still resolves multidimensional coupled sonic and phase exchange effects implicitly by forming a simple Poisson problem for pressure. Because pure time-splitting by physical phenomena was found unsuited to thermal hydraulics problems, a stabilizing corrections method was chosen. An application in nuclear reactor safety analysis is demonstrated.

INTRODUCTION

As nuclear reactor safety analysis becomes more sophisticated, detailed modelling of reactor behavior calls for increasing flexibility and efficiency of numerical calculations. An example in the field of light water reactor thermal-hydraulic analysis is the increasing emphasis on multidimensional calculations of two-phase flow. These problems can be so complicated that, even aside from the many difficult questions about physically modelling multidimensional two-phase flow (e.g., see [1–3]), there appears to be no single numerical method that is best for computing all such problems. At least three numerical approaches have been deployed for various classes of multidimensional two-phase flow problems.

One type of numerical method is the marching algorithm which has been applied where flow in a three-dimensional region is predominately along one coordinate direction. Such is the case within the core barrel of a reactor under normal operating conditions, where coolant enters at the bottom and flows axially upward. An example of a marching method for this application is presented by Masterson [4]; assuming flow conditions known at the inlet, implicit finite difference equations are solved by marching one plane at a time toward the outlet. Done properly, this approach is effective for many reactor core thermal–hydraulic problems with strong axial flow, including some with local flow blockages. It has the advantage of being numerically stable for arbitrarily large time steps. Its limitations lie in the assumptions made in

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order to solve by marching. First, certain transport terms in the multidimensional momentum equations are ignored; claims that these terms may be neglected (e.g., [5, p. 7]) are not in all circumstances convincing. Second, problems with even local flow reversal cannot be treated. Third, propagation of disturbances upstream can be calculated only with restrictions (e.g., assuming completely incompressible flow). As a result, certain natural flow boundary conditions are very difficult to implement. Light water reactor core thermal hydraulics will be the chief interest of this paper, but due to the several shortcomings of marching methods we will seek a different approach.

A second multidimensional calculation method for two-phase flow is that developed for the TRAC code [6]. Part of the motivation for this method was the decision to use a two-fluid model of two-phase flow. (The method has strong advantages even for simpler two-phase flow models such as the homogeneous equilibrium model.) The differential equations of the model are

$$\begin{aligned}
\partial \alpha \rho_v/\partial t + \nabla \cdot \alpha \rho_v \mathbf{v}_v &= \Gamma, \\
\partial (1-\alpha)\rho_l/\partial t + \nabla \cdot (1-\alpha)\rho_l \mathbf{v}_l &= -\Gamma, \\
\alpha \rho_v [\partial \mathbf{v}_v/\partial t + \mathbf{v}_v \cdot \nabla \mathbf{v}_v] + \alpha \nabla P &= -K(\mathbf{v}_v - \mathbf{v}_l) - \mathbf{F}_v \cdot \mathbf{v}_v - \mathbf{g}_v, \\
(1-\alpha)\rho_l [\partial \mathbf{v}_l/\partial t + \mathbf{v}_l \cdot \nabla \mathbf{v}_l] + (1-\alpha)\nabla P &= K(\mathbf{v}_v - \mathbf{v}_l) - \mathbf{F}_l \cdot \mathbf{v}_l - \mathbf{g}_l, \\
\partial \alpha \rho_v e_v/\partial t + \nabla \cdot \alpha \rho_v e_v \mathbf{v}_v + P[\partial \alpha/\partial t + \nabla \cdot \alpha \mathbf{v}_v] &= Q + Q_v, \\
\partial (1-\alpha)\rho_l e_l/\partial t + \nabla \cdot (1-\alpha)\rho_l e_l \mathbf{v}_l + P[-\partial \alpha/\partial t + \nabla \cdot (1-\alpha)\mathbf{v}_l] &= -Q + Q_l,
\end{aligned} \tag{1}$$

which represent local average mass, momentum, and energy balances for the vapor and the liquid phases, with interfacial exchanges governed by the first terms on the right-hand sides (Γ, K, Q). The remaining terms on the right are flow-dependent external sources or sinks. Basic quantities are pressure P, vapor volume fraction α, velocities $\mathbf{v}_v$ and $\mathbf{v}_l$, and phase temperatures; closure comes from specifying the right-hand side, plus equations of state for densities ρ_v, ρ_l and specific internal energies e_v, e_l.

The TRAC method for solving these equations is a semi-implicit finite difference technique that generalizes the ICE method [7] for solving single-phase flow problems. Consider the simplified single-phase equations

$$\begin{aligned}
\rho_t + \nabla \cdot \rho \mathbf{v} &= 0, \\
\rho [\mathbf{v}_t + \mathbf{v} \cdot \nabla \mathbf{v}] + \nabla P &= -\mathbf{g},
\end{aligned}$$

with appropriate boundary conditions (e.g., $\mathbf{v} \cdot \mathbf{n} = 0$ or $P = \text{const.}$ on different portions of the boundary). Taking $\boldsymbol{\xi} = [P, \mathbf{v}]^t$, we can write

$$\mathscr{E}\boldsymbol{\xi}_t + \mathscr{C}\boldsymbol{\xi} + \mathscr{S}\boldsymbol{\xi} = -\mathscr{G},$$

where

$$\mathscr{E} = \begin{bmatrix} c^{-2} & 0 \\ 0 & \rho \end{bmatrix}, \quad \mathscr{C} = \begin{bmatrix} c^{-2}\mathbf{v}\cdot\nabla & 0 \\ 0 & \rho\mathbf{v}\cdot\nabla \end{bmatrix}, \quad \mathscr{S} = \begin{bmatrix} 0 & \rho\nabla\cdot \\ \nabla & 0 \end{bmatrix}, \quad \mathscr{G} = \begin{bmatrix} 0 \\ \mathbf{g} \end{bmatrix}.$$

Here $\mathscr{C}$ represents the effects of convection, and $\mathscr{E}$ and $\mathscr{S}$ govern sonic propagation. Linearizing and introducing appropriate space and time differences in place of derivatives leads to the semi-implicit equation

$$(E + S\Delta t)\xi^{n+1} = (E - C\Delta t)\xi^n - G. \tag{2}$$

The advantage of treating convection terms explicitly is that the problem $(E + S\Delta t)\xi^{n+1} = r \equiv [r_P, \mathbf{r}_v]^t$ can be reduced to the problem of solving

$$[c^{-2} - (\Delta t)^2\nabla^2]P^{n+1} = r_P - \Delta t\nabla\cdot\mathbf{r}_v, \tag{3}$$

a standard elliptic problem which has been extensively studied and for which efficient solution techniques are known. This approach can be generalized to a semi-implicit two-fluid method; let $\xi = [P, \alpha, v_v^x, v_l^x, v_v^z, v_l^z]^t$ and develop linearized difference equations for mass and momentum of the form

$$(E' + S'\Delta t)\xi^{n+1} = (E - C\Delta t)\xi^n - G. \tag{4}$$

Here S' is analogous to S above in representing sonic propagation, C contains all convection terms, and E' may include interfacial exchange terms; one observes that E' is block diagonal with blocks

$$\begin{bmatrix} \alpha c_v^{-2} & \rho_v \\ (1-\alpha)c_l^{-2} & -\rho_l \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \alpha\rho_v + K\Delta t & -K\Delta t \\ -K\Delta t & (1-\alpha)\rho_l + K\Delta t \end{bmatrix} \quad \text{twice.}$$

These blocks are invertible provided only that $0 \leqslant \alpha \leqslant 1$ and the remaining quantities are positive; upon inverting E' and reducing S' we can again reduce (4) to a simple elliptic equation for pressures analogous to (3). This idea extends further to the full set of equations (1). A great deal of elaboration stands beteen this simplified description and practical two-fluid calculations: for example, the mass equation divergences $\nabla\cdot\rho\mathbf{v}$ are approximated by conservative difference expressions; also the linearization alluded to above may be repeated more than once per time step, so that Newton's method is used to solve the nonlinearities in the equations of state and in the exchange terms. Details can be found in Reed and Stewart [8]. By appropriate use of donor cell differencing, the method can be made numerically stable for time steps Δt limited only by the explicit differencing of C, the convection operator. The upper limit for Δt is the least time for either vapor of liquid to travel one spatial mesh width in any direction.

The advantages of this method are the inclusion of all multidimensional transport terms, with the ability to treat arbitrary recirculating or reversed flow patterns, and very general boundary conditions (including functional relationships between flow rate and pressure). The method is efficient because the reduced pressure problem

contains all the coupled effects of interfacial exchanges and sonic propagation in compact form; even when the coupling is very strong, the pressure problem can be solved relatively cheaply. The method is also very robust because it is based on well-understood techniques.

The principal disadvantage of this semi-implicit numerical method is the convective upper limit on time step size. The method was applied in the THERMIT code [8] to thermal-hydraulic analysis of light water reactor cores. For many of the transients such a code might calculate, this convective limit is mildly restrictive; but for some slower transients, one could achieve reasonable accuracy at lower cost if it were possible to take fewer time steps with larger Δt. Our aim in this paper is to present a new method of overcoming the time step limit associated with convection in one direction. This is particularly appropriate for reactor core calculations, where axial flow usually represents a far more restrictive time step limit than transverse flows. Other applications might be the multidimensional calculation of flow in a pipe, or in fast reactor subassemblies [9]. We have chosen a fractional step method in part because it may generalize to overcome convective limits in more than one direction.

A third method has been proposed for multidimensional two-phase flow by Spalding [10]. This method grew out of a technique originally developed for steady single-phase flow; it was then extended to transient problems and finally to two-fluid equations similar to (1). This method also treats all multidimensional transport terms and allows general boundary conditions. The method solves fully implicit difference equations and has therefore no a priori upper limit on time step size. An ingenious iteration scheme is used which requires strong underrelaxation of all variables to obtain convergence. (By strong we mean an underelaxation parameter very near 0.5). Wachspress [11] recently presented an illuminating convergence analysis of this method for steady incompressible single-phase flow. From this analysis one sees that the underrelaxation is needed to resolve the convection operator. A transient in which convection has small effect over each calculational time step (i.e., where the semi-implicit method is most effective) would be calculated inefficiently by this method unless one knew to eliminate the underrelaxation. For transients considered in this paper, where convection effects may be large in one direction but not in the other two, this fully implicit method might well need modification to be as efficient as our proposed method. All this applies to single-phase flow problems; for two-fluid equations the crucial underrelaxation parameters in the fully implicit technique of [10] are chosen ad hoc, with no supportive convergence analysis.

Fractional step methods [12] require only the convergence of solution techniques used in the separate fractional steps. We shall distinguish two types of fractional step methods (among others): time-splitting methods and stabilizing correction methods. In the next section we discuss possible time-splitting methods. In subsequent sections we propose a stabilizing corrections method, examine its numerical stability, and finally compare it to the semi-implicit method for a particular realistic thermal-hydraulic transient. We shall present the method for the two-fluid equations (1), even though like the semi-implicit method it has similar advantages for simpler equation sets (e.g., the homogeneous equilibrium model).

TIME-SPLITTING METHODS

In studying fractional step methods we want to capitalize on the efficiency of the semi-implicit two-fluid calculation method, which distinguishes between sonic propagation and interphase coupling on the one hand, and convection on the other. The former are resolved through implicit differences in an apparently optimal way, with the latter relegated to explicit difference treatment. Fractional step methods (see Yanenko [12] for a survey) separate the generator of an evolution operator into parts and build a solution over each time step out of fractional steps that resolve the different parts separately. Thus, our hope is to apply some variant of the semi-implicit technique in one fractional step, and add another fractional step (or steps) with implicit treatment of convection.

One might object that a simpler way would be to split the two-fluid equations into parts acting in each of the coordinate directions. However, this would abandon the simultaneous multidimensional resolution of pressure disturbances solved so efficiently by the semi-implicit method. Some accuracy would be forfeited, particularly for problems involving interior obstacles ([13]).

To establish terminology, we shall use *fractional step* methods to refer to the broadest class of techniques employing fractional time steps. By *time-splitting* we mean fractional step methods in which each part, or factor of the evolution operator, appears in one fractional step only. *Stabilizing correction* methods may, on the contrary, involve part of the operator differenced explicitly in one fractional step, with adjustment by an implicit resolution in another step. (Which comes "before" and "after" may be a matter of arbitrarily selecting one fractional step as the "first.") While usage of these terms in the literature varies, the above distinctions serve our purposes and appear consistent with [12].

The idea of time-splitting by physical phenomenon is not new; Yanenko [14] reported applying the idea to gas dynamics problems. We shall consider application to two-phase thermal hydraulics problems. Furthermore, we insist on strictly conservative differences approximations, since in closed circuit flow problems the loss of mass or energy for numerical reasons would be intolerable. (Strict numerical conservation of momentum is less important due to the large sources and sinks of momentum in a forced convection loop.) There exist numerous realizations of time-splitting in finite differences, but our particular goals will force the main choices.

Consider for simplicity the one-dimensional form of the single-phase mass conservation equation

$$\partial\rho/\partial t + \partial(\rho v)/\partial z = 0.$$

Adopting the usual staggered spatial mesh, with fluid state variables (density, pressure, temperature, viscosity, etc.) defined at integer-numbered cell centers (e.g., $k, k-1$) and velocities at half-integer numbered cell faces (e.g., $k-\frac{1}{2}$, $k+\frac{1}{2}$), we seek to split

$$\rho_k^{n+1} - \rho_k^n + (\Delta t/\Delta z)(\rho_k^{n+?} v_{k+1/2}^{n+?} - \rho_{k-1}^{n+?} v_{k-1/2}^{n+?}) = 0 \tag{5}$$

into fractional steps

$$\rho_k^{n+1/2} - \rho_k^n + (\Delta t/\Delta z)\rho_k^?(v_{k+1/2}^{n+1/2} - v_{k-1/2}^{n+1/2}) = 0 \tag{6a}$$

and

$$\rho_k^{n+1} - \rho_k^{n+1/2} + (\Delta t/\Delta z)v_{k-1/2}^?(\rho_k^{n+1} - \rho_{k-1}^{n+1}) = 0, \tag{6b}$$

the first relating to sonic propagation and the second to convection. Spatial indices in (6) are chosen so that the sum of the space-difference terms yields the conservative form of (5). We can fill in the question marks as follows. The time level of ρ in Eq. (6a) will be either n or $n-\frac{1}{2}$, the level of v in Eq. (6b) either $n+\frac{1}{2}$ or n. Consider a steady flow solution of (5), that is, $\rho_k^{n+1} = \rho_k^n$; although $\partial \rho v/\partial z = 0$ for steady one-dimensional flows, $\partial v/\partial z$ may certainly be nonzero, so that $\rho_k^{n+1/2} \neq \rho_k^n$ even for steady flow. In order for Eqs. (6) to add up to $\rho_k^{n+1} - \rho_k^n = 0$, we must therefore chose time level n for ρ in Eq. (6a) and $n+\frac{1}{2}$ for v in Eq. (6b). Thus if one wants densities and velocities consistent with mass conservation, one must use density from the convective fractional step and velocity from the sonic fractional step to form the mass flux ρv.

This is an interesting point not mentioned in [14], and might be of little consequence in certain applications; however, in two-phase thermal hydraulics problems it is crucial. Consider, for example, the steady flow of liquid along a heated tube. As the liquid temperature rises, its density decreases and the local velocity increases in order that ρv remain constant. Since the liquid density is little affected by pressure, one can obtain a good approximate solution by discarding the momentum equation and integrating $\partial \rho v/\partial z = 0$ and $\partial \rho v e/\partial z = Q_l$, or $\partial e/\partial z = Q_l/\rho v$. In other words, the conservation of mass and energy essentially determine ρ and v along the tube. Therefore, if one used a time-splitting scheme like Eqs. (6) above, one would have to regard n-level densities as correct and $n+\frac{1}{2}$-level densities as numerical artifice. One can easily seen that for large Courant numbers $v\Delta t/\Delta z$, the difference between ρ_k^{n+1} and $\rho_k^{n+1/2}$ would be larger than the spatial density differences. This wreaks havoc on the treatment of interfacial exchange terms. For example, interfacial drag in the two-fluid momentum equations must be differenced implicitly, so either the correct relative velocity will be balanced against the incorrect pressure gradient, or vice versa.

If there is a way past this dilemma using what we are calling time-splitting methods, we have not found it. Therefore we turn to a second kind of fractional step method, stabilizing corrections.

Stabilizing Corrections Method

The semi-implicit method was symbolized above

$$(E' + S'\Delta t)\xi^{n+1} = (E - C\Delta t)\xi^n - G,$$

where E', S' represent interphase exchange and sonic propagation, and C represents convection. In the same symbolism our stabilizing corrections method can be summarized as follows. Let S', C each be split into two parts, one containing only differences in the z-direction, and another part comprising x- and y-direction differences, thus

$$S' = S'_z + S'_{xy}, \qquad C = C_z + C_{xy}.$$

Our method consists of a first fractional step

$$(E' + S'\Delta t)\xi^{n+1/2} = (E - C\Delta t)\xi^n - G \tag{7}$$

identical to the semi-implicit step, but with Δt larger than the axial convective limit, followed by a correction

$$(E' + S'_z\Delta t + C_z\Delta t)\xi^{n+1} = (E' + S'_z\Delta t)\xi^{n+1/2} + C_z\Delta t\xi^n \tag{8}$$

which "undoes" the axial difference solution of the first step and replaces it by a fully implicit solution in the axial direction. Since C_{xy} is still treated explicitly, the convective limits in the transverse directions must be respected. We note that the numerical stability of this method is not obvious, since the first step by itself would be unstable for $\Delta t > \max(\Delta z/v_v, \Delta z/v_l)$, and since summing Eqs. (7) and (8) does not eliminate $\xi^{n+1/2}$. The question of stability will be discussed in the next section.

The above equations gloss over some important details of solving the nonlinear conservative difference equations. A more complete description is in order.

For simplicity we shall consider the two-dimensional case, and present only the detailed difference equations of the vapor phase; the liquid phase equations are identical in form. The difference equations are based on the usual staggered grid with α, ρ_v, e_v, P defined at cell centers indexed α_{jk}, etc. Index j refers to x-direction, k to z-direction. The velocities v_v^x and v_v^z are defined at cell faces normal to their associated directions, and have indices $(j+\frac{1}{2}, k)$ and $(j, k+\frac{1}{2})$, respectively. In the difference equations below, only spatial indices which differ from the indices of the first (time difference) term are indicated; thus in the mass equation $(\alpha\rho_v)$ means $(\alpha\rho_v)_{jk}$, while in the x-momentum equation $(\alpha\rho_v)$ means $(\alpha\rho_v)_{j+1/2,k}$. The difference equations for the semi-implicit fractional step are

$$(\alpha\rho_v)^{n+1/2} - (\alpha\rho_v)^n + \frac{\Delta t}{V}$$
$$\times \{[(\alpha\rho_v)^n A_x (v_v^x)^{n+1/2}]_{j-1/2}^{j+1/2} + [(\alpha\rho_v)^n A_z (v_v^z)^{n+1/2}]_{k-1/2}^{k+1/2}\} = \Gamma^{n+1/2}\Delta t, \tag{9a}$$

$$(\alpha\rho_v)^n \left\{(v_v^x)^{n+1/2} - (v_v^x)^n + \frac{\Delta t}{\Delta x}(v_v^x)^n[(v_v^x)^n]_{j-1/2}^{j+1/2}\right.$$
$$\left. + \frac{\Delta t}{\Delta z}(v_v^z)^n[(v_v^x)^n]_{k-1}^{k}\right\} + \alpha^n \frac{\Delta t}{\Delta x}[P^{n+1/2}]_j^{j+1}$$
$$= -K\Delta t(v_v^x - v_l^x)^{n+1/2} - F_v^x \Delta t (v_v^x)^{n+1/2}, \tag{9b}$$

$$(\alpha\rho_v)^n \left\{(v_v^z)^{n+1/2} - (v_v^z)^n + \frac{\Delta t}{\Delta x}(v_v^x)^n[(v_v^z)^n]_{j-1}^{j}\right.$$

$$\left. + \frac{\Delta t}{\Delta z}(v_v^z)^n[(v_v^z)^n]_{k-1/2}^{k+1/2}\right\} + \alpha^n \frac{\Delta t}{\Delta z}[P^{n+1/2}]_k^{k+1}$$

$$= -K\Delta t(v_v^z - v_l^z)^{n+1/2} - F_v^z \Delta t(v_v^z)^{n+1/2}, \tag{9c}$$

$$(\alpha\rho_v e_v)^{n+1/2} - (\alpha\rho_v e_v)^n + \frac{\Delta t}{V}\{[(\alpha\rho_v e_v)^n A_x(v_v^x)^{n+1/2}]_{j-1/2}^{j+1/2}$$

$$+ [(\alpha\rho_v e_v)^n A_z(v_v^z)^{n+1/2}]_{k-1/2}^{k+1/2}\} + P^n \left\{\alpha^{n+1/2} - \alpha^n\right.$$

$$\left. + \frac{\Delta t}{V}[\alpha^n A_x(v_v^x)^{n+1/2}]_{j-1/2}^{j+1/2} + \frac{\Delta t}{V}[\alpha^n A_z(v_v^z)^{n+1/2}]_{k-1/2}^{k+1/2}\right\} = (Q + Q_v)^{n+1/2}\Delta t. \tag{9d}$$

Volume V and areas A_x, A_z depend on the space mesh and rod bundle geometry. The notation $[\ ]_{j-1/2}^{j+1/2}$ indicates a spatial difference $(\ )_{j+1/2} - (\ )_{j-1/2}$. Donor cell rules govern the explicit velocity differences in the momentum equations (choices indicated correspond to nonnegative velocities) and also define the cell face values of α, ρ_v, e_v in the mass and energy equation differences. All terms on the right of mass and energy equations may depend on $\alpha^{n+1/2}$, $P^{n+1/2}$, $T_v^{n+1/2}$, $T_l^{n+1/2}$ at node (j, k) and on other variables at time level n. The method used to solve the above equations uses the reduction to a Poisson pressure problem, as sketched in the Introduction and detailed in Reed and Stewart [8].

The second fractional step stabilizes by correcting all *axial* convection terms in the above equations. It turns out that this can be done by solving a series of one-dimensional problems. First we stabilize the axial convection term in the transverse momentum equation by solving

$$(\alpha\rho_v)^n \left\{(v_v^x)^{n+1} - (v_v^x)^{n+1/2} + \frac{\Delta t}{\Delta z}(v_v^z)^n[(v_v^x)^{n+1}]_{k-1}^{k}\right\}$$

$$+ K\Delta t(v_v^x - v_l^x)^{n+1} + F_v^x \Delta t(v_v^x)^{n+1}$$

$$= K\Delta t(v_v^x - v_l^x)^{n+1/2} + F_x^x \Delta t(v_v^x)^{n+1/2} + (\alpha\rho_v)^n \frac{\Delta t}{\Delta z}(v_v^z)^n[(v_v^x)^n]_{k-1}^{k}. \tag{10}$$

We have written unknowns on the left to show that only v_v^x, v_l^x appear at time level $n+1$. Note that the stabilized cross-velocities involve not only implicit convective differences but new implicit exchange terms as well. Equation (10) and its mate for the liquid phase can be solved together. In fact, they form a system of linear equations in which each axial column of nodes can be solved independently by Gaussian elimination of a block tridiagonal matrix with 2×2 blocks.

The remaining stabilizing correction equations are also coupled; they are

$$(\alpha\rho_v)^{n+1} - (\alpha\rho_v)^n + \frac{\Delta t}{V}\left[(\alpha\rho_v)^{n+1}A_z(v_v^z)^{n+1}\right]_{k-1/2}^{k+1/2} - \Gamma^{n+1}\Delta t$$

$$= -\left[(\alpha\rho_v)^n A_x(v_v^x)^{n+1}\right]_{j-1/2}^{j+1/2}, \tag{11a}$$

$$(\alpha\rho_v)^n\left\{(v_v^z)^{n+1} - (v_v^z)^n + \frac{\Delta t}{\Delta z}(v_v^z)^n\left[(v_v^z)^{n+1}\right]_{k-1/2}^{k+1/2}\right\}$$

$$+ \alpha^n\frac{\Delta t}{\Delta z}\left[P^{n+1}\right]_k^{k+1} + K\Delta t(v_v^z - v_l^z)^{n+1} + F_v^z\Delta t(v_v^z)^{n+1}$$

$$= -(\alpha\rho_v)^n\frac{\Delta t}{\Delta x}(v_v^x)^n\left[(v_v^z)^n\right]_{j-1}^{j}, \tag{11b}$$

$$(\alpha\rho_v e_v)^{n+1} - (\alpha\rho_v e_v)^n + \frac{\Delta t}{V}\left[(\alpha\rho_v e_v)^{n+1}A_z(v_v^z)^{n+1}\right]_{k-1/2}^{k+1/2}$$

$$+ P^n\left\{\alpha^{n+1} - \alpha^n + \frac{\Delta t}{V}\left[\alpha^{n+1}A_z(v_v^z)^{n+1}\right]_{k-1/2}^{k+1/2}\right\} - (Q + Q_v)^{n+1}\Delta t$$

$$= -\frac{\Delta t}{V}\left\{\left[(\alpha\rho_v e_v)^n A_x(v_v^x)^{n+1}\right]_{j-1/2}^{j+1/2} + P^n\left[\alpha^n A_x(v_v^x)^{n+1}\right]_{j-1/2}^{j+1/2}\right\}. \tag{11c}$$

Note that the level $n+1$ cross-velocities v_v^x also appear in the mass and energy equations as stabilizing corrections; we have put these terms on the right because they are known at this stage. The terms on the left contain the unknowns at level $n+1$. Closer inspection shows that Eqs. (11), together with their liquid-phase counterparts, can be grouped into separate systems for each axial channel; the channels can thus be solved independently of each other. Furthermore, the structure of the equations for an axial channel is identical to that for a one-dimensional flow problem with fully implicit differencing. Such equations can be and have in the past been solved by a Newton iteration technique in which the Jacobian matrix (a block tridiagonal one with partially filled 6×6 blocks) is directly inverted by Gaussian elimination. Such a one-dimensional fully implicit technique has been used (with equations slightly different from (1)) in the TRAC code [6], for example.

In sum, our method starts with a first fractional step in which semi-implicit difference equations are solved for a time step size Δt above the axial convective stability limit. In the second fractional step, stabilizing corrections are computed first for the cross-velocities (one axial column of nodes at a time), then for axial velocities, densities, energies by a one-dimensional fully implicit method applied to each axial channel. Since inverting the $1-\mathrm{D}$ fully implicit Jacobian takes somewhat more computational effort per node than the semi-implicit method, this stabilizing corrections scheme will be advantageous when Δt is at least twice the axial convective limit.

Numerical Stability

The fractional step method we have chosen has an advantage in accuracy, as will be demonstrated below; however, it is no trivial task to verify the numerical stability of the method. We have carried out a von Neumann local linear stability analysis of the difference equations (9)–(11), neglecting the energy equations and the phase change rate Γ, but including the interfacial drag term for momentum exchange. The reason for this is that the two-fluid equations (1) are known to have a pair of complex characteristic roots, indicating they do not lead to a well-posed initial value problem. (The mathematical theory is not absolutely conclusive, but Lax [15] has shown that solutions of linearized systems with complex characteristics cannot be bounded in terms of initial data, and more recently in [16] has considered non-linear systems.) Hence no consistent numerical scheme for the two-fluid equations (1) will be stable in the usual sense. Notwithstanding their ill-posedness, two-fluid equations can be solved numerically and give well-behaved results, as shown in [17], if interfacial drag is present and mesh spacing is not unreasonably fine.

To carry out a linear stability analysis, we consider the growth of a Fourier mode of the discrete solution of Eqs. (9)–(11) with $\xi^n_{jk} = \xi^n \exp(ijl\,\Delta x) \exp(ikm\,\Delta z)$, where $l\,\Delta x$, $m\,\Delta z$ take values equal to π divided by a positive integer less than or equal to the total number of mesh points in the appropriate direction. This Fourier mode we characterize by the vector $\xi^n = [P^n, \alpha^n, (v_v^x)^n, (v_l^x)^n, (v_v^z)^n, (v_l^z)^n]^t$ at time level n, by ξ^{n+1} at time level $n+1$. After linearizing Eqs. (9a) – (9c) for vapor and liquid we obtain a system of linear equations relating $\xi^{n+1/2}$ to ξ^n; similarly linearizing Eq. (10) leads to a relation amongst ξ^{n+1}, $\xi^{n+1/2}$, and ξ^n, while Eqs. (11a)–(11b) yield a relation between ξ^{n+1} and ξ^n. By eliminating $\xi^{n+1/2}$ from these linear equations, we obtain equations

$$A\xi^{n+1} = B\xi^n$$

from which the amplification factors λ can be found (cf. [18, p. 68ff.]) as the roots of

$$\det(A\lambda - B) = 0. \tag{12}$$

As in [17], our ad hoc condition for a well-behaved numerical procedure is that $|\lambda| < 1$. The characteristic equation (12) was generated with the aid of the MACSYMA symbolic computing system [19]; in the special case $\mathbf{v}_v = \mathbf{v}_l$ and $c_v = c_l = \infty$, the roots are

$$\frac{\alpha(1-\alpha)\rho_v\rho_l(1-u_x)}{\alpha(1-\alpha)\rho_v\rho_l(1+u_z) + K\,\Delta t\,\rho} \qquad \frac{\alpha(1-\alpha)\bar{\rho}(1-u_x)}{\alpha(1-\alpha)\bar{\rho}(1+u_z) + K\Delta t}$$

$(1-u_x)/(1-u_z)$ twice, and zero twice. Here $\rho = \alpha\rho_v + (1-\alpha)\rho_l$, $\bar{\rho} = \alpha\rho_l + (1-\alpha)\rho_v$, $u_x = (v^x\Delta t/\Delta x)[1 - \exp(-il\Delta x)]$, and $u_z = (v^z\Delta t/\Delta z)[1 - \exp(-im\Delta z)]$. For comparison, the equation $\phi_t + v^x\phi_x = 0$ solved by explicit donor-cell differences would give the amplification factor $1 - u_x$, while the equation $\phi_t + v^z\phi_z$ solved by implicit

differences would give $1/(1+u_z)$. Thus the above expression indicates well-behaved numerical solutions ($|\lambda| < 1$) in the equal velocity, incompressible fluids case, provided the Courant–Friedrichs–Lewy condition $|v^x \Delta t/\Delta x| \leqslant 1$ is satisfied for the cross velocities. This holds for all $K \geqslant 0$, since Eqs. (1) have no complex characteristics when $\mathbf{v}_v = \mathbf{v}_l$.

For the more general case we have had to rely on numerical solution of MACSYMA-generated expressions for (12) over the range of expected values of the pressure, void fraction, velocities, and mesh spacing. In all cases we found $|\lambda| < 1$ if the cross-velocites remain below the convective limit and if the fluid velocities are less than or equal to the individual phase sonic velocities. In practice, all our calculations of pressurized water reactor (PWR) core thermal hydraulic transients have been well behaved. An arbitrary test problem at near-atmospheric pressure was also well behaved.

Numerical Example

To test the stabilizing corrections method, we computed a PWR transient with considerable asymmetry in the transverse directions. The test problem involved nine typical channels arranged together in a 3×3 array (cf. Fig. 1). Starting from normal full flow in the axial direction and full-power heat generation in the fuel rods, the transient involved the following sequence of events. (1) At $t = 0$ the inlet velocities begin to decay exponentially until after 60 sec they are 10 % of initial values; this

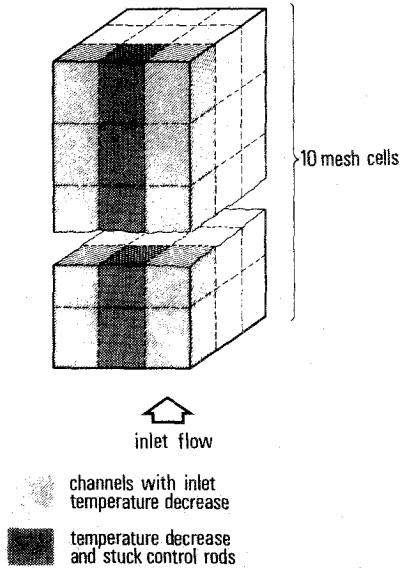

FIG. 1. Test problem configuration.

corresponds to a coastdown of all reactor coolant pumps such as might occur with a loss of AC power at the plant site. (2) At $t = 3$ seconds, the heat generation rate in all fuel rods drops abruptly to about 14 % of full power, and then decays exponentially to about 4 % after 60 sec, except in one channel which has an excess of heat generation equal to 2% of the initial power; this corresponds to reactor scram with one stuck control element assembly. (3) At $t = 4$ sec the inlet temperatures in one row of three channels begin to decrease until at the end of 60 sec they are about 85° C lower than in the other channels; this corresponds to a steamline break in one primary loop. The purpose of this test problem was of course not to analyze the physical modelling of such accident conditions, but only to compare the semi-implicit method with the stabilizing crrections method in terms of numerical accuracy and computing efficiency.

The axial velocities during this transient with the chosen mesh spacing impose maximum time step sizes with the semi-implicit method from about 0.07 sec at full flow to 0.3 sec after 60 sec; we chose 1-second time steps with the stabilizing corrections method except during the initial period of most rapid decrease in the power when smaller time steps were used. The total number of time steps was 364 with the semi-implicit method and 86 with the stabilizing corrections. Both methods used three Newton iterations for the semi-implicit step; the one-dimensional fully implicit iterations reached full convergence in two iterations. The transient required 187 sec of CPU time on a CDC 7600 for the semi-implicit method versus 59 sec for the stabilizing corrections method. (With a relatively simple overlapping storage scheme, the core storage requirements of the two methods are the same.)

Multidimensional two-fluid calculations such as these produce a wealth of information, including three-dimensional velocity vector fields as well as scalar fields for void fraction, pressure, and fluid conditions throughout the transient. Rather than reproduce the results in detail, we summarize the comparison of the two methods. The largest discrepancy was in the void fractions, which rose to about 7 % (accounting for subcooled boiling) at the time of reactor scram; the two calculations disagreed by about 0.5 % in the largest voids. After scram, the voids collapsed and the flow became single-phase; at the end of 60 sec the liquid axial velocities agreed within less than one percent, while the cross-velocities agreed within about 2 % of the largest values. Both methods show the onset of a flow recirculation pattern within the core at about 60 sec. The resulting locally negative axial velocities would cause a breakdown if a marching solution method were used, but the stabilizing corrections method continued to compute the recirculation with no difficulty.

Conclusions

We have shown that a semi-implicit numerical method for two-fluid calculation of two-phase flow can be extended to overcome the convective time step size limitation in one direction. This extension is a fractional step method of the stabilizing corrections type, and can be efficient for slowly evolving transients with flow

predominately in one direction. A realistic themal reactor core thermal–hydraulic problem demonstrated the accuracy and improved computing efficiency of the method.

There are several directions for further development. One involves more efficient solution of the one-dimensional fully implicit equations; although the $1-D$ Newton iterations converged quickly for the problems we have computed, a convergence acceleration technique was recently devised [20] for $1-D$ problems that could be applied to our stabilizing corrections step. Another possibility is that a recently announced two-step method for one-dimensional two-fluid calculations [21] could be used to supplant the one-dimensional fully implicit axial calculations in the stabilizing corrections.

Further development could also lead to overcoming time step limits due to convection in all directions. A natural extension of the fractional step method might for example employ convection-stabilizing corrections successively for each coordinate direction. The result would be a method of the same degree of numerical implicitness as that of Spalding and co-workers [10]. It is an open question which approach would in general be more efficient, and the answer to that question may in part depend on what sort of convergence analysis can be furnished for the latter method in the two-fluid case.

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