

NUMERICAL SOLUTION OF ONE DIMENSIONAL TWO-PHASE DRIFT FLUX
EQUATIONS WITH A BLEND OF PARTIALLY AND FULLY IMPLICIT METHODS

by

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ABSTRACT

A numerical method for treating two-phase flow in pipes is presented which incorporates the use of a partially implicit scheme in regions of relatively low flow velocity and a fully implicit treatment in regions of high velocity. This method takes advantage of the lower cost per iteration of the partially implicit scheme, without being limited by its conditional stability. Applications of this approach to water reactor blowdown calculations produce reductions in computer time by factors of 2 to 4 without a significant loss of accuracy.

INTRODUCTION

The Transient Reactor Analysis Code (TRAC) is currently being developed for the thermal-hydraulic analysis of water reactor accidents. In the early versions of TRAC, the drift-flux equations for one dimensional two phase flow were solved with a partially implicit method described by Liles and Reed.¹ This method is stable as long as the time step is limited by the Courant relation

$$\Delta t \leq \left| \frac{\Delta x}{V} \right| \quad (1)$$

where Δx is the mesh spacing and V the flow velocity. For many problems this stability limit is adequate. However, we have found that accurate reproduction of flow near breaks in blowdown calculations requires relatively fine spacial resolution. Since the flow velocities can be extremely high in these regions, the Courant condition requires time steps which are quite small. In problems with a large total number of mesh cells the cost in computer time for following the full history of a blowdown with such small time steps can be prohibitively high.

One way of increasing the time step size is to use a fully implicit method.^{2,3,4} Results presented later in this paper show that in blowdown calculations, when a fully implicit numerical method is used to avoid stability limitations, the Courant condition (1) can be violated by a factor of 10 without altering the results by more than 1%. Total computational time of course does not decrease by an order of magnitude. Factors of two to four, depending on convergence criteria, are not unusual, however. One reason for this is that with larger time steps, state variables can change more per time step and the number of iterations required to solve the finite difference equations may increase. Another reason is that the fully implicit

method requires nearly twice the computational time per cell per iteration needed for the partially implicit scheme. Therefore, it is worthwhile to design an overall method for which the stability condition (1) can be exceeded in the locations where high velocities occur, but where cheaper procedures are utilized elsewhere.

FLOW EQUATIONS AND NUMERICAL METHODS

The model used to describe two-phase flow in this work requires the simultaneous solution of the following four partial differential equations:^{5,6}

$$\frac{\partial \rho_m}{\partial t} + \mathbf{v} \cdot \rho_m \hat{\mathbf{v}}_m = 0 \quad . \quad (3)$$

$$\frac{\partial(\alpha \rho_v)}{\partial t} + \mathbf{v} \cdot (\alpha \rho_v \hat{\mathbf{v}}_m + \rho_f \hat{\mathbf{v}}_r) = 0 \quad . \quad (4)$$

$$\frac{\partial(\rho_v \mathbf{v}_m)}{\partial t} + \mathbf{v} \cdot (\rho_m \mathbf{v}_m \hat{\mathbf{v}}_m + \rho_f (\mathbf{v}_v - \mathbf{v}_r) \hat{\mathbf{v}}_r) = -p \mathbf{v} \cdot (\hat{\mathbf{v}}_m + \rho_f (\frac{1}{\rho_v} - \frac{1}{\rho_r}) \hat{\mathbf{v}}_r) + q \quad . \quad (5)$$

$$\frac{\partial \hat{\mathbf{v}}_m}{\partial t} + \hat{\mathbf{v}}_m \cdot \mathbf{v} \hat{\mathbf{v}}_m = -\frac{1}{\rho_m} (\nabla p + \mathbf{v} \cdot \rho_f \hat{\mathbf{v}}_r \hat{\mathbf{v}}_r) + \frac{q}{\rho_m} - K \hat{\mathbf{v}}_m |\hat{\mathbf{v}}_m| \quad . \quad (6)$$

where,

$$\rho_m = \alpha \rho_v + (1 - \alpha) \rho_r \quad (6)$$

$$\rho_f = \frac{\alpha(1-\alpha)\rho_v\rho_r}{\rho_m} \quad (7)$$

and

$$e_m = \frac{\alpha \rho_v e_v + (1-\alpha) \rho_l e_l}{\rho_m} \quad (8)$$

Variables appearing in the above equations have the following meanings:

ρ_m	mixture density
ρ_v	vapor density (microscopic)
ρ_l	liquid density (microscopic)
α	vapor volume fraction
v_m	mixture velocity
v_r	relative velocity between phases
e_v	vapor specific internal energy
e_l	liquid specific internal energy
e_m	mixture specific internal energy
Γ	vapor production rate due to phase change
P	pressure
g	force of gravity
k	wall friction coefficient
Q	heat source
T_l	liquid temperature
T_v	vapor temperature

In these equations we have assumed pressure equilibrium between the liquid and vapor phases. In addition, an assumption regarding partition of energy between the phases is needed. For this work it was assumed that the two phases were at the same temperature. Finally, equations of state are specified for both liquid and gas, and correlations used to obtain \dot{v}_r , Q , Γ .

Equations (2) - (5) are solved for one dimensional pipes using a staggered Eulerian mesh, where state variables such as pressure, internal energy, and void fraction are obtained at the center of cells with length Δx_j , and the mean and relative velocities are obtained at the cell boundaries. Because of this staggered mesh, it is necessary to form spacial averages of various quantities to obtain the finite difference form of the divergence operator. To produce stability in the partially implicit method a donor-cell average was used of the form,

$$\langle xv \rangle_{j+\frac{1}{2}} = \begin{cases} x_j v_{j+\frac{1}{2}} & , \text{ for } v_{j+\frac{1}{2}} \geq 0. \\ x_{j+1} v_{j+\frac{1}{2}} & , \text{ for } v_{j+\frac{1}{2}} < 0. \end{cases} \quad (9)$$

where an integer subscript indicates that a quantity is evaluated at a mesh cell center and a half integer denotes that it is obtained at a cell boundary. With this notation the finite difference divergence operator is

$$v_j \cdot (xv) = \left(A_{j+\frac{1}{2}} \langle xv \rangle_{j+\frac{1}{2}} - A_{j-\frac{1}{2}} \langle xv \rangle_{j-\frac{1}{2}} \right) / \text{Vol}_j \quad (10)$$

where A is the pipe's cross-sectional area, and Vol_j is the volume of the j 'th cell. Slight variations of these donor-cell terms appear in the velocity equation. Donor cell averages are of the form:

$$\langle xv_r^2 \rangle_j = \begin{cases} x_j v_r^2 \Big|_{j-\frac{1}{2}} & , \quad v_r \Big|_{j-\frac{1}{2}} \geq 0 \\ x_j v_r^2 \Big|_{j+\frac{1}{2}} & , \quad v_r \Big|_{j+\frac{1}{2}} < 0 \end{cases} \quad (11)$$

and the term $v_m \cdot \nabla v_m$ is donor-called as

$$v_{m,j+\frac{1}{2}} v_{j+\frac{1}{2}} v_m = v_{m,j+\frac{1}{2}} \begin{cases} (v_{m,j+\frac{1}{2}} - v_{m,j-\frac{1}{2}})/\Delta x_j, & v_{m,j+\frac{1}{2}} \geq 0 \\ (v_{m,j+3/2} - v_{m,j+\frac{1}{2}})/\Delta x_{j+1}, & v_{m,j+\frac{1}{2}} < 0 \end{cases} \quad (12) \quad (12)$$

Given the preceding notation, the finite difference equations for the partially implicit method are:

$$(\rho_m^{n+1} - \rho_m^n)_j / \Delta t + v_j \cdot (\rho_m^n v_m^{n+1}) = 0 \quad (13)$$

$$(\alpha^{n+1} \rho_v^{n+1} - \alpha^n \rho_v^n)_j / \Delta t + v_j \cdot (\alpha^n \rho_v^n v_m^{n+1}) + v_j \cdot (\rho_f^n v_r^n) = r^{n+1} \quad (14)$$

$$(\rho_m^{n+1} e_m^{n+1} - \rho_m^n e_m^n)_j / \Delta t + v_j \cdot (e_m^n e_m^n v_m^{n+1}) + v_j \cdot (\rho_f^n (e_v^n - e_t^n) v_r^n) \quad (15)$$

$$= - p_j^{n+1} / v_j + (v_m^{n+1}) + v_j \cdot (\rho_f^n (\frac{1}{\rho_v^n} - \frac{1}{\rho_f^n}) v_r^n) + q_j^n$$

$$(v_m^{n+1} - v_m^n)_{j+\frac{1}{2}} / \Delta t + v_{m,j+\frac{1}{2}} v_{j+\frac{1}{2}} v_m = - [(p_{j+1}^{n+1} - p_j^{n+1}) / \Delta x_{j+\frac{1}{2}} \quad (16)$$

$$- v_{j+\frac{1}{2}} \cdot (\rho_f^n v_r^n)] / \bar{\rho}_{m,j+\frac{1}{2}}^n + \epsilon^n - k^n v_m^{n+1} |v_m^n|$$

where

$$\bar{\Delta x}_{j+\frac{1}{2}} = (\Delta x_j + \Delta x_{j+1}) / 2 \quad (17)$$

and

$$\rho_{m,j+1}^n = (\Delta x_j \rho_{m,j+1}^n + \Delta x_{j+1} \rho_{m,j}^n) / (2 \Delta x_{j+1}) \quad (18)$$

The superscript n indicates that the quantity is evaluated at the "current" time and thus is known, while the superscript $n+1$ indicates that the variable is evaluated at the new time and hence is an unknown for which the equations must be solved. These equations are equivalent to those given by Liles and Reed in the full donor-cell limit, except that the term $\rho_{m,j+1}^n$ in the velocity equation is computed here as a simple spatial interpolation.

When constructing a set of fully implicit finite difference equations, the use of donor cell averaging is no longer necessary for stability, and a straight interpolation is often preferred. However, for reasons which will be discussed later, we chose to use the same donor cell averaging in the fully implicit method that was used previously. As a result the finite difference equations for this method are identical to equations (13) - (18) when the superscripts on all terms not divided by Δt are $n+1$ rather than n .

In a one cell transition zone between a region which is solved partially implicitly and another region solved fully implicitly, the finite difference equations must be altered to maintain conservation of mass and energy. In such a zone the fully implicit formulation is used, except that the divergence terms are altered to the form

$$\nabla_j \cdot (XV_m) = (\Lambda_{j+1} \langle X^{n+1} V_m^{n+1} \rangle_{j+1} - \Lambda_{j-1} \langle X^n V_m^{n+1} \rangle_j) / \text{Vol}_j, \quad (19)$$

where it has been assumed that the fully implicit region is at the higher values of j .

Both sets of finite difference equations are solved with a full Newton-Raphson method rather than the block implicit technique (BIT) described by

Liles and Reed. This involves inserting the mixture property definitions into the finite difference schemes. The resulting expanded algebraic equations are then linearized and the thermal and caloric equations of state for each phase are inserted (see reference 1 for a more detailed description). The basic practical difference between these solution procedures is that the Newton-Raphson requires the inversion of a block tri-diagonal matrix, and the BIT method drops the off-diagonal blocks of this matrix, solving only a block diagonal system. For the fully implicit equations this is absolutely essential, since the BIT can fail to converge if the stability condition given by equation 1) is violated by very much. For the particular one-dimensional equations used in the partially implicit scheme the tridiagonal procedure can be programmed so that it requires essentially the same amount of computing time per iteration as the BIT. However, in many applications the Newton-Raphson will converge to a given tolerance in fewer iterations, reducing the total computational cost per time step, and thus making it the preferred solution method.

NUMERICAL RESULTS

The earliest tests of the combined methods consisted of two pipe segments linked to form a closed loop. One segment was treated fully implicitly and the other partially implicitly. A constant momentum source was applied, wall friction specified, and the system driven to a steady state. The most important result to come from these tests was the observation that for two phase systems where the averages in the fully implicit section were done by spacial interpolation rather than donor-celling, non-physical standing waves occurred in the loop. However, when donor-celling was used in the fully implicit section, no such waves appeared, indicating that the non-physical results were a direct consequence of the interfaces between the two different spacial differencing methods.

The bulk of the tests were run on the blowdown of a pipe (unheated RSR test problem 2, see Kirchner⁷ for details). The noding used for the pipe is

given in Table 1. The system is initially pure liquid with pressures near 9.8 MPa, temperatures of 543 K, and steady state flow consistent with a velocity into cell 16 of 1.4 m/sec. All calculations were initiated by setting a zero velocity boundary condition on the left boundary of cell 1, and atmospheric boundary conditions to the right of cell 16, simulating the simultaneous closing of a valve at one end of the pipe and the opening of a break at the other.

A base calculation was first performed using only the partially implicit procedure with the time step controlled by condition 1) except during the first 0.1 sec., when it was limited to 0.5 milliseconds to resolve the initial rapid depressurization to saturation conditions. This resulted in a time step over the remaining 7.9 seconds of the blowdown which remained fairly constant at about 2 milliseconds. The time histories of pressure for zones 1 and 16 of this run are plotted as solid lines on Figure 1. Though spacial zoning and timestep size are different, the results of this run are basically the same as those presented by Kirchner.⁷

Initial tests of the fully implicit method were performed using a spacial interpolation (central differencing) approach, rather than donor cell averaging. This approach was first applied to the whole pipe with the same zoning and time step size as the base case. During the final 7 seconds of the blowdown, the pressures obtained from this calculation varied by 10% to 50% from those of the base case. To check which calculation was more accurate, calculations were run for both methods with successively smaller mesh spacing. The results of the donor-celled, partially implicit method did not change significantly when the zoning was refined, but the results of the central difference scheme approached those of the base case as the cell lengths were decreased. This is interesting since the spacial error terms of a central difference scheme are of the order Δx^2 , compared to errors of the order Δx for the donor celled method. However, it should not be too surprising because this problem contains large changes in void fraction, pressure, and the spacial derivatives of these

quantities over very short distances. Due to these results and those with the steady state loop problems, donor-cell averaging was adopted for the fully implicit code.

To demonstrate the dependence of accuracy on time step, the blowdown problem was rerun with the fully implicit donor-cell method. Again the time step was fixed at 0.5 milliseconds for the first 0.1 second, but after that the time step was set to 0.04 seconds in one case and 0.2 seconds in another. The results obtained with timesteps of 0.2 seconds are plotted in Fig. 1 as dashed lines. They agree with the base case to within 10% when time steps of 0.04 seconds are used, the results agreed with the base case to within 1%, and could not be distinguished as separate lines in Fig. 1. Hence, excellent accuracy was achieved at 20 times the Courant number.

Finally the full combined method was tested on this problem. Cells 1-10 were treated with the partially implicit equations, cell 11 was the transition zone, and cells 12-16 were computed with the fully implicit equations. The time step was controlled by the velocity between cells 10 and 11, and averaged about 0.02 seconds. As would be expected from previous results, this run agreed with the base case to better than 1% at all times. For this particular problem, the savings in computer time for the final 7.9 seconds was roughly a factor of 3.

In addition to the simple tests which have been described, this technique has been successfully applied to the numerical analysis of the semiscale tests run by the Idaho National Engineering Laboratory.⁸ No direct timing comparisons were made between blended approach and partially implicit method for this problem due to the large amounts of computer time required. However, some indirect comparisons are available. Runs with the blended scheme were done with 30% more mesh cells than the old method. In the regions near the break where velocities were highest, a fully implicit treatment allowed mesh lengths which were

an order of magnitude smaller than those used for the partially implicit method. For calculations which were comparable in all respects except those just mentioned, the blended approach required 25% to 40% less computer time, depending on the total elapsed real time at which the calculations were terminated.

CONCLUSIONS

We have shown that a combination of two finite difference methods with different levels of implicitness can be used effectively to avoid stability problems without sacrificing accuracy. Though a fully implicit set of finite difference equations can be applied to achieve the same end, we have found that for blowdown problems this mixed method is less costly to use.

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TABLE 1

Cell Numbers	Length (m)	Volume (m ³)	Flow Area (m ²)
1-5	2.02	1.08×10^{-3}	5.31×10^{-4}
6-10	.80	2.77×10^{-4}	3.46×10^{-4}
11-13	1.99	4.52×10^{-4}	2.26×10^{-4}
14	1.49	3.39×10^{-4}	2.26×10^{-4}
15-16	.99	2.26×10^{-4}	2.26×10^{-4}

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Figure Captions

**Figure 1. Pressure versus time for pipe blowdown calculations with
 $\Delta t = .002$ and $\Delta t = .2$ seconds.**

