TECHNICAL MEMORANDUM

ANL-CT-76-46
LMFBR Structural Materials
and Design Engineering
(UC-79h)

TWO-STEP EXPLICIT PROCEDURE FORMULATION FOR
FAST DECOMPRESSION OF TWO-PHASE WATER/STEAM MIXTURE*

by

Y. W. SHIN

Components Technology Division

BASE TECHNOLOGY

May 1976

*Work was performed while on temporary foreign assignment at Power Reactor and Nuclear Fuel Development Corporation, Oarai Engineering Center, Japan.

NOTICE
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

This document is
PUBLICLY RELEASABLE

B. C. Steele
Authorizing Official

Date: 7-19-87

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

TABLE OF CONTENTS

	<u>Page</u>
NOMENCLATURE	ii
ABSTRACT	1
I. INTRODUCTION	2
II. GOVERNING DIFFERENTIAL EQUATIONS	4
III. DIFFERENCE FORMULATIONS	7
A. Two-Step Lax-Wendroff Scheme	7
B. Rubin-Burstein Scheme	8
IV. FORMULATION OF BOUNDARY CONDITIONS	9
A. Reservoir-End Boundary	10
B. Break-End Boundary	11
C. Alternate Treatment	12
V. NUMERICAL STABILITY	13
VI. DISCUSSIONS	14
REFERENCES	15

NOMENCLATURE

a	Non-dimensional parameter controlling shock thickness, Eq. (8)
c	Sonic speed
e	Total energy per unit volume, Eq. (11b)
E	Total energy per unit mass, Eq. (4)
F	Flux vector, Eq. (11b)
g	Gravitational acceleration
i	Internal energy per unit mass
j	Grid point index
k	Grid point index for the break-end boundary
K	Pressure loss coefficient, Eq. (18)
K'	Pressure loss coefficient, Eq. (20)
l	Length parameter defined in Eq. (8)
L	Pipe length
m	Momentum per unit volume, Eq. (11a)
n	Time-step index
p	Static pressure
q	Pseudoviscosity
Q	Heat input per unit tube length and per unit cross-sectional area
S	Source vector, Eq. (10c)
t	Time
Δt	Time-step
U	Vector representing independent variables, Eq. (10a)
β	Parameter combination as defined in Eq. (14)
ρ	Density
ρ_0	Density in the reference configuration, Eq. (6)
θ	Tube inclination angle
τ	Wall friction per unit tube length and per unit cross-sectional area

TWO-STEP EXPLICIT PROCEDURE FORMULATION FOR
FAST DECOMPRESSION OF TWO-PHASE WATER/STEAM MIXTURE

by

YONG W. SHIN

ABSTRACT

For numerical solution of fast two-phase decompression taking place in heat transfer tubes following sudden tube rupture, the problem has been formulated in two-step explicit procedures. The basic schemes used are the two-step Lax-Wendroff scheme and the Rubin-Burstein scheme with special treatments provided for boundary condition formulation. The weak numerical instabilities associated with the basic Lax-Wendroff scheme are treated by aid of a pseudoviscous term added in the governing conservation equations. The pseudoviscous term will also spread any sharp discontinuities over a few mesh points so that the shocks are represented approximately.

An earlier approach to this problem using the method of characteristics faced considerable difficulties in handling the flashing transients. The main difficulty was due to the increased nonlinearity, as the sonic speed changes by many factors and the flow accelerates with phase change, that results in large discontinuities which must be handled as internal boundaries. The direct finite difference technique with the pseudoviscosity treatment considered here is one of the approaches chosen to overcome this difficulty. Formulations given in this report include special considerations in the boundary condition treatment in anticipation of potential difficulties at the boundaries. The transient is actually driven from the boundaries and prior works revealed that the boundary treatment is the key problem area.

I. INTRODUCTION

It is generally accepted that, in the design of sodium-heated steam generators, the leak of water/steam into sodium cannot be completely ruled out. Hence, both from design and safety considerations the leak and its consequence must be analyzed to provide adequate guides. The steam generator development and its safety have been important subjects of the LMFBR program and the approach has been by way of computer code development and performing scaled leak experiments. The computer code under development in many countries, including the United States and Japan, is an integral code by which the entire sequence of events following a design basis leak can be calculated. Time-dependent water/steam leak into sodium, the exothermic sodium-water reaction, hydrogen gas generation, pressure-pulse generation and its propagation through the secondary loop, activation of relief systems, subsequent sodium and reaction-products venting, and waterside blowdown together with structural response will all be the capabilities of the integral code on its completion.

This activity is a subtask of the integral code development activity. It will include capabilities for initial fast transient to determine the initial leak rates as well as the longer time blowdown event. Major emphasis will first be placed on the initial transients which will be the determining factor for the initial spike pressure which will, in turn, be the most important design criterion for the steam generator. From existing test data^{1,2} and computer predictions, using TRANSWRAP,³ the time domain of importance for initial waterside transient is in the order of initial 50 msec.

Earlier approaches to this waterside transient used the method of characteristics. This method proved to be accurate and convenient especially in the boundary condition treatment. Unfortunately, however, the method of characteristics was difficult to handle the fast flashing transient accompanying phase change since the drastic change of local sonic speed and flow acceleration due to sudden decompression creates large discontinuities that must be treated as internal boundaries. Some success has been reported by Galluzzo⁴ where the discontinuities were treated approximately by the weak shock theory.⁵ Nevertheless, the effect of this approximation and the degree of nonlinearity that limits the applicability of this approximation technique are difficult to estimate.

This report describes the formulation of the problem of fast waterside decompression for numerical treatment by two-step explicit schemes of a second-order accuracy. The discontinuities existing in the solution are approximated by spreading over a few mesh points by means of the pseudoviscosity technique.⁶ The two-step Lax-Wendroff⁷ scheme was formulated. In order to attain a smooth starting transient, the implicit-like scheme suggested by Rubin and Burstein⁸ is also considered. Special boundary condition formulations are included that are slight variations from the basic schemes for the interior mesh points. Alternate boundary treatments have also been discussed in anticipation of difficulties associated with

the boundary treatment. Choice of any particular boundary formulation will be made on the basis of numerical results and their comparison with analytical and experimental data.

Many computer codes^{9,10,11} exist that are developed for slower decompression phenomena such as the coolant system blowdown of water reactors. These codes can handle phase change as long as the quality remains low and the decompression takes place slowly. Nevertheless, the fast two-phase transient, taking place in a time domain appropriate for the steam generator design and safety considerations, has not as yet been successfully treated and yet remains an open subject. From unreported earlier works, indication was observed that the numerical formulation of the boundary conditions, the reservoir- and break-end boundary conditions in particular, was difficult and usually caused numerical instabilities. The obvious physical conditions alone at these boundaries are not sufficient and additional conditions are needed to carry out the numerical procedure. Choice can be made from a wide variety of conceivable formulations as long as they are consistent with the basic numerical schemes used and physically meaningful. Boundary treatment is an open question requiring guidance from supporting analytical and experimental efforts.

II. GOVERNING DIFFERENTIAL EQUATIONS

The governing equations considered are the one-dimensional compressible flow equations with homogeneous flow properties assuming phase equilibrium. This homogeneous flow model may not be adequate for the starting transient where flow is highly accelerating; however, in light of other uncertainties of the problem, the model is considered satisfactory, especially in the longer time range. The equations include such effects as friction, gravity force, and heat transfer so that the long-time unsteady flow solution converges to the steady-state solution.

Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \rho u = 0. \quad (1)$$

Momentum:

$$\frac{\partial}{\partial t} \rho u + \frac{\partial}{\partial x} (\rho u^2 + p) = \rho g \cos \theta - \tau.$$

Energy:

$$\frac{\partial}{\partial t} \rho E + \frac{\partial}{\partial x} \rho \left(E + \frac{p}{\rho} \right) u = \rho g u \cos \theta - u \tau + Q. \quad (3)$$

The work term in the energy equation associated with the wall-slip is included for the sake of completeness. In the calculation, it may be neglected when no slip is assumed on the wall. Angle θ is the inclination between the positive x -coordinate and the direction of gravity force. τ is the frictional force acting on the pipe wall that corresponds to a unit length and unit cross-sectional area of the pipe. Q is the heat input to the flow per unit volume. The gradient-type heat transfer along the x -coordinate is neglected in comparison to the transverse-type. E is the total energy defined as

$$E = i + \frac{1}{2} u^2 \quad (4)$$

where i is the internal energy.

The form of pseudoviscous term used here is the one including time derivative instead of the spatial derivative.

$$q = \begin{cases} \frac{(\rho_0 \ell)^2}{\rho^3} \left(\frac{\partial \rho}{\partial t} \right)^2 & \text{if } \frac{\partial \rho}{\partial t} < 0 \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

where ρ_0 is a constant density in a reference configuration of the system.

The spatial average density in the initial state may be used as the reference density ρ_0 :

$$\rho_0 = \frac{1}{L} \int_0^L \rho(x) dx \quad (6)$$

where L denotes the pipe length. An equivalent form involving a spatial derivative is as follows:

$$q = \begin{cases} \rho \ell^2 \left(\frac{\partial u}{\partial x} \right)^2 & \text{if } \frac{\partial u}{\partial x} < 0 \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

Use of the form, Eq. (5), eliminates the necessity for numerical evaluation of spatial derivatives which are difficult to evaluate at the boundaries. ℓ is a constant having the dimensions of length by which the shock thickness is controlled:

$$\ell = \alpha \Delta x \quad (8)$$

By choice of the dimensionless constant α between the numerical values of 1.5 and 2.0, the shock thickness is kept around 3 to 5 times the mesh spacing Δx .

The pseudoviscous term is added to the governing differential equations. The effects of the pseudoviscosity are two-folds. The sharp discontinuities are represented by a smooth curve spread over a few meshes while, in the region where the solution is smooth, no significant effects exist. Also, the pseudoviscous term will tend to suppress the spurious oscillations appearing in the result of the basic two-step Lax-Wendroff (L-W) scheme.

For the purpose of formulating in the numerical schemes, the governing differential equations with the pseudoviscous term are written in a generalized transport equation form:

$$\frac{\partial}{\partial t} U + \frac{\partial}{\partial x} F(U) = S(U) \quad ; \quad (9)$$

where U , F , and S are vectors representing the independent variables, their fluxes, and source terms respectively of the transport equations.

$$U = \begin{pmatrix} \rho \\ m \\ e \end{pmatrix} \quad ; \quad (10a)$$

$$F = \begin{pmatrix} m \\ \frac{m^2}{\rho} + p + q \\ \frac{m}{\rho} (e + p + q) \end{pmatrix} \quad ; \quad (10b)$$

$$S = \begin{pmatrix} 0 \\ \rho g \cos\theta - \tau \\ mg \cos\theta - u\tau + Q \end{pmatrix} . \quad (10c)$$

Here, the momentum and the total energy used as independent variables are per unit volume as defined below.

$$m = \rho u; \quad (11a)$$

$$e = \rho E. \quad (11b)$$

III. DIFFERENCE FORMULATIONS

The generalized transport equation, Eq. (9), is written in finite difference relations in both the two-step L-W scheme and the implicit-like scheme by Rubin and Burstein called here Rubin-Burstein (R-B) scheme. The two-step L-W procedure consists of two split time-step integration of an explicit type with a first-order accuracy. The overall accuracy of this scheme, however, is a second-order. The R-B procedure is also a two-step procedure; but, both steps involve the full time-step. The first step calculates explicitly the provisional solution at the advanced time. The provisional solution is next used to construct an implicit procedure to obtain the final solution. The overall accuracy of this scheme is shown also to be of a second-order. Both schemes considered here are basically explicit schemes that require no iterative treatment. The implicit nature of the second step in the R-B scheme enables a smooth start temporally of a sudden starting transient.

A. Two-Step Lax-Wendroff Scheme⁷

First order accurate, provisional values are first obtained at the centers of the rectangular meshes of the $x - t$ plane net. In reference to Figure 1, the difference relations to obtain the provisional values are:

$$U_j^{t+\Delta t/2} = \frac{1}{2} (U_j^t + U_{j+1}^t) + \frac{1}{2}\beta(F_j^t - F_{j+1}^t) + \frac{1}{4}\beta\Delta x(S_j^t + S_{j+1}^t) ; \quad (12a)$$

$$U_{j-1/2}^{t+\Delta t/2} = \frac{1}{2}(U_{j-1}^t + U_j^t) + \frac{1}{2}\beta(F_{j-1}^t - F_j^t) + \frac{1}{4}\beta\Delta x(S_{j-1}^t + S_j^t) . \quad (12b)$$

In the second step, these provisional values are used to form the fluxes and sources that are both centered in both x - and t -coordinate. The final values are obtained by

$$U_j^{t+\Delta t} = U_j^t + \beta(F_{j-1/2}^{t+\Delta t/2} - F_{j+1/2}^{t+\Delta t/2}) + \frac{1}{2}\beta\Delta x(S_{j-1/2}^{t+\Delta t/2} + S_{j+1/2}^{t+\Delta t/2}) . \quad (13)$$

The first-order accurate terms obtained in the first step are subtracted out on the right-hand side of Eq. (13) and, as a result, the second step has truly a second-order accuracy. Here,

$$\beta = \frac{\Delta t}{\Delta x} . \quad (14)$$

The cluster of grid-points appearing in one application of Eqs. (12) and (13) is shown in Figure 1. The small circles in Figure 1 represent the provisional value points while the big circles are the grid-points. The single solid lines connecting the circles are the interaction lines for the first step and the double lines are the interaction lines for the second step.

A slight variation from the above scheme can also be considered. In this variation, provisional values at an additional point (point 1 of Figure 1) can be calculated to replace the source term in Eq. (13) where it is averaged between points 2 and 3.

B. Rubin-Burstein Scheme

A variation from the above L-W procedure as given by Rubin and Burstein⁸ is described below. As can be seen from the interaction molecules shown in Figure 2, this procedure does not consider the intermediate time. Provisional values are first calculated at points 1 and 2 (refer to Figure 2) for use in centering the spatial derivatives of fluxes in the second step:

$$U_{j+1/2}^{t+\Delta t} = \frac{1}{2}(U_j^t + U_{j+1}^t) + \beta(F_j^t - F_{j+1}^t) + \frac{1}{2}\beta\Delta x(S_j^t + S_{j+1}^t) ; \quad (15a)$$

$$U_{j-1/2}^{t+\Delta t} = \frac{1}{2}(U_{j-1}^t + U_j^t) + \beta(F_{j-1}^t - F_j^t) + \frac{1}{2}\beta\Delta x(S_{j-1}^t + S_j^t) . \quad (15b)$$

Provisional values are calculated at an additional point (point D of Figure 2) which will next be used to center the source terms in the second step:

$$U_j^{t+\Delta t} = \frac{1}{2}(U_{j-1}^t + U_{j+1}^t) + \frac{1}{2}\beta(F_{j-1}^t - F_{j+1}^t) + \beta\Delta x S_j^t . \quad (15c)$$

The second-order accurate procedure next centers both the flux terms and source terms using the provisional values as obtained by Eqs. (15):

$$U_j^{t+\Delta t} = U_j^t + \frac{1}{2}\beta\left[\frac{1}{2}(F_{j-1}^t - F_{j+1}^t) + F_{j-1/2}^{t+\Delta t} - F_{j+1/2}^{t+\Delta t}\right] + \frac{1}{2}\beta\Delta x(S_j^t + S_j^{t+\Delta t}) \quad (16)$$

Still, an additional variation of this scheme can be devised in which the source terms are time-centered using the provisional values at points 1 and 2 as obtained by Eqs. (15a) and (15b). In this case, there is no need for Eq. (15c). The interaction molecules for this variation would still be the same as the one shown in Figure 2. The small, large circles, single and double lines in this figure signify the same as described above for Figure 1. The triple lines, however, represent the interaction both for the first- and second-step calculation.

IV. FORMULATION OF BOUNDARY CONDITIONS

In order to carry out the numerical solution of an initial-boundary value problem such as the one on hand, the values of all independent variables are usually needed at the boundary grid points. Two most difficult boundary conditions are discussed; the reservoir-end and break-end condition. Each of the boundary formulations are given that are consistent with each of the two numerical methods considered. The difficulties in the boundary formulations are mainly due to the lack of information at the boundaries. One obvious information at these two boundaries seems to be an energy relation. Even this relation may not apply if the flow region at the boundary is as such that the computational boundary point is not in the region of influence of the external region.

In the following, the boundary conditions are formulated on the basis of the energy relation together with an approximate balance of mass and momentum at the boundary cell. Next, considerations for alternate boundary formulation are discussed. The energy relation between the boundary grid (with no subscript) and the conditions external to the computational domain (with subscript e) is:

$$i + p/\rho + \frac{1}{2}u^2 = i_e + P_e/\rho_e + \frac{1}{2}u_e^2. \quad (17)$$

The change of the form of energy, namely the mechanical energy dissipating to thermal energy is expressed as the pressure losses as the conventional procedure for incompressible conduit flows:

$$i - i_e = \pm K \left(\frac{1}{2}u^2 \right). \quad (18)$$

We assume at this point $u_e \approx 0$ (complete dissipation for the case of break-end) for both boundary conditions. Since the loss takes place in the flow direction, the + sign in Eq. (18) corresponds to the reservoir-end while the - sign corresponds to the break-end boundary. Combination of Eqs. (17) and (18) yields.

$$P/\rho = P_e/\rho_e - (1 \pm K) \frac{1}{2}u^2. \quad (19)$$

Although the above equation has been formally derived, there exists many uncertainties in the practical situation. The loss coefficient K will depend in general on the nature of flow restriction as well as the flow unsteadiness prevailing at the boundaries. There is little information available for the value of K especially when phase change is involved and large unsteadiness exists. In view of these uncertainties, Eq. (19) is further simplified:

$$P = P_e - K' \left(\frac{1}{2}\rho u^2 \right) \quad (20)$$

where $K' = 1 + K$ which depends on the chosen reference density $\bar{\rho}$. K' could include effects of local unsteadiness as shown in Dailyl² et al.

A. Reservoir-End Boundary

For the two missing relations required for the boundary formulation, conservation of mass and momentum is used for the half size cell at the boundary (e.g., cell length $\Delta x/2$). The procedure consists of two split steps.

The L-W method is first described. Figure 3 depicts the interaction molecules for the reservoir- and break-end. The big circles represent the grid points while the small circles the provisional value points. The interior calculations are first completed before the boundary points so that the values at the solid circles are known. The values at points for which all adjacent values are known are determined first by an algebraic means of adjacent values. Point F, for example, is the mean of points D, B, E, and G. Likewise, point C is the mean of A and B. In the first step, conservation of mass and momentum is taken for the half cell, ACD1:

$$U_{1\frac{1}{2}}^{t+\Delta t/2} - U_{1\frac{1}{2}}^t = \beta(F_1^t - F_{1\frac{1}{2}}^t) + \frac{1}{2} \beta \Delta x S_{1\frac{1}{2}}^t.$$

Here, the terms involving values at points $j = 1\frac{1}{2}$ are eliminated by a linear spatial distribution to obtain the values at point 1:

$$U_1^{t+\Delta t/2} = U_1^t + U_{1\frac{1}{2}}^t - U_{1\frac{1}{2}}^{t+\Delta t/2} + 2\beta(F_1^t - F_{1\frac{1}{2}}^t) + \frac{1}{2} \beta \Delta x (S_1^t + S_{1\frac{1}{2}}^t). \quad (21a)$$

Similarly, the second step involves the conservation for the half cell, 1D23, and yields:

$$U_1^{t+\Delta t} = U_1^{t+\Delta t/2} + U_{1\frac{1}{2}}^{t+\Delta t/2} - U_{1\frac{1}{2}}^{t+\Delta t} + 2\beta(F_1^{t+\Delta t/2} - F_{1\frac{1}{2}}^{t+\Delta t/2}) + \frac{1}{2} \beta \Delta x (S_1^{t+\Delta t/2} + S_{1\frac{1}{2}}^{t+\Delta t/2}). \quad (21b)$$

This equation involves values at point 2. This point value can be calculated by Eq. (12a) or (12b) except that the time indices will have to be advanced by $\frac{1}{2}$ throughout.

Once density and velocity are calculated by Eqs. (21) as above, the boundary pressure is calculated by Eq. (20). In fact, Eq. (20) is used twice at each time step calculation; once for point 1 and next for point 3.

The formulation for the Rubin-Burstein procedure is devised basically in two steps also but here the fluxes and sources are time-centered in each step. This time-centering is considered to improve the accuracy, especially at the boundaries where rapid transients exist. This time-centering is also consistent with the time-centering associated with the basic scheme for the interior grids. The first step takes a balance for a half cell, AC12, to yield the following result (see Figure 4):

$$U_1^{t+\Delta t/2} = U_1^t + U_{1\frac{1}{2}}^t - U_{1\frac{1}{2}}^{t+\Delta t/2} + \beta(F_1^t - F_{1\frac{1}{2}}^t + F_1^{t+\Delta t/2} - F_{1\frac{1}{2}}^{t+\Delta t/2}) + \frac{1}{2}\beta\Delta x(S_1^t + S_{1\frac{1}{2}}^t + S_1^{t+\Delta t/2} + S_{1\frac{1}{2}}^{t+\Delta t/2}) \quad (22a)$$

Here again, a linear distribution of variables is assumed between grid points $j = 1$ and 2 . Eq. (22) requires values at point 1. This point is calculated by Eq. (12a). The second step procedure is essentially the same as the first and can be obtained from Eq. (22) by advancing the time superscripts by $\Delta t/2$. The resulting equation reads:

$$U_1^{t+\Delta t} = U_1^{t+\Delta t/2} + U_{1\frac{1}{2}}^{t+\Delta t/2} - U_{1\frac{1}{2}}^{t+\Delta t} + \beta(F_1^{t+\Delta t/2} - F_{1\frac{1}{2}}^{t+\Delta t/2} + F_1^{t+\Delta t} - F_{1\frac{1}{2}}^{t+\Delta t}) + \frac{1}{2}\beta\Delta x(S_1^{t+\Delta t/2} + S_{1\frac{1}{2}}^{t+\Delta t/2} + S_1^{t+\Delta t} + S_{1\frac{1}{2}}^{t+\Delta t}). \quad (22b)$$

Point 3 values appearing in Eq. (22b) are calculated by Eq. (15a).

B. Break-End Boundary

The break-end boundary conditions are formulated essentially the same way as the reservoir-end. Hence the final equations only are written down. Reference should be made to Figures 3 and 4 for the L-W and R-B procedures respectively.

For the L-W procedure:

$$U_k^{t+\Delta t/2} = U_{k-\frac{1}{2}}^t + U_k^t - U_{k-\frac{1}{2}}^{t+\Delta t/2} + 2\beta(F_{k-\frac{1}{2}}^t - F_k^t) + \frac{1}{2}\beta\Delta x(S_{k-\frac{1}{2}}^t + S_k^t); \quad (23a)$$

$$U_k^{t+\Delta t} = U_{k-\frac{1}{2}}^{t+\Delta t/2} + U_k^{t+\Delta t/2} - U_{k-\frac{1}{2}}^{t+\Delta t} + 2\beta(F_{k-\frac{1}{2}}^{t+\Delta t/2} - F_k^{t+\Delta t/2}) + \frac{1}{2}\beta\Delta x(S_{k-\frac{1}{2}}^{t+\Delta t/2} + S_k^{t+\Delta t/2}) \quad (23b)$$

And for the R-B procedure,

$$U_k^{t+\Delta t/2} = U_{k-\frac{1}{2}}^t + U_k^t - U_{k-\frac{1}{2}}^{t+\Delta t/2} + \beta (F_{k-\frac{1}{2}}^t - F_k^t + F_{k-\frac{1}{2}}^{t+\Delta t/2} - F_k^{t+\Delta t/2}) \\ + \frac{1}{2} \beta \Delta x (S_{k-\frac{1}{2}}^t + S_k^t + S_{k-\frac{1}{2}}^{t+\Delta t/2} + S_k^{t+\Delta t/2}); \quad (24a)$$

$$U_k^{t+\Delta t} = U_{k-\frac{1}{2}}^{t+\Delta t/2} + U_k^{t+\Delta t/2} - U_{k-\frac{1}{2}}^{t+\Delta t} + \beta (F_{k-\frac{1}{2}}^{t+\Delta t/2} - F_k^{t+\Delta t/2} + F_{k-\frac{1}{2}}^{t+\Delta t} - F_k^{t+\Delta t}) \\ + \frac{1}{2} \beta \Delta x (S_{k-\frac{1}{2}}^{t+\Delta t/2} + S_k^{t+\Delta t/2} + S_{k-\frac{1}{2}}^{t+\Delta t} + S_k^{t+\Delta t}). \quad (24b)$$

C. Alternate Treatment

In view of the potential problem associated with the boundary condition treatment, the above described formulations may have to be regarded as first proposition. The difficulties of proper boundary treatment have been recognized earlier.^{13, 14} Numerical instabilities resulting from some types of boundary formulations have been noted. Basically, three types of boundary formulations have been considered; algebraic extrapolation, characteristic extrapolation, and schemes based on the governing equations of conservation. The test problem considered for these various schemes was one that has no discontinuities. A review of open literature on this subject seems to indicate that there is no obvious method of devising computational boundary conditions. The subject still remains as a widely open question. A final choice of one particular boundary treatment should be made by numerical experimentation together with supporting effort based on analytical and experimental results.

Another aspect that can not be left out is the consideration of critical flows¹⁵ in two-phase flows. Depending on the computational results obtained, this consideration may turn out to be important. The situation of the criticality in a transient two-phase flow appears to be an open area yet.

V. NUMERICAL STABILITY

It has been shown^{7,8} that both the L-W and R-B procedures are dictated in their numerical stability by the Courant-Friedrichs-Lewy (CFL)¹² condition. CFL condition defines the necessary condition for hyperbolic systems. It states that the numerical domain must include the physical domain of dependence so that:

$$\Delta x \geq (c + |u|) \Delta t. \quad (25)$$

The governing differential systems considered in this report are of mixed hyperbolic-parabolic type; the equations include terms that are essentially dissipative and make the system parabolic. In a purely parabolic system such as the heat equation, the centered differencing both in time and space resulted in an unstable situation; however, forward time-differencing has a stabilizing effect which makes the difference system stable if $\sigma \Delta t / (\Delta x)^2 \leq \frac{1}{2}$ (σ is the diffusion coefficient).

In the present problem, the fast transient is of primary interest and the hyperbolicity of the problem is considered to be the dominant phenomenon. Hence, above stability criterion will be a valid condition. Any discrepancy resulting from the partial parabolic nature can easily be taken care of in the numerical procedure. More important than this is the computational difficulty associated with the greatly varying sonic speed due to phase change. Since the uniform spatial mesh is the most convenient, this situation can result in a significant numerical dispersion effects locally so that the hyperbolicity of the problem is numerically suppressed. In this condition, a variable mesh system may have to be employed in order to minimize the undesirable smoothing effects. For the first coding, however, a uniform mesh system is recommended.

VI. DISCUSSIONS

The problem of rapid decompression of compressed water poses a rather difficult problem since the computational domain includes a large range of flow regimes, from the nearly incompressible liquid phase transient (waterhammer) to the compressible high quality steam flow. The phase change at the liquid saturation accompanies a rapid change in the flow regime because of the discontinuous change of the sonic speed. Moreover, the waterhammer calculations require accurate procedure for mass conservation (if the numerical scheme uses the mass conservation equation explicitly) since a small error in the density calculation results in a large error in the pressure. In consideration of these requirements, Harlow and Amsden's¹⁷ Implicit-Continuous-Eulerian (ICE) technique was first chosen. ICE technique calculates the pressure field implicitly by an exact satisfaction of mass conservation and as a result it is capable of handling a wide range of flow regimes without any special treatment. On the other hand, it uses a cell-grid system which are not easily amenable to boundary formulation. Moreover, the numerical stability consideration of this method is not straight-forward.

It is from these two reasons that the simple explicit schemes discussed in this report are considered also. These simple codes are intended to be guides for the proper boundary condition formulations as well as provide the intercode comparison needed for future code validation. The procedures considered here solve the density explicitly and how the procedures would work in actual calculation in the compressed water flow regime, in particular, is difficult to predict. This consideration is especially important at the boundaries where rapid acceleration or deceleration takes place.

REFERENCES

1. M. Hori, M. Sato, H. Nei, T. Harasaki, M. Hishida, and T. Saito, "Sodium-Water Reaction Studies for Monju Steam Generators", IAEA Study Group Meeting on Steam Generators for LMFBR's (October, 1974).
2. M. Sato, H. Hiroi, and M. Hori, "Large Scale Sodium-Water Reaction Tests for Monju Steam Generators", Int. Conf. on Liq. Metal Tech. in Energy Production, Champion, Pa. (May, 1976).
3. C. R. Bell and M. P. Heisler, "TRANSWRAP--A Compressible Hydrodynamic Code for Large-Leak Sodium/Water Reaction Analysis," Report No. TI-001-130-025, Atomics International, (Feb. 1973).
4. N. G. Galluzzo, "Unsteady Water Injection Models for Analysis of Sodium/Water Reactions in Steam Generators", ASME Paper No. 75-PVP-67 2nd National. Cong. on Press. Vessels and Piping, San Francisco, Ca. (June, 1975).
5. A. H. Shapiro, "The dynamics and Thermodynamics of Compressible Fluid Flow", Vol. 2, Ronald Press, N.Y. (1954).
6. J. VonNeumann and R. D. Richtmyer, "A Method for the Numerical Calculation of Hydrodynamic Shocks", J. Appl. Phys. 21, 232-237 (March 1950).
7. R. D. Richtmyer, "A Survey of Difference Methods for Non-Steady Fluid Dynamics", National Center for Atmospheric Research, Technical Note 63.2 (1963).
8. E. L. Rubin and S. Burstein, "Difference Methods for the Inviscid and Viscous Equations of a Compressible Gas", J. Comp. Phys. 2, 178-196, (1967).
9. K. Namatame and K. Kobayashi, "Subcooled Decompression Analysis in PWR LOCA", Trans. ASME, J. Heat Transfer, 12-18, (Feb. 1976).
10. R. P. Rose, G. H. Harrison and G. A. Jayne, "Hydrodynamics Describing Acoustic Phenomena During Reactor Coolant System Blowdown", IDO-17254 Phillips Petroleum, Idaho (July, 1967).
11. S. Fabric, "Computer Program WHAM for Calculation of Pressure, Velocity, and Force Transients in Liquid Filled Piping Network", Kaiser Engineers Report No. 67-49-R, Kaiser Industries, IL (Nov, 1967)
12. J. W. Daily, W. L. Hankey, Jr., R. W. Olive, and J. M. Jordann, Jr., "Resistance Coefficients for Accelerated and Decelerated Flows Through Smooth Tubes and Orifices", Trans. ASME (July, 1956).

13. C. K. Chu and A. Sereny, "Boundary Conditions in Finite Difference Fluid Dynamic Codes", J. Comp. Phys. 15, 476-491, (1974).
14. J. H. Chen, "Numerical Boundary Conditions and Computational Modes", J. Comp. Phys. 13, 522-535, (1973).
15. F. J. Moody, "Maximum Flow Rate of a Single Component, Two-Phase Mixture", Trans. ASME, J. Heat Transfer, 134-142 (Feb. 1965).
16. R. Courant, K. Friedrichs, and H. Lewy, "Über the Partiellen Differenzial-gleichungen der Mathematischen Physik", Math. Ann. 100, 32-74, (1928).
17. F. H. Harlow and A. A. Amsden, "A Numerical Fluid Dynamics Calculation Method for All Flow Speeds", J. Comp. Phys. 8, 197-213, (1971).

Fig. 1. Grid Index System and Interaction Molecules for the Two-Step L-W Procedure

Fig. 2. Grid Index System and Interaction Molecules for the R-B Procedure.

(a) Reservoir-End

(b) Break-End

Fig. 3. Interaction Molecules for Boundary Formulations of Two-Step L-W Procedure.

Fig. 4. Interaction Molecules for Boundary Formulations of R-B Procedure.