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NRC Research and Technical Assistance Report

NUMERICAL BEHAVIOR OF THOR-LIKE MASS/ENERGY EQUATIONS UPON FLOW REVERSAL*

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1. Background

L. D. Eisenhart has been engaged in a study of the numerical behavior of a simplified (three-region core) set of THOR difference equations. Certain puzzling numerical irregularities occur near the time of flow reversal. The study reported herein is aimed at finding possible causes for such irregularities.

I've based information on THOR on an incomplete examination of various sources (e.g. Refs. a through d). I've defined a relatively simple problem similar to that studied by Eisenhart in an effort to clear away details that are hopefully unimportant. I've also used sort of a conglomorate notation, borrowing a little from various THOR sources, but also using notations from references that are more familiar to me.

2. Simplified Problem

Consider the three region (one dimensional) geometry shown in Figure 2.1.

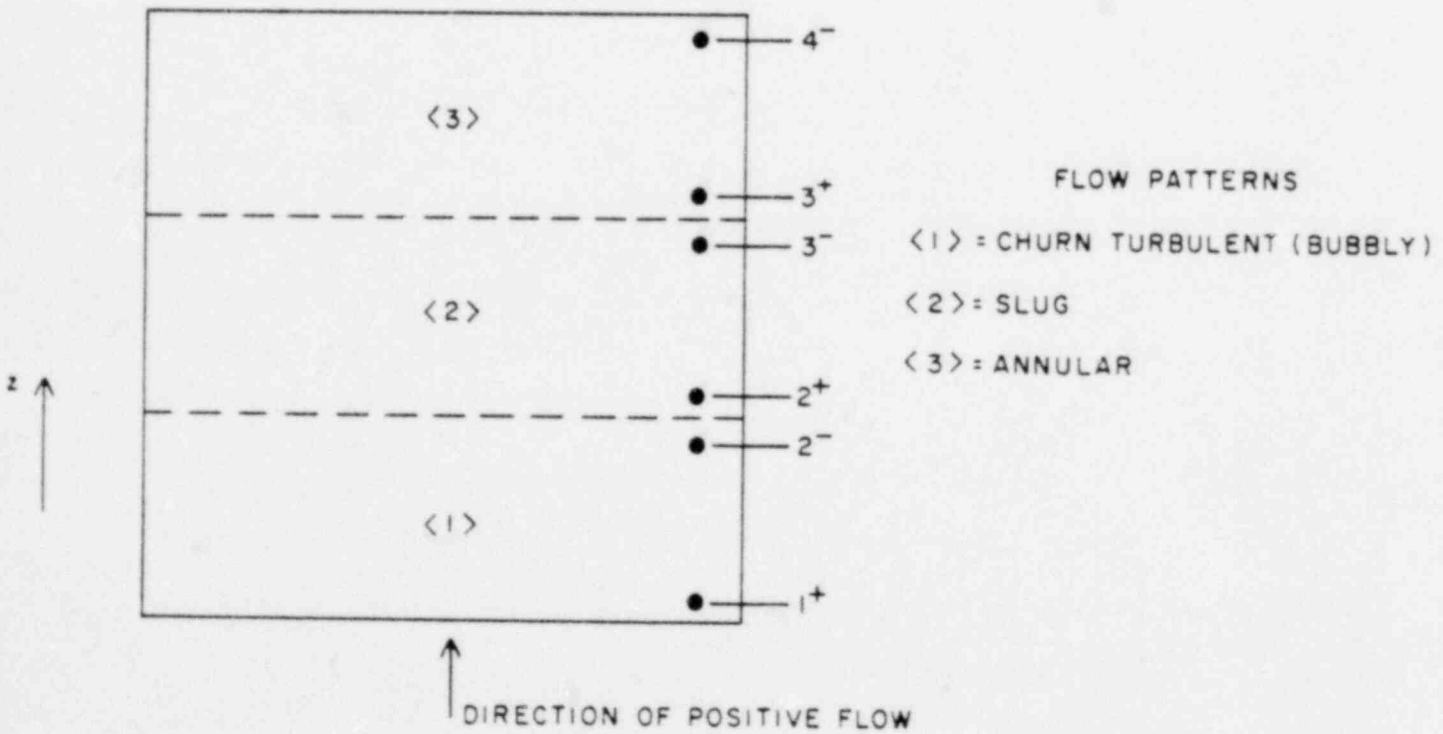

Figure 2.1

Consider a three-zone problem used by L. D. Eisenhart for numerical studies:

- the total length is short (0.17 m);
- an initial steady state (at t=10.0s) is achieved in which all flow patterns of Figure 2.1 are initially present;
- a flow reduction transient is initiated following t=10s by ramping down the inlet plenum pressure; and
- the change in average flow path pressure (the pressure for property evaluation) during the transient is fairly modest (from 7698 kPa at t=10s to 7695 kPa at t=10.16s).

Calculated results are illustrated in Figure 2.2. Mass velocities fall to an inlet flow reversal near t=10.17s. All three flow patterns are still present at that time.

The observed solution behavior is:

- until the time of flow reversal, all variables seem to behave well for time steps at least as long as 5 ms; and
- after that time, a variety of problem stops occur (such as negative enthalpy (~ -4000 kJ/kg) values or crossing of flow pattern interfaces) as various methods of time step control and fixes are attempted.

My investigation of these difficulties has been based on a feeling that the difficulties would still be present if the following additional problem simplifications were made:

a) Rather than initiating the transient by changing the plenum-to-plenum pressure drop, I'll consider that the inlet mass velocity (G_1^+) is a known function of time, as given in Figure 2.2a.

b) I'll neglect all changes with time in the reference pressure for property evaluation.

c) I'll study the equations which are differenced in space but still differential equations in time. These $(DE)_t/(\Delta E)_z$ equations are given by Ruger (Ref. b).

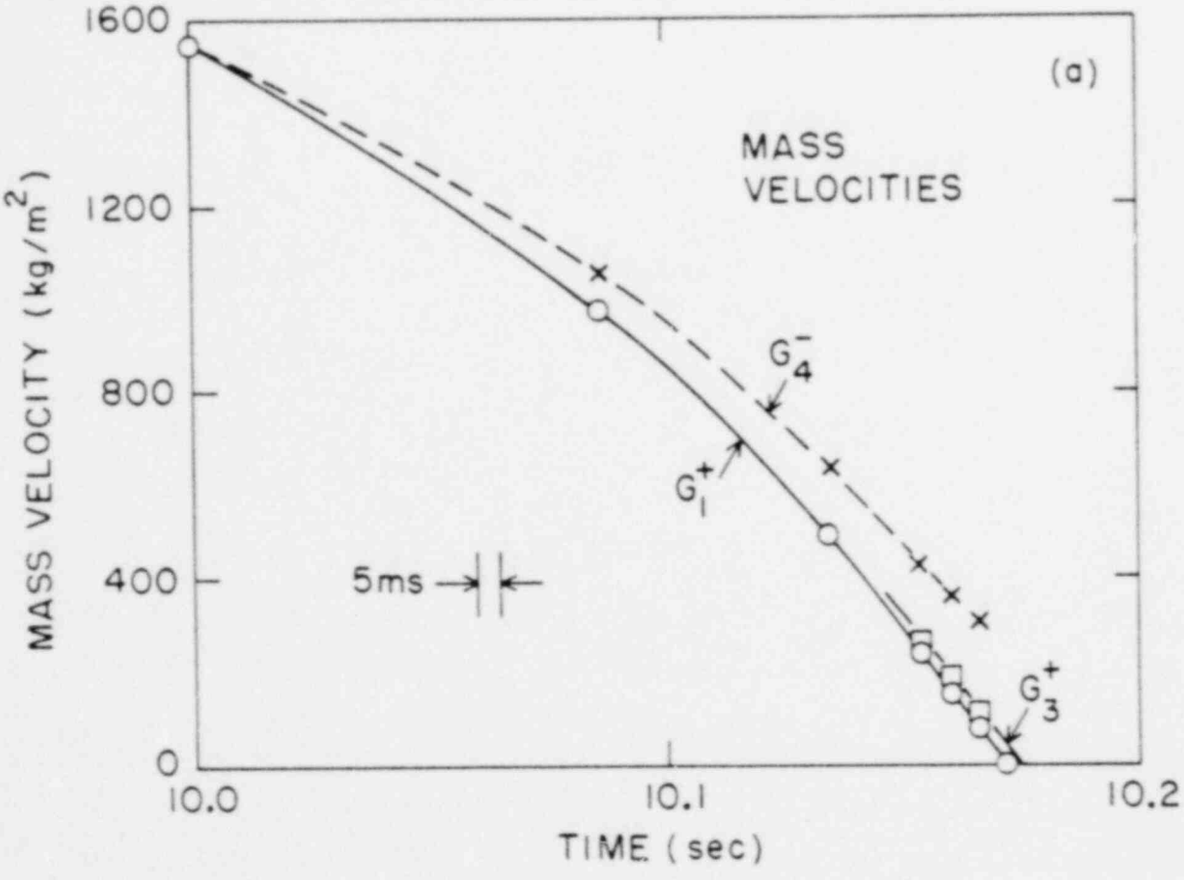

Figure 2.2

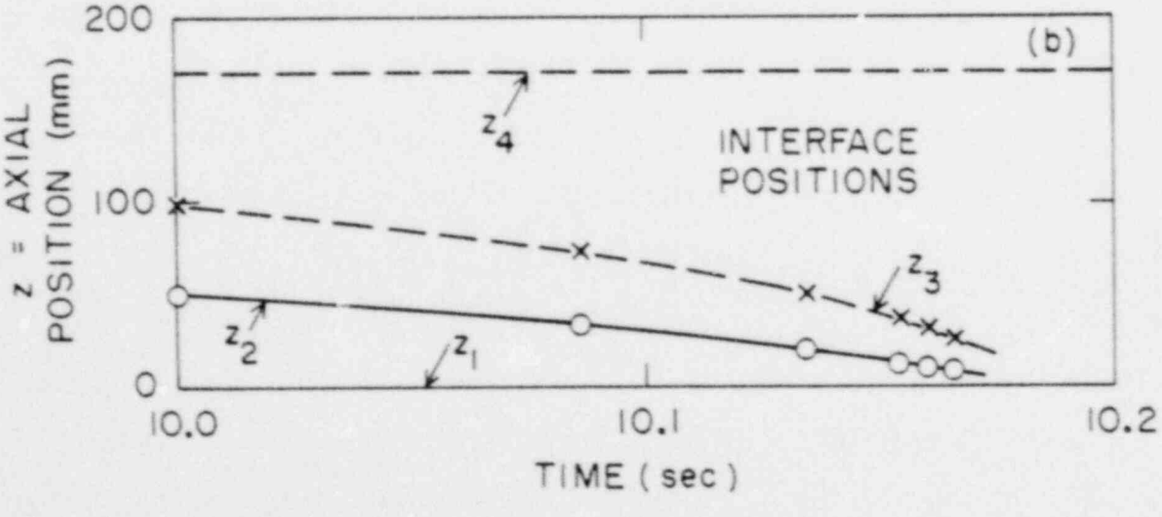

Figure 2.2a

d) As in Ref. b, all properties will be evaluated at saturation conditions, so that no vapor mass equation will be required.

3. Partial Differential Equations

This section contains a brief presentation of conservation laws based on a combination of concepts and notations from a variety of sources (chiefly Ref. a through e and Ref. f, pp. 5 and 65-71).

a) Conservation of Mass

For one-dimensional flow through a constant area flow channel:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial G}{\partial z} = 0, \tag{3.1}$$

where

$$\bar{\rho} = \frac{1}{A}\int_A \rho \, dA; \tag{3.2}$$

$$G = \frac{1}{A}\int_A \rho u \, dA; \tag{3.3}$$

u = local velocity (in the positive z direction);

ρ = local density;

A = flow area;

$\bar{\rho}$ = volume weighted density;

G = mass velocity;

t = time; and

z = axial position.

b) Conservation of Energy

$$\frac{\partial}{\partial t}(\bar{\rho}\,\bar{H}) + \frac{\partial}{\partial z}(GH') = 0 \tag{3.4}$$

where:

$$\overline{H} = \frac{1}{\overline{\rho}A}\int \rho\, H\, dA; \tag{3.5}$$

$$H' = \frac{1}{GA}\int \rho\, u\, H\, dA; \tag{3.6}$$

H = local enthalpy;

$\overline{H}$ = volume weighted or static enthalpy;

H' = flow weighted or mixing cup enthalpy;

Q = heat input per unit volume;

and where various terms have been neglected as indicated in Ref. e in a manner consistent with Ruger (Ref. b).

An alternate form of the energy equation can be obtained by multiplying Eq. 3.1 by $\overline{H}$ and subtracting from Eq. 3.4:

$$\overline{\rho}\frac{\partial \overline{H}}{\partial t} + G\frac{\partial \overline{H}}{\partial z} + \frac{\partial}{\partial z}\left[G(H'-\overline{H})\right] = Q. \tag{3.7}$$

c) Separated Flow Representation

Adopt a single value each for density, enthalpy, and velocity to represent all liquid in the channel at a given axial level. Denote these values by ρ_ℓ, H_ℓ, and u_ℓ. Denote also the corresponding quantities for vapor as ρ_v, H_v, and u_v. Finally, designate the fraction of the flow area occupied by vapor as α (static vapor fraction). Then the quantities defined in Eqs. 3.2, 3.3, 3.5 and 3.6 become:

$$\overline{\rho} = \alpha\rho_v + (1-\alpha)\,\rho_\ell \quad ; \tag{3.8}$$

$$G = \alpha\rho_v u_v + (1-\alpha)\,\rho_\ell u_\ell \quad ; \tag{3.9}$$

$$\overline{H} = \frac{1}{\overline{\rho}}\left[\alpha\rho_v H_v + (1-\alpha)\rho_\ell H_\ell\right] \quad ; \tag{3.10}$$

and

$$H' = \frac{1}{G}\left[\alpha\rho_v u_v H_v + (1-\alpha)\rho_\ell u_\ell H_\ell\right]. \tag{3.11}$$

In the simplified case defined in Section 2, the quantities ρ_v, ρ_ℓ, H_v, and H_ℓ are all evaluated at saturation conditions corresponding to a pressure which is independent of time. In this case, $\bar{\rho}$ from Eq. 3.8 and $\bar{H}$ from Eq. 3.10 depend only upon α. Or equivalently, $\bar{\rho}$ is a function of $\bar{H}$ only. Therefore, the mass equation (Eq. 3.1) can be rewritten

$$\frac{d\bar{\rho}}{d\bar{H}} \frac{\partial \bar{H}}{\partial t} + \frac{\partial G}{\partial z} = 0 \quad ; \tag{3.12}$$

or by combining with Eq. (3.7):

$$\frac{\partial G}{\partial z} = - \frac{1}{\bar{\rho}} \left(\frac{d\bar{\rho}}{d\bar{H}} \right) \left\{ Q - \left[G \frac{\partial \bar{H}}{\partial z} - \frac{\partial}{\partial z} G(H'-\bar{H}) \right] \right\} . \tag{3.13}$$

Separated flow quantities and equations of interest include:

Let Y = the static quality (the vapor mass concentration denoted by c in Wulff, Ref. d):

$$Y = (\alpha \rho_v / \bar{\rho}) \quad ; \tag{3.14}$$

or equivalently

$$\alpha = \frac{\rho_\ell Y}{\rho_\ell Y + \rho_v (1-Y)} \quad ; \tag{3.15}$$

and

$$\bar{H} = Y H_v + (1-Y) H_\ell . \tag{3.16}$$

Let X = the flowing quality (the mass flow rate of vapor divided by the total mass flow rate):

$$X = (\alpha \rho_v u_v / G) \quad ; \tag{3.17}$$

and let β = the flowing vapor fraction (the volume flow rate of vapor divided by the total volume flow rate):

$$\beta = (j_v / j) \quad ; \tag{3.18}$$

where j_v is the superficial velocity of vapor,

$$j_v = (XG / \rho_v) \quad , \tag{3.19}$$

where j_ℓ is the superficial velocity of liquid,

$$j_\ell = \left[(1-X)\ G/\rho_\ell\right] ; \tag{3.20}$$

and the volumetric flux j is

$$j = j_v + j_\ell \ . \tag{3.21}$$

The interrelation between β and X is similar to that between α and Y. That is,

$$\beta = \left[\frac{\rho_\ell X}{\rho_\ell\ X + \rho_v (1-X)}\right] \quad . \tag{3.22}$$

Also,

$$H' = X\ H_v + (1-X)\ H_\ell \ . \tag{3.23}$$

d) Drift Flux Representation

A drift flux representation can be considered as an empirical relation between static and flowing vapor fractions. That is,

$$\beta = \left[c_o + (u_{vj} / j)\right] \alpha \ , \tag{3.24}$$

where c_o = an empirical flow distribution parameter;

and u_{vj} = the weighted mean drift velocity, another empirical parameter.

The relation can be combined with the various separated flow relations (and a great deal of algebra) to obtain the relation:

$$G(H'-\overline{H}) = \left\{\frac{\rho_v \rho_\ell \left[u_{vj} + \frac{G}{\rho}\ (c_o - 1)\right]}{\left[\rho_v - (c_o-1)\ Y\ (\rho_v-\rho_\ell)\right]}\right\}(\overline{H}-H_\ell) \quad . \tag{3.25}$$

In the cases for which $c_o = 1$, the above relation can be greatly simplified as done by Ruger in Ref. b:

$$G(H'-\overline{H}) = \rho_\ell\ u_{vj}\ (\overline{H}-H_\ell) \quad . \tag{3.26}$$

Knowledge of the quantity $G(H'-\overline{H})$ is needed for the solution of Eqs. 3.7 and 3.13.

4. Spatially Differenced Equations

Mass Equation with Moving Boundaries

Use i as an index to describe the positions in Fig. 2.1. Integrate the conservation of mass equation (Eq. 3.1) over axial region i, and incorporate moving boundaries by the techniques of Mulff (Ref. d, Eq. 21):

$$\frac{d}{dt}\left[\langle\rho\rangle_i \Delta z_i\right] + \left[G - \overline{\rho}\ \dot{z}\right]_{i+1}^{-} - \left[G - \overline{\rho}\ \dot{z}\right]_i^{+} = 0 \quad ; \tag{4.1}$$

where $\Delta z_i = z_{i+1} - z_i$. (4.2)

b) Energy Equation with Moving Boundaries

In a similar manner, integrate the conservation of energy equation (Eq. 3.4) to obtain:

$$\frac{d}{dt}\left[\langle\overline{\rho}\ \overline{H}\rangle_i\right] + \left[GH' - \overline{\rho}\ \overline{H}\ \dot{z}\right]_{i+1}^{-} - \left[GH' - \overline{\rho}\ \overline{H}\ \dot{z}\right]_i^{+} = \langle Q\rangle_i \Delta z_i \tag{4.3}$$

c) Interface Equations

By writing equations similar to 4.1 and 4.3 for a region interface of zero thickness, it is found that the following quantities are continuous at each interface i:

$$\left[G - \overline{\rho}\ \dot{z}\right]_i^{+} = \left[G - \overline{\rho}\ \dot{z}\right]_i^{-} \quad ; \tag{4.4}$$

$$\left[GH' - \overline{\rho}\ \overline{H}\ \dot{z}\right]_i^{+} = \left[GH' - \overline{\rho}\ \overline{H}\ \dot{z}\right]_i^{-} \quad . \tag{4.5}$$

d) Summary of Ruger Equations

Ruger's equations of Ref. b can be keyed to the equations developed in this report as follows:

- 1 (Overall Momentum) - not needed here since inlet flow is specified.
- 2, 5, 8 IGAE (Integrated Algebraic Mass Flux) - not needed here since these are profile equations to relate $\langle G \rangle_i$ to $(G)_i^+$ and $(G)_{i+1}^-$. We do not need $\langle G \rangle_i$.
- 3, 6, 9 GAE (Mass Velocity Algebraic Equation) - This set of equations is equivalent to the following difference form for Eq. 3.13:

$$\left[\frac{(G)_{i+1}^- - (G)_i^+}{\Delta z_i}\right] = -\frac{1}{(\bar{\rho})_i} + \left[\frac{(\bar{\rho})_{i+1}^- - (\bar{\rho})_i^+}{\Delta \bar{H}_i}\right] \left\{A\right\}$$

where

$$\left\{A\right\} = \left\{\langle G \rangle_i - \frac{\left[(G)_i' + (\rho_\ell u_{vj})_i\right] \Delta \bar{H}_i}{\Delta z_i}\right\} \quad ; \qquad (4.6)$$

where

$$\Delta \bar{H}_i = (\bar{H})_{i+1}^- - (\bar{H})_i^+ \quad ; \qquad (4.7)$$

where Eq. 3.26 has been incorporated and where $(\rho_\ell u_{vj})$ is constant through Region i.

- 4, 7 SHM (Mass Jump at Interface) - the same as Eq. 4.4.
- 10, 13, 16 EN (Energy Equation) - an approximation to Eq. 3.7 with $\bar{\rho} \frac{\partial \bar{H}}{\partial t}$ given by

$$\bar{\rho} \frac{\partial \bar{H}}{\partial t} \cong (\rho)_i^- \left\{ \langle \dot{\bar{H}} \rangle_i - \frac{\Delta H_i}{\Delta z_i} \left[\frac{1}{2} (\dot{z}_{i+1} + \dot{z}_i)\right]\right\} \qquad (4.8)$$

where

$$\langle \overline{H} \rangle_i = \frac{1}{2} \left[(\overline{H})^-_{i+1} + (\overline{H})^+_i \right] \tag{4.9}$$

has been employed.

The convective term has been approximated by

$$G \frac{\partial \overline{H}}{\partial z} + \frac{\partial}{\partial z} \left[G(H' - \overline{H}) \right] \cong \left[(G)^+_i + (\rho_\ell u_{vj})_i \right] \frac{\Delta \overline{H}_i}{\Delta z_i} \quad ; \tag{4.10}$$

where Eq. 3.26 has been incorporated and where $(\rho_\ell u_{vj})$ is constant through Region i.

- 11, 14 IF (Interface Definition) - the enthalpy $(H)^-_i$ is supplied at each interior interface (i=2 and i=3) to define the conditions for flow pattern changes.
- 12, 15 SHE (Energy Jump at Interface) - obtained by combining Eqs. 3.26, 4.4 and 4.5:

$$\left[(\overline{H})^+_i - H_\ell \right] \left[(G)^+_i + (\rho_\ell u_{vj})_i - (\overline{\rho} \dot{z})^+_i \right] =$$

$$\left[(\overline{H})^-_i - H_\ell \right] \left[(G)^-_i + (\rho_\ell u_{vj})_{i-1} - (\overline{\rho} \dot{z})^-_i \right] . \tag{4.11}$$

- 17, 18, 19 HPRO (Enthalpy Profile)

  - for through flow the linear profile Equation 4.9 is used;
  - for both inflows to a region, no profile equation is required; and
  - for both outflows from a region the old slope of enthalpy with respect to position z is retained.

(4.12)

- 20, 21, 22 BC (Boundary Conditions)

  - P_1, P_6 are not required for the simplified problem; $(G_1)^+$ must, however, be specified as a function of time.
  - $(\overline{H})^-_1$ is required as a function of time for any time the flow at interface 1 is directed from the inlet plenum into the channel.

(4.13)

- $(\overline{H})_4^+$ is required as a function of time for any time that the flow at interface 4 is directed from the exit plenum back into the channel. (4.14)

5. Comments

a) Calculations with Flow Reversal

- CHIC experiences - I'm familiar with some numerical studies performed by G. Birkhoff and T. F. Kimes using the CHIC (Convection of Heat In Channels) Code (Ref. g). Several numerical approaches were studied. One of them, program II, (CHIC-2), is relevant here. It uses a "box method" for representing the convection (energy) equation and is, therefore, a method akin to the linear profile approach of Eqs. 4.8 and 4.9. CHIC-2 results showed:
  - the predictor-corrector feature did not provide significantly improved accuracy; and
  - improvements to the mass equation treatment were required.

These findings were incorporated in subsequent thermal hydraulic developments. In addition, and more pertinent to our present discussion, the mathematical ideas incorporated in CHIC-2 concerning flow reversal (Equations E2 through E4, Ref. g) were used as a basis for subsequent developments. The following approach was felt to be mathematically sound*:

- Each mesh cell is assigned a single mass velocity to be used in the energy equation solution (e.g. an average of inlet and exit mass velocities);
- If that "characteristic velocity" is positive, then the cell is an upflow cell; if negative it is a downflow cel., and I'll omit from this discussion the unlikely case of zero flow;

*A difference from THOR is that these are for mesh cells with fixed, not moving, boundaries. I'd expect they could also be used as a guide in the moving boundary case.

- For upflow cells, the enthalpy at the bottom interface must be taken from the cell below it;
- For downflow cells, the top interface enthalpy must be taken from the cell above it;
- If a downflow cell is above an upflow cell then two enthalpies can be obtained at the common interface and some energetically equivalent average of the two should be adopted; and
- If an upflow cell is above a downflow cell then an extra artificial cell is temporarily (one time step) introduced at a position corresponding to zero velocity in order to obtain the enthalpy information needed for both cells.

• THOR Reverse Flow Logic - the reverse flow logic defined by Eqs. 4.12 through 4.14 seems to be mathematically quite different than the above approach. Possible deficiencies and possible remedies include:

- With the box method and for energy equation numerics a cell is either upflow or downflow. The categories "through flow," "both inflow," or "both outflow" are not meaningful.
- The "characteristic velocity" that, in the present case, should be used for deciding whether a box is upflow or downflow, is the bracketed term on the right hand side of Eq. 4.10,

$$\left[(G)_i^+ + (\rho_\ell\, u_{vj})_i\right] . \qquad (5.1)$$

- A rederivation of the difference equations probably should be performed to obtain a more centered characteristic velocity such as

$$\left\{\left[\frac{1}{2}(G)_i^+ + \frac{1}{2}(G)_{i+1}^-\right] + (\rho_\ell\, u_{vj})_i\right\} . \qquad (5.2)$$

- The adoption of expression 5.2 is a mathematical refinement and unnecessary for obtaining reasonably good answers. The other considerations concerning characteristic velocities and cell nature are however essential to obtaining valid numerical solutions (though other fixes than those suggested here may also work).

Spatial Ringing Difficulties

- The use of a box differencing method has at least one other difficulty for which there seems to be no easy fix. Consider a case where the top cell in a channel has had upflow then switches to downflow. If at this time, the exit plenum has an enthalpy much different than the exit enthalpy of the top cell at the previous time step, then a violent enthalpy "ringing" can occur spatially, and by interaction with other (especially two phase) relations can destroy the numerical solution.
- This latter difficulty suggests adopting more robust approaches (e.g., a change from box to donor cell differencing was employed in the SSC-L steam generator calculations, Ref. h).

b) Enthalpy Jump Singularities

The enthalpy jump relation (Eq. 4.11) could conceivably give strange behavior in a numerical solution. This would occur if the expression

$$\left[(G)_i^+ + (\rho_\ell u_{vj})_i - (\overline{\rho}\,\dot{z})_i^+\right]$$

approached zero during the solution or was at least much smaller in magnitude than

$$\left[(G)_i^- + (\rho_\ell u_{vj})_{i-1} - (\overline{\rho}\,\dot{z})_i^-\right] .$$

I suspect this was the immediate cause of the problem stops from negative enthalpy that were observed by Eisenhart (Section 2 and Ref. a). Quantitative

estimates from program output though, indicate that if $\dot{z}_f$ behaved well then this equation would have caused no difficulties for mass velocity values greater than approximately -500 kg/m^{2}s. It is likely then that other difficulties, such as those discussed in Section 5a, caused poor values of $\dot{z}_f$ to be calculated, which in turn resulted in enthalpy disasters through the jump relation (Eq. 4.11).

c) Alternate Formulation

I can see advantages to following liquid levels and mixture levels by kinematic jumps (Ref. c, Section 1.2.3.2). I am not convinced that it is a good idea to treat flow pattern boundaries as kinematic jumps. An alternate approach that seems attractive from a numerical standpoint, and good enough from a physical standpoint is as follows:

- use spatially fixed control volumes (computational cells);
- use integrals of Eq. 3.7 (or 3.4) to obtain spatially differenced equations to represent convective processes;
- require that at each pressure the enthalpy H' be a continuous function of $\overline{H}$ (and G and geometric variables), though first derivatives could be discontinuous;
- use drift flux formulations and flow patterns considerations to define the best H' relations that are consistent with mathematical continuity; and
- define information such as wall friction profiles within a cell to be consistent with flow pattern changes expected on the basis of G and H values at the two ends of the cell.

d) "Don't Tamper" Time Step Control

I think it's possible, in problems of this type, that efforts to obtain time steps from calculated information can amplify numerical irregularities that would otherwise be only temporary. I am an advocate of user selected time

steps that are chosen on the basis of transient speed. This of course does require some user knowledge about what is happening during the transient. I'd rather rely on user knowledge about transient speed than rely on him being able to detect when a complicated internal time step selection routine was giving him trouble.

6. Summary

In order to suggest possible causes for numerical irregularities observed by L.D. Eisenhart, I've defined a simpler but related problem for study. I've then written the differential equations and the difference equations for this problem as a basis for discussion. A prime suspect for the irregularities is given in Section 5a. Other comments are also supplied.

7. References

a) Conversations with L.D. Eisenhart, July 1978 through September 1978.

b) C. Ruger, "3 Zone Core Eqn's. All 2¢," Handwritten Notes, 12/12/77.

c) W. Wulff, D.C. Jones, Jr., et al., "THOR-1 (PWR): A Computer Code for Predicting the Thermal Hydraulic Behavior of Nuclear Reactor Systems," BNL-NUREG-24760, Volumes 1 through 4, August 14, 1978.

d) W. Wulff, "Lumped-Parameter Modeling of One-Dimensional Two-Phase Flow," BNL-24483, presented at Second OECD Meeting for Specialists in Transient Two-Phase Flow, Paris 1978.

e) J. E. Meyer, "Conservation Laws in One-Dimensional Hydrodynamics," in "Bettis Technical Review," WAPD-BT-20, September 1960, pp. 61-72.

f) J. G. Collier, "Convective Boiling and Condensation," McGraw Hill, London, 1972.

g) G. Birkhoff and T.F. Kimes, "CHIC Program for Thermal Transients," WAPD-TM-245, February 1962.

h) W. L. Weaver III, J.E. Meyer, and A.K. Agrawal, "A Few Pressure Model for Transient Two-Phase Flows," Trans. Am. Nucl. Soc. 28, 273-274 (1978).

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