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DEVELOPMENT OF A COMPUTER CODE FOR THERMAL HYDRAULICS OF REACTORS (THOR)

EIGHTH QUARTERLY PROGRESS REPORT
JULY - SEPTEMBER 1976

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THERMAL REACTOR SAFETY DIVISION, DEPARTMENT OF APPLIED SCIENCE
BROOKHAVEN NATIONAL LABORATORY, ASSOCIATED UNIVERSITIES, INC.
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JULY - SEPTEMBER 1976

Contributors:

Arnold Dubow	Upendra S. Rohatgi
Donald Garber	Charles Ruger
Peter G. Kroeger	G.S. Srikantiah
Stanley V. Lekach	William J. Turner
M. Reocreux	Wolfgang Wulff

Programmers AMD

Edited by: M.M. LEVINE

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FOREWORD

This Eighth Quarterly Progress Report covers the advanced code development work performed during the time from July 1, 1976 through September 30, 1976 in the Thermal Reactor Safety Division, Department of Applied Science at Brookhaven National Laboratory, under Contract No. EY-76-C-02-0016 for the Analysis Development Branch of the United States Nuclear Regulatory Commission. The Department of Applied Mathematics assisted in this work with computer program coding.

ABSTRACT

The purpose of the advanced code development work reported here is to construct a computer code for the prediction of thermohydraulic transients in water-cooled nuclear reactor systems. The fundamental formulation of fluid dynamics is to be based on the one-dimensional drift flux model for non-homogeneous, non-equilibrium flows of two-phase mixtures. Particular emphasis is placed on component modeling, automatic prediction of initial steady state conditions, inclusion of one-dimensional transient neutron kinetics, freedom in the selection of computed spatial detail, development of reliable constitutive descriptions, and modular code structure.

Activities During Eighth Reporting Period, July 1, 1976 thru September 30, 1976

A wall conduction model has been implemented in the distributed pipe program. Supplemented with a heat transfer coefficient routine this program was used for calculating Standard Problem Number 2.

A stand-alone program has been written and checked out to calculate V_{gm} for a number of flow regimes.

Coding and de-bugging has continued on sub-programs for the reactor core.

A lumped parameter model has been developed for the pressurizer and surge line, and coding for a stand-alone computer program for model verification was initiated. Analysis has been continued on the lumped steam generator model.

The steady state model developed earlier was modified for implementation in the present host code. The network model has been examined for fuller understanding of the constraints imposed on component modeling by the integration scheme to be used.

The host code was extended to provide the user with control over boundary and trip conditions. A design was begun for an optimizer routine in the host code to eliminate many of the algebraic equations prior to transient execution time.

A method for coupling components which allows different components to advance with different size time steps has been devised.

A lumped plenum model has been set up and is being programmed.

A lumped pipe model has been developed with various possible choices for profile computation.

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1. INTRODUCTION

Computer codes are required to simulate accident-induced nuclear reactor system transients for the purpose of predicting times and locations for the possible occurrences of excessive temperatures and pressures, following postulated accidents, such as a loss of coolant accident (LOCA), or during anticipated system transient without scram (ATWS). The program discussed here deals primarily with thermohydraulic aspects of water-cooled reactor system transients.

1.1 Program Objectives

This research program is designed to produce an advanced computer code for the prediction of accident-induced thermohydraulic transients in water-cooled nuclear reactors which meets six primary objectives, as presented in detail in Reference [1]^{*} and summarized below.

- (i) The fluid dynamics equations in the code must account for thermodynamic non-equilibrium between the vapor and liquid phases and for unequal phase velocities.
- (ii) Reactor system components must be modeled individually to describe specific processes in particular geometries.
- (iii) The axial variation of the transient fission power must be predicted.
- (iv) The initial steady state of the reactor hydraulic system must be automatically predicted.
- (v) Material descriptions and correlations must be developed for economical computing and continuing updating.

* Numbers in brackets refer to the Bibliography.

- (vi) The code structure must be modular and must accommodate, through both lumped- and discrete parameter descriptions of reactor system components, a flexible compromise between computing speed and detail.

The requirements which must be met to achieve these objectives have been detailed in Reference [1]. The equations of motion for the transient two-phase mixture are based on the one-dimensional drift-flux model [2,3]. The drift-flux model as used here has been revised and is presented in Appendix A of this report.

1.2 Plan of Research

The present research program is being carried out in twenty-two distinct tasks, some of which are continuations of previous efforts.

<u>Task</u>	<u>Task</u>
1. Modeling of Pipe Break	12. Modeling of Steam Separator
2. Thermodynamic Properties	13. Modeling of Steam Dryer
3. Heat Transfer Coefficients	14. Pressurizer
4. Friction Factor	15. Steam Generator
5. Drift Velocity	16. Power Generation and Neutron Kinetics
6. Vapor Source/Sink	17. Fuel Rod Temperature
7. Steady State Conditions	18. Modeling of Component Interfaces
8. Reactor Core Modeling	19. System Modeling
9. Modeling of Downcomer Flow	20. Code Assembly
10. Prediction of Pump Performance	21. Lumped Pipe
11. Modeling of Jet Pump	22. Plenum

Detailed task objectives have been presented earlier in Reference [1] for Tasks 1 through 6, 16 and 18, and in Reference [2], for Task 7, in Reference [3] for Tasks 8 through 15 and 17, and in Reference [4], for Tasks 19 and 20.

Task 21 has the aim of producing a lumped model representation of an adiabatic constant area pipe. This serves two purposes: First it provides a component which may be needed for system assembly for reactor systems. Second, in its simplest form as a component with few processes taking place - no heating, no moving interfaces, etc. - it provides a useful tool for testing models of system assembly. Questions dealing with profiles, component connection and boundary conditions, time advancement procedures, etc. can be addressed with one or more pipe sections in appropriate arrays without the complication that other components may offer.

Task 22 is to provide a lumped model for describing the upper and lower plena of a reactor core. This component is characterized by a volume with uniform pressure and internal velocities which are small with respect to the in- and out flux velocities. At the same time, the lower plenum must have suitable connections to the downcomer and the core.

2. SUMMARY OF CURRENT ACHIEVEMENTS

2.1 Modeling of Pipe Break (S. Lekach)

The thermal conduction module has been implemented in the hydraulic finite difference in a radial wall conduction model with linear coefficients evaluated for present time step values (analogous to the hydraulic model). The thermal conductivity is taken as a function of the temperature. The model allows the temperature to be obtained either implicitly or explicitly with the hydraulic vector $\underline{y}$. The heat transfer coefficient as well can be expressed either implicitly or explicitly in terms of the hydraulic vector $\underline{y}$. Coupling between the wall temperatures and the hydraulics is expressed as follows:

$$\phi' = \phi + \frac{\partial \phi}{\partial \underline{y}} (\underline{y}' - \underline{y}) + \frac{\partial \phi}{\partial T_{\text{wall}}} (T'_{\text{wall}} - T_{\text{wall}})$$

where the dashed quantities are the future (unknown) values; the surface heat flux $\phi = h (T_{\text{wall}} - T_{\text{fluid}})$, and

$$\underline{y} = \begin{pmatrix} h_m \\ p \\ v_m \\ c \end{pmatrix}$$

Currently the thermal conduction calculation uses the same time step as the hydraulic module. We expect to include a modification that will allow different size time steps and will still retain the fully implicit feature of the temperature calculation.

As part of the calculations for Standard Problem Number 2, and as part of the temperature module, we wrote a heat transfer coefficient routine. This routine is strictly for temporary use until a more complete and up-to-date

version is obtained thru R.S.R. Currently the in-house routine contains five correlations (Dittus-Boelter, Thom, Jens-Lottes, single phase vapor Dittus-Boelter, Dougall-Rosenhow stable film boiling) and two critical heat flux correlations (Bernath and Biasi).

Since the numerical algorithm is fully implicit large time steps can be chosen with concern only for accuracy, not stability. The following variable-time stepping scheme is used:

Define $N = \max_{\text{all } k} \left\{ \left| \frac{y'_k - y_k}{y_k} \right| \right\}$ where y_k is the hydraulic vector at node k , y'_k is the new y .

If, at the completion of a time step, $N \leq \delta$, (where δ is chosen by the user) we double the time step and continue to advance. If $N > \delta$, we halve the time step and repeat the step until the criterion is satisfied. There are, of course, lower and upper limits for the time step.

With this approach we have run Standard Problem Number 2 with 24-48 nodes in about 80 to 350 cpu seconds on the CDC 7600 depending on the thermal conduction model chosen and on whether the heat transfer coefficient is taken to be an implicit or explicit function of the hydraulic vector y . δ was taken to be 1%. The real time simulated was 5 seconds.

Two choking criteria are being developed. In one the determinant of the coefficient matrix $\underline{b}$ in

$$\underline{a} \frac{\partial y}{\partial t} + \underline{b} \frac{\partial y}{\partial z} + \underline{c} y = \underline{d}$$

is evaluated and the hydraulic state y_c is found such that

$$\det [\underline{b}(y_c)] = 0$$

at the choking break.

In the other, still under evaluation and not yet in use, an iteration is performed to find the hydraulic vector for which the mixture velocity equals the choking velocity.

We expect both alternatives to work equally well and will test to see which is faster.

2.2 Drift Velocity (A. Dubow)

A stand-alone program was written and checked out to calculate V_{gm} for turbulent bubbly flow, slug flow, and annular flow in a duct.

2.3 Reactor Core Modeling (T. Wang, W. Wulff)

Coding and debugging has been continued on the subroutines for the steady-state prediction in the stand-alone program for testing the core model. The individual transient momentum balances, associated with the flow and heat transfer regimes in the core have been replaced by a single momentum balance for the entire core.

2.4 Pressurizer (B. Martin and W. Wulff)

Approach

The newly developed lumped-parameter model for the pressurizer and its surge line have been developed along the outline presented in Reference [1], Section 8.2.2.

The processes anticipated during blowdown are (i) bulk condensation in the vapor dome at the top of the vessel, (ii) flashing in the lower liquid zone, starting at the interface between the vapor dome and the liquid zone and then progressing

downward through the surge line, and (iii) discharge through the surge line of pure liquid first, then of low-void, two-phase mixture, and finally of high-void vapor. Flashing occurs when the local pressure falls below the saturation pressure corresponding to the local enthalpy of the liquid.

Three flow regimes, separated by two moving horizontal interfaces at vertical positions $z = Z_1$ and Z_2 have been identified for the vessel. The interface at Z_1 separates the top zone, occupied by a stagnant, high-void mixture of dispersed droplets and saturated vapor, from the middle zone of dispersed bubbles in liquid. The interface at Z_2 separates the middle zone from the bottom zone of pure liquid.

The same three flow regimes are expected in the surge line. Flashing is expected, upward from an interface at $z = Z_3$ near the top of the surge line, even before the interface at $z = Z_2$ reaches the surge line because of the pressure drop caused by the mixture acceleration from the vessel to the surge line. The three flow regimes in the surge line are treated as the three regimes in the vessel, except that the dynamics of the high-void zone are analyzed as the mixture of dispersed droplets and vapor enters the surge line.

The thermodynamic properties in the top zone are considered to be uniform. A single profile function has been estimated for the low-void middle zone. This profile function describes the normalized axial distribution of vapor mass concentration and has been used to compute the axial variations of mixture enthalpy, mixture mass flux and vapor void fraction. The axial variation of enthalpy in the pure liquid zone is estimated from the prescribed initial conditions; the liquid density is a function of enthalpy alone.

The one-dimensional balance equations have been averaged along the axial direction as required, by using the profile estimates. The transient mixture

mass and the transient vapor mass balances have been combined and integrated analytically for the low-void middle mixture zone. A single momentum balance was derived for the fluid in both the vessel and the surge line.

Eight ordinary differential equations govern the transients in the pressurizer, three for the motion of interfaces at $z = Z_1, Z_2$, and Z_3 , and one each for the volume averages of pressure and mixture enthalpy in the top zone, of vapor mass concentrations for the low void zones in vessel and surge line and one for the total momentum in vessel and surge line.

Results

The principal profile function for the low-void zone has been derived from the combination of the steady balance equations for mixture mass, mixture momentum and mixture thermal energy and from the steady vapor mass balance with a constant vapor production term. The vapor production term has been computed from the homogeneous equilibrium vapor generation rate

$$\Gamma_{HEM} = \rho_m \left(\frac{\partial c}{\partial p} \right)_{sm} \frac{Dp}{D\tau} \approx \rho_m \left(\frac{\partial c}{\partial p} \right)_{sm} \left[\dot{\langle p \rangle} + \frac{G_m}{\rho_m} \frac{\partial p}{\partial z} \right] \quad (2.41)$$

where ρ , c , p , s and G represent, respectively, density, vapor mass concentration, pressure, entropy and mass flux, the subscript m denotes mixture properties, the superscripted dot denotes time differentiation, $D/D\tau$ denotes Lagrangian differentiation and $\langle p \rangle$ stands for the volume-averaged pressure. The integration of the four balance equations yields, for constant depressurization $\langle p \rangle$ the vapor mass concentration

$$c(\delta) = -A + \sqrt{B + C\zeta} \quad (2.42)$$

Here A , B , C are non-dimensional groups which depend only on volume-averaged properties and the concentration $c(0)$ at the normalized axial coordinate $\zeta = 0$.

Averaging of Equation (2.4.2) yields a relation between $\langle c \rangle$ and $c(0)$. Substitution of $\zeta=1$ into Equation (2.4.2) yields a second relation, namely between $\langle c \rangle$ and $c(1)$. Thus, the terminal values $c(0)$ and $c(1)$ of the vapor mass concentration c have been related to the volume averaged concentration $\langle c \rangle$. Moreover, Equation (2.4.2) can be used to carry out all quadratures in the transient, volume-averaged balance equations.

Equation (2.4.2) has been compared with experimental data from a transient blowdown test [2] whose characteristic time (time required for pressure reduction to 63% of initial (pressure) is ninety seconds. The instantaneous parameters $\langle p \rangle = 42 \times 10^5 \text{ N/m}^2$, $\dot{\langle p \rangle} = -4.31 \times 10^4 \text{ N/(m}^2\text{s)}$ and $\langle G_m \rangle = -3.4 \text{ kg/(m}^2\text{s)}$ were used to compute the groups A, B and C in Equation (2.4.2). The comparison showed that with the quasi-steady analysis one overpredicts the transient void fraction near the top of the low-void zone by approximately 3%. This means that the local storage of mass and momentum are not very significant. Equation (2.4.2) appears sufficiently accurate to predict the shape (normalized axial variation) of the vapor mass concentration. Further comparison of Equation (2.4.2) with experimental results is required.

The volume-averaging of the balance equations is routine and not discussed in detail. Closed-form integrations have been obtained by computing saturation properties for mixture properties from a single, time-dependent pressure $\langle p \rangle$.

Equations of motion have been derived for two kinds of interfaces. The velocity of the interface at $z = Z_1$, between low and high-void fraction zones, is computed from the vapor and mixture mass balances and from mixture conditions just above and below the interface. The velocity of the interface at $z = Z_2$, between pure liquid and low-void zones, is computed from the interface definition as the axial position where the local pressure equals the saturation pressure

corresponding to the local liquid enthalpy. The evaluation of this velocity involves the liquid thermal energy balance and the momentum balance.

Future Work

Programming of a code should be continued to test the pressurizer model by comparing computed with experimental results.

2.5 Steam Generator Modeling (C. Ruger)

The hydraulics of the lumped steam generator model are based on the one-dimensional drift flux model of Reference 3. The approach uses order of magnitude considerations to simplify the conservation equations, division of the flow channels by fixed or moving boundaries to separate, respectively, structural elements and flow and heat transfer regimes, closed form solution or volume-averaging the conservation equation and introduction of appropriate profile functions to relate volume averaged state variables to their terminal values.

The four balance equations consist of the mixture mass, vapor mass, mixture momentum and mixture enthalpy. The principal dependent variables have been chosen as pressure, p ; mixture specific enthalpy, h_m ; mixture mass flux, G ; and vapor mass fraction, c .

Prior to volume-averaging the mixture mass and mixture enthalpy equations were combined by elimination of the storage term $\partial h_m / \partial \tau$ between them. This elimination uses the thermal equation of state and also takes advantage of the above mentioned approximation of neglecting the spacial derivative of pressure.

The spacial derivatives of enthalpy appearing in the resulting equations have been evaluated by introduction of a normalized quasi-steady mixture enthalpy distribution in the axial direction - the so called enthalpy profile. This is obtained as a function of the wall heating from the steady mixture enthalpy balance with specifications of either thermodynamic equilibrium or the spacial deviation of liquid enthalpy from equilibrium.

Substitution of the enthalpy profile relocation allows closed form axial integration of the combined balance equation to yield the normalized axial distribution of mixture momentum in terms of the entrance value of mass flux and

the time derivative of average pressure. Two independent algebraic expressions have been obtained by evaluation of this result at the exit terminal and by integration over the channel length.

Since two of the balance equations were combined to obtain these results, only three independent balance equations remain to be volume-averaged. The mixture momentum equation has been averaged over the entire (fixed) channel length, resulting in a single ordinary differential equation not involving moving boundaries. The vapor mass and mixture enthalpy balance equations have been averaged over each flow regime separately. The Leibnitz rule is applied to the time derivative terms to obtain a set of ordinary differential equations. Following is an example of the results - in this case for the energy balance:

$$\langle \dot{h}_m \rangle - \int_0^L \frac{1}{\rho_{m,i}} dL \langle \dot{p} \rangle$$

= moving boundary terms ($\dot{Z}_i$)

+ heating terms

+ convection terms

An additional set of ordinary differential equations describing the locations of the moving regime boundaries have been obtained from the definition of the boundary by the void fraction and the vapor mass balance equation in each regime.

Future Work

Analysis of the heat transfer in the tubes between the primary and secondary flow channels is to be carried out. In addition, logic must be developed to keep track of the nature of adjuent flow regimes in the primary and secondary zones, in order to choose the proper heat transfer coefficients. Coding is to be initiated for a stand-alone steam generator model.

2.6 System Modeling (G. Srikantiah)

System Balance Equations and Explicit Integration:

The network balance equations form an algebraic system made up of the following sets of equations:

(i) Component Balance equations:

$$F_1(\dot{Y}, Y_1, Y_2, \dots) = 0$$

(ii) Component profile equations:

$$F_2(Y_1, Y_2, \dot{Y}, \dots) = 0$$

(iii) Nodal (interface) continuity equations:

$$\sum W_{ij} = 0 \text{ at node } j$$

It has been established that the profile equations should be derived such that they conform with the propagation of information in the fluid at the component interfaces. The explicit integration scheme requires the computation of the derivatives, $\dot{Y}$ at each step. In this scheme $\dot{Y}$'s must be obtained by solving the algebraic system. As the following example shows, the system of algebraic equations must be formulated carefully if it is to yield proper solutions.

Figure 1.

Consider a simple four component network as in Figure 1. The number of edges n_e is four, and the number of vertices n_v is four. For this example we shall consider simplified, volume averaged balance equations for pressure p and mass flux G only.

(i) Balance equations:

$$p_1 - p_2 = L_a \langle \dot{G}_a \rangle + f_a (\langle G_a \rangle, \rho_a)$$

$$G_{1a} - G_{a2} = \alpha_a \langle \dot{p}_a \rangle$$

where $\rho_a = \rho_a (\langle p_a \rangle)$;

(ii) Profile equations

$$f_{ap} (p_1, p_2, \langle p_a \rangle) = 0$$

$$f_{aG} (G_{1a}, G_{a2}, \langle G_a \rangle) = 0, \text{ etc.}$$

Note that the balance equations do not form part of the simultaneous set since the terms involving $\langle \dot{p}_a \rangle$, $\langle \dot{G}_a \rangle$, etc. do not occur in the other equations. There will be a total of $2n_e$ profile equations and n_v equations at the component interfaces of the type:

$$\sum_i W_{ij} = 0 \text{ (at node } j)$$

Here the flow rate W is the product of area A and mass flux G . Examination of the equation set reveals that the equations (profile) involving p 's are independent of the equations involving G 's, and the two sets can be solved in principle, separately. This will be the case so long as the network has the same number of components as interfaces, i.e., $n_e = n_v$. If we now consider a network of five components formed by adding a component e to the above network connecting the interfaces 2 and 4, the additional equations (profile) are,

$$f_{ep} (p_2, p_4, \langle p_e \rangle) = 0$$

$$f_{eG}(G_{2e}, G_{e4}, \langle G_e \rangle) = 0$$

The continuity equations at the interfaces are modified at vertices 2 and 4 but their number remains the same. The total number of equations are $2n_e + n_v$, where $n_e = 5$ and $n_v = 4$; the variables are four p's and ten G's. However, the profile equations for p are independent of those for G. There are five p-profiles to determine four p's and nine G-profiles and interface balances to solve for ten G's. The specification of profile equations in this way always lead to an overdetermined system for p's and an underdetermined system for G's. By analogy with the steady-state balance equations, we may specify that the p-profiles be functionally dependent on the G's. When this condition is fulfilled, it is possible to find a solution for the total system.

Implicit Scheme:

Consider a first order implicit scheme in which the derivative $\dot{\langle Y \rangle}$ is replaced by

$$\dot{\langle Y \rangle} = \frac{\langle Y' \rangle - \langle Y \rangle}{\delta t}$$

where the prime indicates advanced time. The profile and balance equations for any element of the five component network above take the form (for the component e, for example),

$$\left. \begin{aligned} f_{ep}(p_2', p_4', \langle p_e' \rangle) &= 0 \\ f_{eG}(G_{2e}', G_{e4}', \langle G_e' \rangle) &= 0 \end{aligned} \right\} \text{profile;}$$

$$\left. \begin{aligned} P_2' - P_4' &= \frac{L_e}{\delta t} (\langle G_e \rangle' - \langle G_e \rangle + f_a (\langle G_e' \rangle, \rho_e')) \\ G_{2e}' - G_{e4}' &= \frac{\alpha_e}{\delta t} (\langle P_e \rangle' - \langle P_e \rangle) \end{aligned} \right\} \text{Balance;}$$

These equations are written in their simplest form and are of the same form for the other components. The continuity equations at the interfaces are:

$$\sum_i w_{ij}' = 0 \quad (\text{at node } j).$$

Detailed examination of this set of equations reveals that this system, where all primed quantities are unknowns, appear to be solvable. The profile equations no longer have the constraints which appear in the explicit case.

2.7 Code Assembly (D. Garber)

2.7.1 Host Code

Current Developments

Objectives and Activities:

1. The Code User has been provided with the ability of specifying an IF, AND, OR, THEN, ELSE, etc. logic to control boundary and trip condition specification. This control is flexible since the object of the IF, AND, OR Logic test is any global item in the large common memory array (referenced by the Data Base Manager). If during the calculation the above logic is .TRUE, a consequence equation(s) (THEN, etc.) is implemented.
2. Since the equations that appear in the Host code are strings of address pointers, substitution of a given equation for a variable can be accomplished by redirection of pointers. The efficiency and logic of such a system has been studied for some sample problems

3. An algebraic equation processor (SYMBOLANG) has been implemented and introduced to members of the THOR group. This FORTRAN based language allows for FORMAC-like manipulation of equations on the computer.
4. A study has begun as to how the code can be modified to implement an implicit problem formulation.

Future Work

Begin implementation of the Optimization routine. Design and implement a variety of output routines for the Host code.

2.7.2 Coupling of Lumped and Discrete Parameterized Components (W. Turner)

The THOR code will include both a lumped parameter and a distributor parameter description of most components. Thus, a THOR simulation of a particular thermal hydraulic system will usually be partly by means of lumped models and partly by means of distributed models of components. Hence it is necessary to couple the two component types. This coupling problem will be discussed here in terms of the more general problem of coupling two time stepping digital computer simulations of compressible hydraulics one of which requires significantly smaller time steps than the other. It is desirable that this coupling be done in such a way that different size time steps can be used in each calculation, as then each hydraulic simulation can proceed at maximum efficiency. Desirable as this might be, it has not, as far as we have been able to determine, been incorporated in any water cooled reactor code at the present time (9, 10, 11, 12). Different time step sizes have of course been used for coupled hydraulic simulation in some fast reactor codes (SAS3A), however, in these cases incompressible flow is assumed in at least one of the simulations. Other than with the method of characteristics, no method has been found for coupling two simulations of compressible hydraulics.

The method proposed here will first be discussed for the solution of the simple hyperbolic equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial z} = 0$$

where the characteristic velocity is positive and constant. Then the method will be extended to the coupling of two numerical simulations of compressible hydraulic systems described by a hyperbolic set of conservation equations.

One Conservation Equation

Consider the loop shown in Figure 2. The loop is divided into two regions:

Figure 2.

region A which is solved by method A using time step Δt ; and region B which is solved by method B using time steps δt (assumed not larger than Δt). The two regions are bounded by their common interfaces at z_1 and z_2 where u takes the values

$$u_1(t) = u(z_1, t) \quad \text{and} \quad u_2(t) = u(z_2, t)$$

In region A the entire solution from t^0 to $t^0 + \Delta t$ is determined if the boundary condition u_1 is known over the time interval t^0 to $t^0 + \Delta t$ and the initial condition at time t^0 . We choose the time step Δt sufficiently small that u_1

and u_2 can be assumed to vary linearly i.e.,

$$u_1(t) = \frac{(\Delta t - t + t^0) u_1^0 + (t - t^0) u_1'}{\Delta t}$$

Thus given the initial condition at t^0 , the only further parameter required for solution in region A at $t = t' = t^0 + \Delta t$ is u_1' i.e.,

$$u(z, t') = f(u_1', z) \text{ in region A.}$$

thus $u_2(t') = u_2' = g(u_1')$.

If solution method A requires the linearization of the equations used to solve region A, then a linear approximation to function g will be available;

$$u_2' = b u_1' + d \quad (2.7.2.1)$$

If the equations of method A are not linear in the values of u at the unknown time t' then a best estimate $\bar{u}_1'$ for u_1' must be obtained. This estimate is probably best obtained by extrapolation from the last two time steps. Then the function g is linearized at about this point.

$$u_2' = g(\bar{u}_1') + \frac{dg}{du_1'} (u_1' - \bar{u}_1') \quad (2.7.2.2)$$

giving values for b and d . Thus

$$u_2(t) = b u_1(t) + d \text{ at } t = t^0 + \Delta t$$

$$\text{and } u_2(t) = u_2^0 \quad \text{at } t = t^0$$

Since the behavior of u_1 and u_2 is approximately linear over Δt we obtain by linear interpolation in t

$$u_2(t) = \left[(t^0 + \Delta t - t) u_2^0 + (b u_1' + d) (t - t^0) \right] / \Delta t$$

$$\text{for } t^0 < t \leq t^0 + \Delta t$$

This is now the boundary condition for region B. At each time step δt this equation and the equations used in solution method B are solved for u within region B and for u_1 and u_2 . Eventually a δt must be chosen so that a region B solution is obtained at time $t^0 + \Delta t$. The u_1 and u_2 obtained as part of the region B solution for this time are consistent with the region A equations. The $u_1(t^0 + \Delta t)$ is then used in solution method A to find the solution for region A. Consider the u_1, u_2 plane shown in Figure 3.

Figure 3.

In this example solution method B for region B required three time steps to cover the single large time step used in method A for region A. The lines on Figure 3 are determined by the region A solution; the points P, Q, R are determined from the region B solution and the lines.

n Conservation Equations

The extension to n conservation equations is fairly obvious and will not be given in detail. Let u be a vector with components

$x_1, x_2, \dots, x_n$ at point 1 and

$y_1, y_2, \dots, y_n$ at point 2; these being the values of the basic

variables (G, P, h, c for THOR) of the problem at points 1 and 2.

We again consider the loop of Figure 2. Let r and s be the number of positive characteristics at points 1 and 2 respectively. Thus the region A linearized boundary conditions are

$$\begin{aligned} \eta_i &= \sum_j \alpha_{ij} x'_j, & i &= 1, 2, \dots, r \\ x_k &= \sum_j \beta_{kj} y'_j, & k &= 1, 2, \dots, n-s \end{aligned} \quad (2.7.2.4)$$

for $t = t^0 + \Delta t$

In general η and χ are quantities that are required to be continuous at the boundary e.g. flow rates of the conserved quantities. As the boundary condition equations must be sufficient to complete the set of equations for region A, the linearized solution for $t = t^0 + \Delta t$ can be obtained and written

$$u_1(t^0 + \Delta t) = A_1 \eta + B_1 \chi + E_1$$

$$u_2(t^0 + \Delta t) = A_2 \eta + B_2 \chi + E_2$$

where η and χ are vectors with components η_i and χ_k respectively and A and B are r and $(n-s)$ by n matrixes respectively. The values of u_1 and u_2 at time t^0 are known

$$u_1(t^0) = u_1^0$$

$$u_2(t^0) = u_2^0$$

The time step is sufficiently small to allow linear interpolation, thus

$$\begin{aligned} u_1(t) &= \frac{(t^0 + \Delta t - t) u_1^0 + (A_1 \eta + B_1 \chi + E_1) (t - t^0)}{\Delta t} \\ u_2(t) &= \frac{(t^0 + \Delta t - t) u_2^0 + (A_2 \eta + B_2 \chi + E_2) (t - t^0)}{\Delta t} \end{aligned} \quad (2.7.2.5)$$

$$\text{for } t^0 \leq t \leq t^0 + \Delta t$$

are the boundary conditions for region B. Note that these 2 n equations do not

contain $2n$ boundary conditions. If the $n+r-s$ unknowns (χ, n) are eliminated for the $2n$ equations, $n+s-r$ equations will be obtained relating components of u_1 and u_2 . These are the boundary conditions on region B imposed by region A. As required, the number of these conditions ($n+s-r$) is equal to the number of characteristics crossing into region B from region A. Thus the equation for region B plus these boundary conditions are a complete set and can be solved for u_1 , u_2 , χ , n and conditions within region B at each δt . Once the region B solution is determined up to Δt , the boundary conditions for region A (Equation 2.7.2.4) are known and the large time step Δt can be calculated for region A.

2.8 Lumped Pipe (U.S. Rohatgi)

A lumped parameter model for an adiabatic, constant area pipe has been developed. The drift flux formulation is used, where it is assumed that the non-equilibrium vapor generation term is proportional to the homogeneous equilibrium (HEM) vapor generation rate, and the mixture densities are a function only of average instantaneous pressure and local instantaneous vapor mass concentration. The thermal energy balance and the vapor mass balance are simplified by approximating the $\frac{\partial p}{\partial t}$ term by $\frac{\partial \langle p \rangle}{\partial t}$. Three of these equations, the mixture momentum balance, vapor mass balance and thermal energy balance, are integrated over the pipe length. The integration of the last requires profiles for pressure (p), enthalpy (h) and vapor mass concentration (c). In what follows, three different models are described, which differ in the way the profiles are computed and in how the balance equations are simplified.

A. First Approach:

In the first approach, the drift flux velocity is assumed to depend on averaged quantities, and the profiles for p and c are obtained from steady-state

vapor mass and mixture momentum balances. The enthalpy profile is obtained from the caloric equation of state. All three profiles turn out to be linear after certain simplifications. The mixture mass balance is not volume averaged in the usual way, instead the $\frac{\partial c}{\partial t}$ term is substituted from the vapor mass balance equation to give an ordinary differential equation for the mass flux $G(z,t)$. This G distribution gives two relationships among the inlet, outlet and average mass fluxes. Thus a system of eight equations is obtained, which along with four boundary conditions completely specify the problem in twelve variables, average, inlet and outlet values of p , h , c and G .

2.8.2 Second Approach

In the second approach the p profile is obtained from the transient mixture momentum balance. The h and c profiles, and the integrated vapor mass balance, thermal energy equations are the same as above. In the mixture mass and the balance, the density is approximated as a function of average pressure $\langle p \rangle$ and average concentration $\langle c \rangle$. This is a good approximation at high pressure for all concentration and at low pressures for high concentrations. This gives a linear profile for G , with its slope given as a function of $\frac{d\langle p \rangle}{dt}$ and $\frac{d\langle c \rangle}{dt}$. It also gives two relationships among inlet, outlet and average mass flux. This G distribution is used to integrate the mixture momentum equation. The first integration relates p_1 , p_2 , and $\frac{d\langle G \rangle}{dt}$, while the second relates $\langle p \rangle$, p , and $\int_0^L \frac{\partial G}{\partial t} dz$. The main difficulty in this approach is with unsteady inertia term. A linear G profile leads to terms in $\frac{d^2\langle p \rangle}{dt^2}$, $\frac{d^2\langle c \rangle}{dt^2}$, increasing the order of the system. On the other hand if the integral of unsteady inertia is approximated by $\frac{L^2}{2} \frac{d\langle G \rangle}{dt}$, then the system is complete without higher order derivative. However, this simplification restricts this model to the following constraint

$$\dot{G}_1 \ll 4\langle \dot{G} \rangle$$

2.8.3 Third Approach

As both these approaches give systems of complex equations to be solved, additional simplifications are advantageous. Here all the coefficients, the density, the gravity in the friction terms are computed from averaged variables, and the second procedure is repeated. This gives a simplified model for the pipe. In a numerical test of this approach the V_{gm} terms were neglected, and the system of eight equations is first solved by a non-linear algebraic equation solver (ZSYSTEM) for the time derivatives of the average variables and their boundary values. These time derivatives are integrated by a fourth-order Runge-Kutta method. In a test case the inlet pressure, enthalpy and concentration were kept constant, while the exit pressure was decreased. The system of equations was found to be stiff requiring a time step size of .001 seconds. The origin of this stiffness is in the differential equation for $\langle p \rangle$. This stiffness was removed by assuming a linear profile for p and computing $\frac{d\langle p \rangle}{dt}$ from the boundary conditions. The procedure removed the differential equation for $\langle p \rangle$ from the system and the allowable step size went up to .2 second. In another attempt to improve the step size, the analysis was completed for an implicit solution method. Programming for this approach has not been completed.

The third approach comes the closest to the finite difference method with two nodes. The difference lies in the pressure profile, which is taken to be linear in the finite difference case, and in the method of time integration. There is now a need to test these three models with a finite difference solution in order to determine the accuracy and speed of computation gained by different formulations.

2.9 Plenum (P. Kroeger)

The following plenum model has been set up as an initial model and within the constraints of our present time schedule to be improved and modified as experience is obtained, regarding this model and its interaction with the neighboring component models.

The plena are to be considered as relatively large volumes, such that within each such volume the pressure is uniform in space, and internal velocities are small with respect to the inflow and outflow velocities. (A vertical pressure gradient due to gravity can be added later, if required.)

During a substantial part of the LOCA transient superheated or high void fraction saturated vapor will flow from the core via the lower plenum into the downcomer. At the same time, subcooled liquid or a low void fraction two-phase mixture may enter the plenum from the downcomer and replenish the remaining low void fraction two-phase mixture at the bottom of the lower plenum. To represent these effects the existence of two distinct regions separated by an interface is assumed. The lower region will in general be occupied by subcooled liquid or a low void fraction two-phase mixture, while the upper region in general contains a high void fraction two-phase mixture or superheated steam. If applicable, either region could be of zero volume, in which case the plenum is effectively composed of one region only.

Presently the fluid in either region is assumed to be in thermal equilibrium and in a uniform state, but in general unequal to the state of the other region. The upper (high void fraction) region is also assumed to be homogeneous.

For each region the conservation equations for mass and energy are applied. Including the effect of bubbles rising from the lower region into the upper region, and with the interface itself moving these conservation equations are:

Conservation of Mass for region j:

$$\dot{M} = \frac{d}{dt} (\rho_j V_j) = \sum (G_i A_i) - \rho_k (v_k - \dot{z}_e) \bar{\alpha}_k A_e \quad (2.9.1)$$

Conservation of Energy for region j (neglecting kinetic energy, dissipation, and work of body forces):

$$\dot{E} = \frac{d}{dt} (\rho_j e_j V_j) = \sum (G_i A_i h_i) - p \dot{V}_j - \rho_k h_k (v_k - \dot{z}_e) \bar{\alpha}_k A_e + Q_{exj} \quad (2.9.2)$$

where

V_j	volume
M	total mass
E	total internal energy
e	specific internal energy
G_i	mass flux across stationary inlet i
A_i	cross sectional area of stationary inlet i
A_e	area of interface separating regions
z_e	vertical position of interface
p	pressure
h	enthalpy
ρ	density
v	velocity
Q_{ex}	heat addition from the exterior
$\bar{\alpha}_k$	volume fraction of phase k
α_j	average volume void fraction of region j
index i	index for stationary inlet or outlet connected to region j
index j	region j (j = 1 lower region, j = 2 upper region)
index k	index for phase crossing the interface

With the assumption of homogeneous flow in the upper region (i.e. neglecting falling droplets) only vapor from the lower region will cross the interface.

The optional bypass of liquid from the downcomer into the lower region will be described below). In this case the interface velocity $\dot{z}_e$ must be equal to the liquid velocity in the lower region. For a given constitutive relationship for the vapor drift velocity V_{gj} , the vapor mass flux across the interface is

$$\alpha_1 \rho_{v1} (\dot{v}_{v1} - \dot{z}_e) = c_1 \rho_{m1} (\dot{v}_{v1} - \dot{v}_\ell) = \frac{c_1}{1-c_1} \rho_{\ell 1} V_{gj} \quad (2.9.3)$$

where c is static quality and all region 1 data refer to the uniform average state of region 1. The total plenum volume is constant, i.e.,

$$\dot{V}_1 + \dot{V}_2 = A_e \dot{z}_{e1} - A_e \dot{z}_{e2} = 0 \quad (2.9.4)$$

The plenum geometry can be prescribed as $A(z) = \text{constant}$ or as a variable array, with $A(z)$ and $V(z)$ then computed by interpolation. With (3) and (4) into (1) and (2), replacing ρ_e by $\rho h_m - p$ in (2) and using $\rho = \rho(h, p)$ one obtains from (1) and (2) a set of four ordinary differential equations for the dependent variables

$$A \dot{y} = f \quad (2.9.5)$$

where the dependent variable vector is

$$y = (P, z_e, h_{m1}, h_{m2})^T \quad (2.9.6)$$

For the general case in which both regions exist the coefficient matrix can be written as

$$A = \begin{Bmatrix} V_1/a_{o1}^2 & \rho_{m1} A_e & 0 & 0 \\ V_2/a_{o2}^2 & -\rho_{m2} A_e & 0 & 0 \\ -V_1 & 0 & \rho_{m1} V_1 & 0 \\ -V_2 & 0 & 0 & \rho_{m2} V_2 \end{Bmatrix} \quad (2.9.7)$$

and the right hand side vector f is given by

$$\left\{ \begin{array}{l} \sum_1 (G_i A_i) - \frac{c_1}{1-c_1} \rho_{\ell 1} V_{gj1} A_e - \frac{1}{\rho_{m1}} \left(\frac{\partial \rho_{m1}}{\partial h_{m1}} \right)_p f_3 \\ \sum_2 (G_i A_i) + \frac{c_1}{1-c_1} \rho_{\ell 1} V_{gz1} A_e - \frac{1}{\rho_{m2}} \left(\frac{\partial \rho_{m2}}{\partial h_{m2}} \right)_p f_4 \\ \sum_1 (h_i - h_{m1}) G_i A_i - (h_{v1} - h_{m1}) \frac{c_1}{1-c_1} \rho_{\ell 1} V_{gj1} A_e + Q_{ex1} \\ \sum_2 (h_i - h_{m2}) G_i A_i + (h_{v1} - h_{m2}) \frac{c_1}{1-c_1} \rho_{\ell 1} V_{gj1} A_e + Q_{ex2} \end{array} \right\} = f \quad (2.98)$$

For the special cases of only region one or only region two existing, a corresponding simpler set of equations is obtained.

In general all inflows and outflows will enter or leave the region they are connected to, i.e. depending on whether the inlet/outlet location z_i is above or below the interface level z_x . However, to accomodate such effects as subcooled liquid from the downcomer being injected above the interface but flowing (thru the upper region) into the lower region, upper region inflows can, as an option, be permitted to flow into the lower region directly.

To accomodate the fact that the fraction of the downcomer/plenum interface over which liquid is flowing down, or vapor is flowing up will change during the transient, the areas A_i of the stationary inlet/outlet can change with time.

The treatment of the plena differs from the corresponding RELAP [4,5,6] or FLASH [7,8] treatment in that separate mass and energy conservations are

solved here for each of the two regions, permitting different states in these regions. In contrast, RELAP and FLASH solve one energy and one mass conservation equation for the state in the whole volume and obtain a level within this volume from a separate mass balance for the vapor in the lower region, assuming all the liquid to be in the lower region and the vapor in the upper region to be at saturation.

The model is presently being programmed as a free standing program, for preliminary evaluation, before it is to be included into the code itself.

It is expected that extensions and modifications will be made as experience is obtained regarding the model itself and in particular its interactions with the neighboring modules.

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