COMPUTER SIMULATION OF TWO-PHASE FLOW IN NUCLEAR REACTORS

Wolfgang Wulff
Brookhaven National Laboratory* / BNL--47783

DE92 040565

STI

ABSTRACT

Two-phase flow models dominate the economic resource requirements for development and use of computer codes for analyzing thermohydraulic transients in nuclear power plants. Six principles are presented on mathematical modeling and selection of numerical methods, along with suggestions on programming and machine selection, all aimed at reducing the cost of analysis.

Computer simulation is contrasted with traditional computer calculation. The advantages of run-time interactive access operation in a simulation environment are demonstrated.

It is explained that the drift-flux model is better suited for two-phase flow analysis in nuclear reactors than the two-fluid model, because of the latter's closure problems. The advantage of analytical over numerical integration is demonstrated. Modeling and programming techniques are presented which minimize the number of needed arithmetical and logical operations and thereby increase the simulation speed, while decreasing the cost.

1. INTRODUCTION

The cost of computing, that is of executing arithmetical and logical operations on an electronic digital computer, has dramatically declined in recent years, but the total cost of analyzing transient two-phase flow phenomena in, and the dynamic behavior of, complicated nuclear reactor systems has not significantly decreased. The cost of initial capital investment, maintenance and operation of newly available workstations are small compared to those for the equivalent computing capacity in previously used supercomputers. The overall cost of analyzing complex systems has not decreased, because it is dominated by the analyst's salary, which in turn is dictated by the time it takes to prepare, execute, analyze and document the several computer calculations normally needed to assess a single reactor transient and the uncertainty associated with the analysis.

Efforts of analyzing normal and accident transients in nuclear reactor power plants are dominated by the difficulty to model and numerically simulate a vast number of multiphase flow phenomena in the reactor coolant and possibly in the core melt. Multiphase, and particularly two-phase flow issues will therefore be the focus of this paper.

There are three fundamental reasons for the widely experienced, painfully large expenses of nuclear reactor analyses: (i) the demand for growth of scope and detail of the analyses could not be compensated for by advances in computing speed, (ii) the models and computer codes currently used for reactor analyses are largely inefficient, and (iii) the analysis methods are oriented toward computer calculation, rather than toward faster, more expeditious, convenient and efficient computer simulation.

Reason (i) arises from the need to account for an increasing number of more and more complicated phenomena in the analysis. This need will remain and must be dealt with, as reactor technologies advance and

*This work was performed under the auspices of the U. S. Department of Energy.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER

as the objectives expand from design base to severe accident analyses. The expectation, however, of solving the problems of high cost and long execution time for computer analyses, by waiting for low-cost computers of "ultimate" speed, is not realistic on the basis in history.

Reasons (ii) and (iii) are the subject of this paper. It will be demonstrated that engineering judgement in selecting and formulating models, in selecting established and documented numerical methods, and that working in what will be described as a simulation environment, can significantly improve the quality of two-phase flow analyses, while reducing the time and cost that they require.

BWR stability analyses performed recently by Wulff et al [1,2,3], in the simulation environment of the BNL Engineering Plant Analyzer [4] on the one hand, and with INEL's standard FORTRAN code TRAC-BF1 [5], run on the CRAY general-purpose supercomputer, had the same objectives: to analyze (with point kinetics) core wide oscillations related to those that had occurred at the LaSalle-2 Power Station in March of 1989. Approximately the same time and expenditures provided from the simulation environment over ninety different, complete plant transient analyses, including all systems feedback effects [1], and from the standard FORTRAN computing method the effects of four parameter variations on open loop (reactor core channel) calculations with imposed boundary conditions. By working in a simulation, rather than in a computing environment, and by appropriate modeling techniques, one could reduce the total effort of analyzing reactor transients by about two orders of magnitude.

The objectives of this paper are to explain the difference between computing and simulation, to present six principles of modeling and numerical methods, all of which are aimed at reducing the computational effort. It is also the objective of this paper to suggest three coding requirements and to present the important features of the simulation computer environment. Lastly, it will be shown why modeling and numerical methods need to be optimized with the computer architecture as a whole. A given computer code, when optimized for a given computer, cannot achieve the same degree of optimization on another computer, primarily when intensive input and output processing is involved.

2. COMPUTING VERSUS SIMULATION

Traditional computer analyses of nuclear reactor transients, involving two-phase flow and proceeding both under normal and postulated accident conditions, have been performed by computer calculation. Computer calculations are carried out on general purpose computers (super, mainframe, minicomputers or workstations), using an operating system, a FORTRAN compiler and a standard FORTRAN computer code, such as RETRAN [6,7,8], RELAP5 [9,10,11] or TRAC [12,13]. The codes are executed in batch mode, and the results are post-processed with a graphics code to display them conveniently.

In contrast, computer simulation is carried out in a simulation environment, consisting, not necessarily but preferably, of a special-purpose simulation computer, and consisting always of an interactive simulation software system, a simulation language and a simulation code which describes the physics of the system to be analyzed. The interactive simulation software system is the most distinctive characteristic of the simulation environment, followed by the input and output processing hardware components of the simulation computer, and then by the simulation language.

Computer simulation is carried out in-line, interactively. Herein lies the main reason for its efficiency. It provides the analyst with run-time control for setting parameters, activating simulated component functions or failures, resetting initial conditions, further for reselecting integration algorithms and display features. All of this is achieved without reloading and recompiling the program. The analyst can participate in the simulation, by monitoring and influencing the same, in-line, during its execution. This is very important for the assessment of operator actions and for carrying out efficiently large numbers of scoping calculations.

Hardware, such as analog or digital sensors and control systems, can be tested and optimized in the computational loop of a simulation facility. Any program variable can be displayed versus any other variable or time, without preprogramming or reloading the program, and in any form, such as the trend on an oscilloscope, or in tabular form. Herein lies the simulation environment's strength for code development.

The simulation language, such as EASY5 [14], ACSL [15] or ADSIM [16], is state variable oriented and has a large number of simulation-specific constructs, including a choice of proven and documented methods for numerical integration and matrix algebra, and for multidimensional table generation and interpolation.

Computer simulation is today most efficiently achieved with special purpose computers, such as the AD-100 [17] in the BNL Engineering Plant Analyzer. Still, no alternative can reach its convenience and computing speed, primarily because of its superior input and output data processing. However, today's special-purpose simulation computer capabilities can be achieved on advanced workstations, once their simulation systems software is developed and the high-speed, high capacity input processing capabilities (hardware and software) are available.

3. SIMULATION PRINCIPLES

The four elements of simulation are the mathematical models which define the physical system to be simulated, the numerical methods with which to integrate and solve the equations of the mathematical model, the simulation language which facilitates the execution of the numerical methods on a computer, and an interactive computing facility.

3.1 Modeling Principles

Three modeling principles are presented here to promote modeling efficiency, which is achieved when the greatest possible simulation fidelity is obtained with the smallest possible number of arithmetical and logical operations.

3.1.1 Principle of Model Selection

Model selection for gas-liquid two-phase flow simulation is important, because a variety of models with differing modeling detail and complexity is available, and the choice one takes has a profound impact on modeling fidelity and simulation cost. Two-phase flow models are categorized by the number of conservation equations employed for mass, momentum and energy conservation in the liquid and the gas, and the related numbers of implied constraints and needed transfer laws for closure.

Wulff [18] related in 1981 systematically the number of conservation equations to the numbers of constraining assumptions and transfer laws needed to relax constraints. He covered the range from the simplest three-equation model for homogeneous equilibrium two-phase flow, which carries the maximum of three limiting constraints of equal pressures, equal temperatures and equal velocities for both phases, to the most complex, six-equation two-fluid model for nonhomogeneous, nonequilibrium two-phase flow, which has no constraints.

The three-equation model requires two transfer laws, one each for wall shear and wall heat transfer. The six-equation model requires seven laws, three for mass, momentum and energy transfer between the phases, and two each for momentum and energy transfer between the wall and each phase. In general, multiphase flows with n phases, modeled by $3n$ conservation equations, require $n(3n+1)/2$ flow pattern-dependent transfer laws.

Complete closure requires additional constitutive laws for material descriptions and interface conditions. Ishii established in 1975 [19], that the two-fluid model formulation contains thirty-two variables and requires twenty-six closure relations.

The principle of model selection is that one should choose the least complicated model which accommodates all available experimental information and the phenomena of interest.

Irrespective of its complexity, no model can produce more information than is contained in its data base, which includes the closure laws. On the other hand, intolerable simplifying assumptions (such as homogeneous vertical flow) render a model inadequate.

Modeling complexity is linked to computational complexity and corresponding efforts of computing. Models which cannot produce information commensurate with their complexity squander computing resources.

The application of the principle of model selection to two-phase flow modeling leads to the conclusion that the two-fluid model can be justified at this time only for separated flows, where the interface geometry is known and amenable to boundary layer analyses. Transfer laws for momentum exchange between phases and a review of the currently inadequate capability of predicting interfacial area density for the two-fluid model were published by Ishii [20]. The two fluid model is also suitable for testing modeling hypotheses, and for linking theory with experiments.

For the chaotically deforming interfaces of two-phase flow patterns occurring in nuclear reactors, however, there is still no experimental basis for supporting the two-fluid model by developing transfer laws to describe the split of total into phasic momentum and energy transfers at the wall; there is still no suitable instrumentation available for developing such transfer laws.

The four-equation drift flux model introduced by Zuber and Findlay [21] in 1965 is a mixture model, akin to the familiar multispecies model of chemical engineering. It accommodates directly better than any other two-phase flow model the available experimental information. Relative phasic velocities are predicted in terms of two flow-regime dependent parameters: the drift velocity and the distribution parameter, as published by Ishii [22]. According to Bouré [23], the drift-flux model is especially well suited for predicting the propagation of thermal and kinematic disturbances, which are precisely the objectives of thermohydraulics simulations. The comparison of the performances of the drift-flux model and the two-fluid model, as documented in references [1] through [4] on the one hand and in [5] on the other, supports this conclusion.

The closure problem for the drift-flux model is smaller: there is no wall shear and wall heat flux splitting required. The integration of four equations requires obviously fewer resources than that of six equations. The drift-flux model is superior to the two-fluid model for the prediction of flows with tightly coupled phases and stochastically deforming interfaces.

3.1.2 Scaling and Model Simplification

The second modeling principle calls for an order of magnitude comparison, to be performed on all the terms of the governing model equations and, based on it, for the elimination of all terms which represent irrelevant phenomena.

This model simplification is subject to the requirement that well-posedness must be preserved: the elimination of seemingly unimportant dissipative terms must not change a well-posed parabolic into an ill-posed hyperbolic system of partial differential equations having complex characteristics.

Typical simplifications are the elimination of virtual mass effects, except where large local accelerations are to be modeled, and the complete elimination of acoustic effects from thermohydraulic codes (by setting $v_p=0$ in mass and energy balances), unless these are to predict dynamic interactions between fluid and structure.

The suggested simplification process is similar to the normalization of the governing equations, normally performed for scaling and the purpose of compacting the large number of constants in the equations into a much smaller number of scaling groups. Just as only two scaling groups, the normalized wall roughness and the Reynolds number suffice completely to describe wall shear in all circular tubes and for all liquids and gases, so also facilitate scaling groups a significant reduction in the number of needed arithmetical operations. Thus, scaling of equations reduces the computational effort, even without the simplification of equations.

Finally, scaling in computer analyses would focus attention on the need to cover the range of full-scale reactor plant conditions both by small-scale experiments and by selecting correlations for the models.

3.1.3 Use of Analytical Methods

The third modeling principle urges that analytical rather than numerical integration be used, whenever that is feasible, and that analytical solutions be dynamically evaluated on the computer for the conditions evolving during a transient.

Analytical solutions are easy to assess regarding the effects of, and uncertainties from, simplifying assumptions, all of which are enumerable. Analytical solutions are free from effects of numerical diffusion and raise no concerns about convergence.

The analytical integrations over space of the mixture momentum and mass balances are explained below to demonstrate the benefits from analytical methods in two-phase flow simulation.

The analytical integration of the mixture momentum equation around every closed loop in the system is based on Meyer's momentum integral model [24] and has been used in the BNL Engineering Plant Analyzer [4] with great success to reduce over fifty partial difference to just three ordinary differential equations, one for every closed loop in the system. The loop momentum is defined as

$$M = \oint \frac{W_m dz}{A} \quad , \quad (1)$$

and computed from the loop integral of the momentum balance:

$$\begin{aligned} \frac{dM}{dt} = & \Delta P_P - \sum_{k=1}^N (\Delta \Psi_m)_k - \oint g_z \rho_m dz - \sum_{k=1}^N (L \langle f_r \rangle)_k \\ & - \sum_{j=1}^{N+1} (\Delta P_D)_j + (\Psi_m)_{inj} \frac{A_{inj}}{A} \cos \theta \quad . \end{aligned} \quad (2)$$

In Eq.1, A and W_m stand for the flow cross-sectional area and mixture mass flow rate, respectively, while z denotes the coordinate axis along the direction of flow. In Eq.2, the first term on the right is the pressure rise across the pumps. The second term is the change of mixture momentum flux $\Psi_m = w_l G_l + w_v G_v$ in a loop component of constant cross-section; here w and G stand for velocity and mass flux, respectively, subscripts l and v denote liquid and vapor. The third term represents gravity, the fourth term mixture wall shear, the fifth term form losses, and the last term the momentum change due to injection.

It can be seen that there are no restrictions introduced by deriving Eq.2. The evaluation of Eq.2 implies, however, that phasic densities are computed with the local enthalpy and volume average pressure; the insignificant dependence on local pressure variation is ignored. Therefore, pressure wave propagation cannot be predicted; pressure signals are modeled to propagate instantly around the loop.

There are four advantages of integrating Eq.2 instead of the original partial differential equation: (i) As any closed contour integral of the pressure gradient is zero, Eq.2 has no pressure term; (ii) Equation 2 reduces a partial to an ordinary differential equation and quadratures over space, therefore, it reduces the computational effort of integrating the momentum balance; (iii) the numerical stiffness of Eq.2, dominated by loop length over flow cross-sectional area, is sharply reduced relative to that of the corresponding set of finite difference equations, high-frequency ringing is eliminated, larger integration time step sizes are permitted, and (iv) Eq.2 introduces no numerical dissipation from discretizing the momentum flux term.

Equation 2 is needed to model, with the help of the mixture mass balance and drift velocity correlations, the time-dependent phasic velocity variations throughout the two-phase flow system. Equation 2 produces a loop momentum M for every closed loop of a system, each M depending linearly on the volumetric mixture flow rate $(\beta_m)_0$ at a conveniently chosen loop location $z=0$. A set of n momenta yields therefore one volumetric mixture flow rate for each of n loops, and this flow rate $(\beta_m)_0$ serves as the needed integration constant for the spatial integration of the mixture mass balance, formulated as the mixture flux divergence equation.

This is easy to see, because in the drift-flux formulation, the mass flow rate W_m in Eq.1 depends on the volumetric flow rates β_m of mixture and vapor β_v , which are expressed in terms of the phasic density difference $\Delta\rho = \rho_l - \rho_v$, the vapor void fraction α , the distribution parameter C_0 and the void weighted, area averaged drift velocity $\langle v_{gj} \rangle$ as follows:

$$\begin{aligned} W_m &= \rho_l \beta_m - \Delta\rho \beta_v \\ &= (\rho_l - \alpha C_0 \Delta\rho) \beta_m - \alpha \Delta\rho \langle v_{gj} \rangle A \end{aligned} \quad (3)$$

and $\beta_m(z,t)$ is known from the mixture mass balance only up to the integration constant $\beta_m(0,t) = (\beta_m)_0$.

This leads to the analytical integration of the mixture mass balance, the second example for demonstrating the advantages of analytical over numerical methods in two-phase flow modeling. After defining the mixture and phasic fluxes $j_m = j_l + j_v = (1-\alpha)v_l + \alpha v_v$, the two-phase mixture mass balance is written as the mixture volumetric flux divergence equation

$$\nabla \cdot \vec{j}_m = \frac{\rho_l - \rho_v}{\rho_l \rho_v} \Gamma_v - \frac{\alpha}{\rho_v} \frac{D_v \rho_v}{Dt} - \frac{1-\alpha}{\rho_l} \frac{D_l \rho_l}{Dt} \quad (4)$$

where Γ_v is the vapor generation rate and D_k/Dt is the substantial derivative, computed with the k -phase velocity.

The substantial derivatives are evaluated with the thermal equations of state, in terms of pressure and energy derivatives, and the latter are eliminated with the phasic energy equations. The result is first integrated over the system volume to yield the rate of pressure change. For the vapor at saturation (at low vapor void fractions), one finds, with the Gauss divergence theorem, the time rate of pressure change

$$\frac{dp_{sys}}{dt} = \frac{\iiint (F_{\Gamma}\Gamma_v - F_q(1-\alpha) q_1''') dV - \sum_{outflow} \beta_m + \sum_{comp.} F_q \oint \vec{q}_w d\vec{A}}{\iiint F_p dV} \quad (5)$$

where

$$\begin{aligned} F_{\Gamma} &= \frac{\rho_l - \rho_v}{\rho_l \rho_v} + F_q (h_g - h_l) \\ F_p &= \frac{\alpha}{\rho_g} \frac{d\rho_g}{dp} + \frac{1-\alpha}{\rho_l} \left(\frac{\partial \rho_l}{\partial p} \right)_u \\ F_q &= \frac{1}{\rho_l^2} \left(\frac{\partial \rho_l}{\partial u_l} \right)_p \end{aligned} \quad (6)$$

The numerator of Eq.5 contains the dilation effects from phase change and gamma heating, from net-discharges and from wall heating, in that order, while the denominator contains the system compressibility.

The previous result is integrated a second time, now over any portion of the system volume, such that the enclosing surfaces are crossed only by known and one unknown volume flow rates $\beta_m = A j_m$, to give

$$\begin{aligned} \beta_m(z, t) &= (\beta_m)_0(t) - \frac{dp_{sys}}{dt} \iiint F_p dV + \iiint F_{\Gamma}\Gamma_v dV - \sum F_q q_w'' A_w \\ &\quad - \iiint F_q (1-\alpha) q_1''' dV \end{aligned} \quad (7)$$

Equation 7 constitutes the integral of the mixture mass balance and predicts the mixture volumetric flow rate at any location in the loop, in terms of the loop integration constants $(\beta_m)_0$, which are defined by the loop mixture momentum balances, and the mixture mass balances for suitable branch points. The branch points for PWR simulation are the connection of the hot legs with the upper plenum, and the core entrance; for BWR simulation, the branch point is the core entrance.

The advantages of Eq.7 over a finite difference equation are: (i) it reduces a partial to an ordinary differential equation and quadratures over space, therefore, it reduces the computational effort of integrating the mixture mass balance, and (ii) it introduces no numerical dissipation from discretizing the density and velocity gradients in the mass balance. An even greater advantage arises from Eq.7 due to the choice of volumetric, rather than mass flow rates, because the volumetric flow rate β_m is continuous under most circumstances across discontinuities of void fraction, such as a liquid or a mixture level.

The phasic volumetric flow rates are computed everywhere and for both flow directions from the above mixture volumetric flow rates and drift-flux correlations. To accommodate flow reversal at branch points, one needs to find the individual vapor flow rates. If the flows are taken positive in the trunk (subscript 1) toward the plane of the branch and in the branches (subscript k) away from the plane, then one gets from the vapor and mixture mass balances, for perfect lateral mixing in, and no phasic density change across, the plane of branching

$$\begin{aligned}(\beta_v)_1 &= 1/2 A_1 \left[(j_v)_1^+ + |(j_v)_1^+| + \alpha_i [(j_m)_1 - |(j_m)_1|] \right] \\(\beta_v)_k &= 1/2 A_k \left[\alpha_i [(j_m)_k + |(j_m)_k|] + (j_v)_k^+ - |(j_v)_k^+| \right],\end{aligned}\quad (8)$$

where the superscripted plus sign denotes flow rates evaluated with fluid properties extrapolated from the channel interior, in the direction of flow, to just before the plane of branching. The void fraction at the plane is

$$\alpha_i = \frac{(\beta_v)_i^{tot}}{(\beta_m)_i^{tot}}, \quad (9)$$

where the net incoming vapor and mixture volumetric flow rates arriving at the plane are

$$\begin{aligned}(\beta_v)_i^{tot} &= 1/2 \left[A_1 [(j_v)_1^+ + |(j_v)_1^+|] - \sum_{all\ branches} [A_k [(j_v)_k^+ - |(j_v)_k^+|]] \right] \\(\beta_m)_i^{tot} &= 1/2 \left[A_1 [(j_m)_1 + |(j_m)_1|] - \sum_{all\ branches} [A_k [(j_m)_k - |(j_m)_k|]] \right].\end{aligned}\quad (10)$$

Equations 7 through 10 demonstrate that the flux divergence equation is a powerful basis for simulating two-phase flow in multichannel, multiloop systems with flow reversals. It is also shown that analytical integration can reduce significantly the task of integrating partial differential equations of two-phase flow models. Analytical integration works equally well for heat transfer in structures and fuel [24, 25] and balance of plant components [4].

3.2 Selection of Numerical Methods

Computing efficiency is achieved when the best possible approximation to the solution of the modeling equations is found with the smallest possible number of arithmetical and logical operations, because that produces answers in the shortest possible time. The following three principles of selecting and implementing numerical methods were shown to improve computing efficiency.

3.2.1 Elimination of Iterations

The first numerical methods principle calls for the elimination of iterative procedures, by pretabulating the results of iterations in terms of state, or subsidiary variables, which are known when the results are needed in a computational cycle.

State variables form the minimum set of variables which define completely the state of the simulated system; they appear as the key time derivatives in the conservation equations and are always known at the beginning of a computational cycle, when a state equation oriented simulation computer language is used. Subsidiary variables depend on state variables through algebraic or transcendental equations.

Coupled, nonlinear systems of equations occur always. An example is the dependence of wall temperature T_{wall} on the convective heat transfer coefficient or Biot number N_{Bi} , which depends also on the wall temperature.

$$T_{wall} - T_{fluid} = \frac{(\langle T \rangle - T_{fluid})}{[1 + N_{Bi} (C_g + F_{pr})]} \quad (11)$$

The symbols T_{fluid} , $\langle T \rangle$, C_g and F_{pr} in Eq.11 denote, respectively, the coolant temperature, the volume-averaged structural temperature, a geometric constant and a property function [4, p.3-29]. The dependence of T_{wall} in Eq.11 is complicated, because branching is needed for flow regimes and because of complex correlations. The wall temperature can be found only by iteration.

Through the first numerical methods principle, one utilizes now available, inexpensive computer memory; one replaces during the simulation large numbers of time consuming arithmetical and logical operations by a linear table interpolation on a multidimensional hypersurface, and one obtains directly the needed result.

In the above example, one would tabulate the needed wall heat flux directly in terms of coolant and structural temperatures (which are given through energy balances), of flow rate and void fraction (given through momentum and vapor mass balances). There is no need during the simulation for computing Reynolds, Prandtl, Nusselt and Biot numbers, nor for branching into the appropriate heat transfer regime, nor for computing heat transfer coefficients, nor for continuing to repeat that computation until the boundary condition of surface heat flux continuity in Eq.11 is satisfied.

3.2.2 Use of Pretabulations

The second numerical methods principle calls for the pretabulation of complex expressions as multidimensional functions in terms of state, or subsidiary variables, which are known when the results are needed in a computational cycle.

While all parameters combining geometric constants are routinely precomputed as constant coefficients, possibly embedded in scaling groups, and while thermophysical properties had been pretabulated in the past, this numerical methods principle goes further. It serves to reduce, in principle, the computation of each element in the coefficient matrices A_{ij} , B_{ijk} and C_i ,

$$A_{ij} \frac{\partial y_j}{\partial t} = B_{ijk} \frac{\partial y_j}{\partial x_k} + C_i \quad (12)$$

of the governing conservation equations to a linear, multidimensional table interpolation. In praxis, however, the principle leads more likely to the pretabulation of complicated expressions, containing a combination of thermophysical properties and their derivatives [4, pp.3-100 and 3-105].

Pretabulation saves computing resources when (i) table interpolation takes less computing time than the needed arithmetical and logical operations and (ii) the needed number of table entries can be accommodated with the available memory capacity. Up to three function arguments present no memory problems in currently available minicomputers. The execution time of table interpolation for a function of a fixed number of arguments (table entries) is independent of the function complexity.

3.2.3 Integration Methods

The experience gained over the last decade has shown that there is a compelling advantage in employing well established and well documented algorithms for integrating the partial or ordinary (in time)

differential equations of two-phase flow. One should use algorithms for which capabilities, limitations, discretization errors and convergence criteria are documented and can be used to control the computational error.

3.2.3.1 Partial versus Ordinary Differential Equations

The governing conservation equations for two-phase flow are modeled in lumped or discrete parameter form, and formulated either as ordinary or partial differential equations, respectively. As ordinary differential equations they are differential equations with respect to time and can be integrated by standard methods. Partial differential equations can be discretized in space and integrated over time as ordinary differential equations, or they can be completely discretized and integrated by solving a system of implicitly coupled nonlinear equations.

The simultaneous solution of large systems of coupled nonlinear equations requires iterations, is therefore time consuming and not recommended for simulation, except for very slow system response and steady state simulations. A precise recommendation for addressing system response frequency from the computational point of view is given next.

3.2.3.2 Explicit versus Implicit Integration

The choice between implicit and explicit numerical integration has a profound effect on computing efficiency. One must select that integration method which achieves the larger speed ratio $S = \Delta t_{ist} / \Delta t_{frm}$, of permissible integration step size Δt_{ist} over frame time Δt_{frm} . Here, the integration time step is

$$\Delta t_{ist} = \text{Min}(\Delta t_{acc}, \Delta t_{stb}, \Delta t_{sys}) \quad (13)$$

where Δt_{acc} is the maximum time step permitted by discretization errors, Δt_{stb} is the maximum step size permitted by stability constraints, and Δt_{sys} is the characteristic time (fraction of period) of the relevant system response. Relevant system response time in two-phase flow is the period of thermohydraulic oscillation, not of driving neutron kinetics transients.

The frame time is the time it takes the computer to complete a computational cycle, that is to advance from one time level to the next, by Δt_{ist} . The permissible integration step size Δt_{ist} increases with decreasing system response frequency, as the discretization error is proportional to the leading time derivative; for explicit integration it increases only up to the stability limit. Since implicit integration is unconditionally stable, Δt_{stb} is infinite for implicit integration. However, the accuracy restricted Δt_{acc} is always larger for explicit than for implicit integration. It has been shown by Wulff [26], that for the same time and space discretization with donor-cell differencing, implicit integration has for all choices of time and space intervals always the greater numerical dissipation. Explicit integration methods for ordinary differential equations afford higher-order accuracy (by fourth-order Runge-Kutta method, for example) than first-order implicit solution schemes for the integration of space discretized partial differential equations of two-phase flow.

The frame time Δt_{frm} is independent of the system response time as it depends only on the number of programmed operations and the computer's execution speed. The frame time Δt_{frm} is always much smaller for the direct computations of explicit, than for the iterative computations of implicit integration, the more so the larger the number of governing equations is.

For most transients (Large and Small Break Loss of Coolant Accidents, for example), one finds that $\Delta t_{acc} \leq \Delta t_{stb}$, and that explicit is superior to implicit numerical integration. Only for near steady-state conditions can Δt_{acc} exceed Δt_{stb} well enough to compensate for its frame time disadvantage and render the implicit better than the explicit method [26].

3.3 Programming Principles

Programming principles advance and support the development of simulation capabilities and, even more their applications.

3.3.1 Quality Assurance

Quality Assurance (QA) procedures have been developed for the nuclear industry, to document and audit code preparations, completion, checking, the control of code modifications and applications [27]. Aside from criteria of compliance between mathematical model formulation and coding, and from criteria of input data validation, the quality standards are subjective. The following two supplementary coding principles have been found to expedite code development and simulation.

3.3.2 Simulation Languages

High-level simulation languages for computer programming have been recognized as superior to standard FORTRAN, when the application objective is simulation. Most simulation languages, such as EASY5 [14], ACSL [15] and ADSIM [16] compile on general-purpose computers through automatic translation into FORTRAN and are therefore transportable; ADSIM is at this time restricted to VAX computers and advanced workstations, but executes best on the special-purpose simulation computer AD-100 [16], which provides the integrated simulation environment described above in Chapter 2.

Simulation languages are specifically designed to minimize the task of translating mathematical models for physical systems into a computer program. They are state equation-oriented and have simulation-specific language constructs which facilitate code development, code validation, code documentation. A simulation program written in simulation language can be completely self-documenting and may be only half as long as the corresponding well written FORTRAN program. The vapor mass balance, for example, written in ADSIM, reads

$$Mv_j' = Wv_{j-1} - Wv_j + V_j * GAMMAv_j$$

and resembles the modeler's notes. Each term could stand for a vector. There is no need to program, test and document an algorithm for integrating the above differential equation, as the superscripted prime automatically invokes, either a default or a deliberately selected, built-in integration procedure.

Simulation languages have the modular structure to assemble model blocks, function blocks and program regions with systematically identified interfaces. Simulation languages provide the capability to vary automatically key parameters and generate an output envelope by recycling through a set of simulations.

Simulation languages provide interactive run-time access for resetting system and program controls without interrupting the simulation. For these reasons, the use of simulation languages takes fewer economic resources to develop simulation code and to simulate, than the use of standard scientific programming languages.

3.3.3 Self-Documenting Codes

Simulation code should be self-documenting, or cite by page and equation numbers directly the model and its numerical implementation in the code documentation. All input parameters should be prompted on the monitor screen with engineering descriptions, including units, and stored automatically in the same record for auditing, simulation and hard copy documentation. All output displays, graphical or tabular, should be self-explanatory.

The preparation of input data, and the interpretation of tabulated output data still require for most large systems codes extensive, time and resource consuming consultations of a user's manual. Small efforts for improving code commenting and input and output labelling could improve the efficiency of code use.

3.4 Simulation Computer Architecture

Simulation computers have simulation task-specific processors, working in parallel to provide run-time interactive access, to carry out operations of arithmetic and logic, multidimensional table interpolation, integration, etc. These processors have their own built-in instructions (firm ware) and they interact with minimum overhead, in lockstep and through broadcasting over a high-speed bus.

The most distinguishing feature of simulation computers is their separate and dedicated communications bus which, in conjunction with an input-output processor, affords high-speed digital and analog signal transmissions to and from peripheral devices. This hardware and the associated special input-output software, along with the software for run-time interactive access make the simulation computer superior to high-speed general-purpose computers, including workstations, because its input and output processing does not reduce the simulation speed. Moreover, a simulation computer provides for simulation with, and testing of, hardware in the loop.

4. SYNERGY OF SIMULATION ELEMENTS

Experience has shown that efforts to vectorize an existing code, or to add on post-processing for graphic displays, generate only modest improvements in efficiency. The most efficient simulation performance is achieved when model formulation, numerical methods, programming language and the computer are optimized as an integrated system. This means that one selects at first the simulation system and utilizes its advantages in the formulation of the mathematical model and in selecting the computing methods.

The integrated simulation facility of hardware and software must then operate until more advanced experimental results lead to advanced modeling methods and justify the acquisition of, and programming for, the next generation of simulation facility. It is more likely, however that the software of today's optimized integration facility will outperform current standard FORTRAN codes also on future computing platforms.

5. SUMMARY

It was demonstrated that engineering judgement in selecting and formulating models, in selecting established and documented numerical methods, and that working in a simulation environment, can significantly improve the quality of two-phase flow analyses, while reducing the time and cost that they require.

The paper explains the difference between computing and simulation and presents six principles of modeling and numerical methods, all of which were demonstrated to successfully reduce the computational effort. Three coding requirements are presented, and the important features of the simulation computer environment, primarily for intensive input and output processing. Lastly, it is shown why modeling and numerical methods need to be optimized with the computer architecture as a whole.

REFERENCES

- [1] W. Wulff, H.S. Cheng, A.N. Mallen and U.S. Rohatgi, BWR stability analysis with the BNL Engineering Plant Analyzer, USNRC Report, Brookhaven National Laboratory, NUREG/CR-5816 (November 1991).

- [2] W. Wulff, H.S. Cheng, and A.N. Mallen, Causes of instability at LaSalle and consequences from postulated scram failure, Proc. OECD International Workshop on Boiling Water Reactor Stability, Holtsville, NY, CSNI Report 178 (October 1990).
- [3] W. Wulff, H.S. Cheng, and A.N. Mallen, Effect of power oscillations on suppression pool heating during ATWS conditions, Proc. OECD International Workshop on Boiling Water Reactor Stability, Holtsville, NY, CSNI Report 178 (October 1990).
- [4] W. Wulff, H.S. Cheng, S.V. Lekach and A.N. Mallen, The BWR Plant Analyzer, USNRC Report, Brookhaven National Laboratory, NUREG/CR-3943 (August 1984).
- [5] G. Johnsen, S. Rouhani and R. Schumway, A parametric study of variables affecting BWR stability, Proc. OECD International Workshop on Boiling Water Reactor Stability, Holtsville, NY, CSNI Report 178 (October 1990).
- [6] J.H. McFadden et al, RETRAN-02, A program for transient thermal-hydraulic analysis of complex fluid flow systems, Electric Power Research Institute Report NP-1850 (1981) EPRI Palo Alto, CA.
- [7] M.P. Paulsen and E.D. Hughes, Nonequilibrium model for operational transient analysis, Nuclear Technology, Vol. 61, No. 2 (1983).
- [8] E.D. Hughes and K.R. Katsma, Numerical methods improvements for RETRAN, Nuclear Technology, Vol. 61, No. 2 (1983) 167.
- [9] V.H. Ransom et al, RELAP5/MOD2 code manual, USNRC Report NUREG/CR-4312, Idaho National Engineering Laboratory, EG&G Idaho, Inc., Idaho Falls, ID (1985).
- [10] R.A. Dimenna et al, RELAP5/MOD2 models and correlations, USNRC Report NUREG/CR-5194, Idaho National Engineering Laboratory, EG&G Idaho Inc., Idaho Falls, ID (1985).
- [11] J.A. Trapp and R.A. Riemeke, Completion of nearly implicit hydrodynamic numerical scheme for RELAP5/MOD2, Internal Technical Report SE-RSTD-85-006, Idaho National Engineering Laboratory, EG&G Idaho Inc., Idaho Falls, ID (1985).
- [12] TRAC-PF1: an advanced best-estimate computer code for pressurized water reactor analysis, USNRC Report NUREG/CR-3567, Los Alamos National Laboratory, Los Alamos, NM (1984).
- [13] D.R. Liles et al, TRAC-PF1 correlations and models, USNRC Report NUREG/CR-5096, Los Alamos National Laboratory, Los Alamos, NM (1988).
- [14] L. Mainstream, EKS EASY5 dynamic analysis system, Users guide, Boeing Computer Services Company, 1st Edition (March 1980).
- [15] Mitchell and Gauthier, Assoc. Inc., Advanced Continuous System Simulation Language (ACSL) - User Guide and Reference Manual, 3rd Ed. (1981).
- [16] Applied Dynamics International (ADI), ADSIM Reference Manual, Version 7.1, (May 1990); ADI, Ann Arbor, MI.
- [17] E.J. Fadden, L.H. Michaels and A. Haraldsdottir, The Applied Dynamics International SYSTEM 100: an integrated continuous system simulation environment, Proc. Microprocessor and Array Processor Conference, Tampa, FL (1989).

- [18] W. Wulff, Major systems codes, capabilities and limitations, Proc. Simulation Methods for Nuclear Power Systems, Tucson, AZ, US Nuclear Regulatory Commission and Electric Power Research Institute, EPRI WS-81 (May 1981).
- [19] M. Ishii, Thermo-fluid dynamic theory of two-phase flow, Collection de la Direction des Etudes et Recherches d'Electricité de France, Eyrolles, Paris (1975) p. 189.
- [20] M. Ishii, Two-fluid model for two-phase flow, in: Multiphase Science and Technology, Vol. V, ed. G.F. Hewitt, J.M. Delhaye and N. Zuber (Hemisphere Publishing Corporation, New York, Washington, Philadelphia, London, 1990) pp. 1-63.
- [21] N. Zuber and A.J. Findlay, Average volumetric concentrations in two-phase flow systems, Journal of Heat Transfer, 87 (1965) 453.
- [22] M. Ishii, One-dimensional drift-flux model and constitutive equations for relative motion between phases in various two-phase flow regimes, Argonne National Laboratory Report ANL-77-47 (October 1977).
- [23] J. A. Bouré, Wave phenomena and one-dimensional two-phase flow models, in: Multiphase Science and Technology, Parts 1, 2 and 3, Vol. VII, ed. G.F. Hewitt, J.M. Delhaye and N. Zuber (Hemisphere Publishing Corporation, New York, Washington, Philadelphia, London, 1991).
- [24] J.E. Meyer and R.P. Rose, Application of a momentum integral model to the study of parallel channel boiling flow oscillations, Trans. ASME, J. Heat Transfer 85 (1963) 1-9.
- [25] W. Wulff, Lumped parameter models for transient conduction in nuclear reactor components, USNRC Report NUREG/CR-1540, BNL-NUREG-35944, Brookhaven National Laboratory, Upton, NY 11973.
- [26] W. Wulff, H.S. Cheng and A.N. Mallen, Analytical modeling techniques for efficient heat transfer simulation in nuclear power plant transients, ANS Thermal Hydraulics Proc. 1985 National Heat Transfer Conference, Denver CO, (Aug. 1985), BNL-NUREG-35944, Brookhaven National Laboratory, Upton, NY 11973.
- [27] W. Wulff, Computational Methods for Multiphase Flow, in: Multiphase Science and Technology, Vol. V, ed. G.F. Hewitt, J.M. Delhaye and N. Zuber (Hemisphere Publishing Corporation, New York, Washington, Philadelphia, London, 1990) pp. 85-238 (see table 8.1 on p.155).
- [28] J.L. Bryant and N.P. Wilburn, Handbook of software quality assurance techniques applicable to the nuclear industry, Pacific Northwest Laboratory Report, NUREG/CR-4640 (August 1987).

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.

END

**DATE
FILMED**

10 / 30 / 92