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Computational Methods in Thermal Reactor Safety

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COMPUTATIONAL METHODS IN THERMAL REACTOR SAFETY

by

R. J. Pryor

ABSTRACT

A discussion of the WRAP system and the TRAC thermal reactor safety computer code is given. Emphasis is placed on numerical methods used to solve the one- and three-dimensional fluid flow equations in TRAC and the fuel rod conduction equations during reflood. An ATWS neutronics model is also discussed.

In just a few short years there has been a dramatic increase in the complexity and detail of thermal reactor safety calculations. Three-dimensional flow calculations with multifluid models are rapidly replacing one-dimensional, homogeneous equilibrium models for use in these calculations. New numerical methods and approximations for fluid flow abound in the literature. While a comprehensive review of methods for thermal reactor safety computation is beyond the scope of this paper, a summary of some important aspects of the subject will be given. By necessity, this paper is limited to two main subjects, a unique program to incorporate existing computer codes into a single unified system and the work being done on an advanced, best estimate, reactor safety analysis code called TRAC.^{1,2} Most of the discussion centers about calculations required for analysis of a large-break loss-of-coolant accident (LOCA).

LOCA calculations have absorbed the attention and imagination of safety analysts for most of the past 10 years. Although the probability of such an accident is exceedingly small, it must be demonstrated that should a LOCA occur the nuclear fuel can be cooled before the cladding melts and allows release of highly radioactive gases. Historically, the accident sequence is divided into three phases, starting with blowdown when the break occurs.

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During this phase, escape of reactor coolant through the break depressurizes the system. Almost immediately, the core dries out and fuel temperatures begin to rise. Later in the blowdown the emergency core coolant systems (BCCS) are activated and they force liquid to re-enter the system. The refill phase begins once the liquid penetrates the downcomer and it continues until the lower plenum is filled. The final phase, called reflood, begins when the liquid level reaches the bottom of the core. In this phase, the core is rewetted and the fuel temperature rise is halted.

From a modeling point of view, each phase is quite different and may be modeled separately. It is easy to see why the development of computer codes followed this modeling viewpoint and specialized on a part of, or a single phase of, the LOCA. The models required in each code could thus be minimized and the coding logic could be simplified. A number of such codes are widely used today. Pressurized water reactors (PWRs), for example, require computer codes such as RELAP, 3 FRAP, 4 and FLOOD 5 for a complete LOCA analysis. RELAT calculations are used to model the blowdown and part of the refill phases of the transient. FRAP calculations are used to model the fuelcladding dynamics, including thermal ex ansion and deformation. Finally, FLOOD calculations are used to predict the reflood stage of the transient. The various code calculations are linked together and iterated upon until a converged solution is obtained. During each iteration, results obtained using one code are passed to another as boundary conditions. The difficulty of performing LOCA calculations in this manner lies in the iteration process. Results from one code are determined by reading printed output, and input to the next code is prepared by punching computer cards. In the best of circumstances, such calculations are cumbersome, difficult to document, and almost impossible to reproduce.

At least one effort is being made to unify these calculations in a single computational package called WRAP.⁶ This is being done at the Savannah River Laboratory. In the WRAP system, the codes needed for LOCA analysis are linked together through a common data base called WIDS, as shown schematically in Fig. 1. A computational procedure is defined at input and is executed by a control program. The control program automatically interprets results, prepares input, and executes the required codes in a logical sequence. The essential parts of the WRAP system are computer codes commonly used for LOCA analyses, a file management system, and a generalized input processor. The

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Fig. 1. The PWR version of WRAP

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input processor allows a single system description to be defined, instead of requiring a separate input data deck for each code.

Development of the TRAC computer code at Los Alamos Scientific Laboratory is the first major effort to put all of the required LOCA models into a single, advanced, best estimate computer code. TRAC computes all phases of a LOCA continuously and consistently. TRAC is chosen as the subject of this discussion since the methods and approximations used in this code are typical of those in use today. The fluid dynamics methods are of greatest interest; the reflood model is discussed in less detail.

An area of considerable concern, besides hyperbolicity and wellposedness, is how many field equations are required to adequately treat the three phases of a LOCA. A rudimentary set would include three: a mixture continuity equation, a mixture energy equation, and a mixture momentum equation. Such a set is used in earlier versions of RELAP. Certain assumptions, such as homogeneous flow and equal temperatures of vapor and liquid, are made in writing these equations. Another set of approximations that uses the same number of equations is drift-flux flow with the least massive phase at the saturation temperature. Increasing the number of field equations provides more generality for the aphasic masses, temperatures, and velocities. In a six-equation set, separate continuity, energy, and momentum equations are written for the liquid and vapor phases. The price of more generality, however, is that additional constitutive laws are needed for closure. For example, in the six-equation set, interfacial exchange terms, such as areas, heat transfer coefficients, and drag forces (in all directions), must be specified, along with wall exchange terms for each phase.

In the TRAC code a three-dimensional flow model is used for the vessel and a one-dimensional flow model is used for all system components outside the vessel, such as pipes. A full six-equation model is used to describe flow in the vessel, and a five-equation drift-flux model is used for one-dimensional components. The five-equation model includes two energy equations, a mixture momentum equation, and two continuity equations. The drift between the phases in the one-dimensional model is prescribed by a standard set of correlations. A flow regime map is used for identifying the local flow regime and selecting the corresponding constitutive laws.

The choice of equations and mixture of one- and three-dimensional calculations was dictated by available computer resources and by the type of

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phenomena that occur during the LOCA. Clearly, homogeneous flow or onedimensional calculations could not predict ECCS downcomer bypass. Also, an equal temperature assumption is difficult to justify in describing ECCS injection of subcooled liquid into pipes containing superheated vapor. This is not to say that even a six-equation model is adequate, for some argue that entrained liquid drops should be treated separately from the liquid film on walls. The NORCOOL code⁷ and the latest version of COBRA-TF⁸ model a separate droplet field in addition to a film and vapor fields. Treating drops and films separately in full detail requires a nine-equation set. While this issue effects the number of equations which must be solved (and possibly the results of a LOCA calculation), it is not pertinent to the methods discussion which follows.

As an example of how the field equations are solved, consider computation of one-dimensional flow with the five-equation drift-flux model used in TRAC. These equations appear adequate for treating flow in pipes. These equations are as follows.

MIXTURE MASS:

$$\frac{\partial}{\partial t}(\rho_m) + \frac{\partial}{\partial z}(\rho_m v_m) = 0$$
.

VAPOR MASS:

$$\frac{\partial}{\partial t} (\alpha \rho_{v}) + \frac{\partial}{\partial z} (\alpha \rho_{v} v_{m}) + \frac{\partial}{\partial z} \left[\frac{\alpha \rho_{v} (1-\alpha) \rho_{l} v_{r}}{\rho_{m}} \right] = \Gamma$$

MIXTURE MOMENTUM:

$$\frac{\partial}{\partial t} (v_m) + v_m \frac{\partial}{\partial z} (v_m) + \frac{1}{\rho_m} \frac{\partial}{\partial z} \left[\frac{\alpha \rho_v (1-\alpha) \rho_v v_r^2}{\rho_m} \right]$$
$$= -\frac{1}{\rho_m} \frac{\partial \rho}{\partial z} - \frac{c_v}{h_d} v_m |v_m|.$$

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 $\begin{array}{rcl} & & & \\ & & \frac{\partial}{\partial t} & (\alpha \rho_{V} e_{V}) & + & \frac{\partial}{\partial z} & (\alpha \rho_{V} v_{m} e_{V}) & + & \frac{\partial}{\partial z} & \left[\frac{\alpha \rho_{V} (1-\alpha) \rho_{\ell} v_{r} e_{V}}{\rho_{m}} \right] \\ & & & + & p & \frac{\partial}{\partial z} & (\alpha v_{m}) & + & p & \frac{\partial}{\partial z} & \left[\frac{\alpha (1-\alpha) \rho_{\ell}}{\rho_{m}} v_{V} \right] \\ & & & = & q_{WV} & - & p & \frac{\partial \alpha}{\partial t} & + & \Gamma h_{sV} \end{array}$

MIXTURE ENERGY:

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$$\frac{\partial}{\partial t} (\rho_m e_m) + \frac{\partial}{\partial z} (\rho_m e_m v_m) + \frac{\partial}{\partial z} \left[\frac{(1-\alpha)\rho_{\ell} \alpha \rho_v (e_v - e_{\ell})}{\rho_m} v_r \right] \\ + p \frac{\partial v_m}{\partial z} + p \frac{\partial}{\partial z} \left[\frac{\alpha (1-\alpha) (\rho_{\ell} - \rho_v)}{\rho_m} v_r \right] = q_{wv} + q_{w\ell} .$$

The variables that appear in the above equations have the following meanings.

° m	mixture density
° v	vapor density
° _L	liquid density
α	vapor volume fraction
V _m	mixture velocity
Vr	relative velocity between phases
e _v	vapor specific internal energy
e ₂	liquid specific internal energy
em	mixture specific internal energy
Ē.	vapor production rate due to phase change
p	pressure
ġ	force of gravity
K	wall friction coefficient

	wall heat source of vapor									
aw 2	wall heat source of liquid									
Τ _l	liquid temperature									
Tv	vapor temperature									
h _{sv}	saturation enthalpy of vapor									

Common practice is to use a finite difference approximation to convert these partial differential equations into a set of linear algebraic equations that can be solved on a computer. Liles and Reed⁹ first developed the strategy for solving these equations in TRAC, and Mahaffy¹⁰ improved upon it later. This paper discusses the improved solution strategy which is called the Network Solution Method (NSM).

The matrix of unknowns that must be solved at each time step is large, especially if three-dimensional calculations are made. NSM is just one method of reducing this single large matrix into a few smaller ones that can be solved in less overall computer time. RELAP uses a similar method for the same purpose. Most analysts will develop a method in conjunction with, or based on, the structure of the matrix. The NSM method is based on a structure in which coupling between neighboring mesh cells (in the finite difference sense) can be limited to pressure variations. Such coupling is obtained by making a so-called semi-implicit approximation in time. This approximation is best illustrated by considering the time levels associated with the mixture continuity equation

 $\frac{\rho_m^{n+1} - \rho_m^n}{\partial t} + \frac{\partial}{\partial x} \left(\rho_m^n \ V_m^{n+1} \right) = 0 ,$

where the superscript n implies quantities evaluated at the last time step and thus known, and superscript n+1 denotes quantities evaluated at the current time step and thus unknown. Note the manner in which the convection term in this equation is formulated. Only the velocity is computed at the new time level. The convection terms in the vapor mass, vapor energy, and mixture energy equations are treated similarily. In the momentum equation, the V7V term is treated totally explicitly.

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Fig. 2. Positions of variables in mesh cell j of a finite difference mesh.

A finite difference approximation is now made on a staggered Eulerian mesh as shown in Fig. 2. State variables such as pressure, temperature, and void fraction are defined at the center of mesh cells, and the mean and relative velocities are defined at the cell boundaries. With these assumptions, the finite difference divergence operator is

$$\frac{\partial}{\partial z} (uv) = \left[A_{j+\frac{1}{2}}(uv)_{j+\frac{1}{2}} - A_{j-\frac{1}{2}}(uv)_{j-\frac{1}{2}} \right] / Vol_{j}$$

where u is any state variable, A is the cross-sectional area, and VOL_j is the volume of the jth cell. To provide stability in the partially implicit method, an up-wind or donor-cell average is used to evaluate properties convected across cell boundaries.

$$(uv)_{j+l_{2}} = \begin{cases} u_{j}v_{j+l_{2}} & \text{for } v > 0 \\ \\ u_{j-1}v_{j+l_{2}} & \text{for } v < 0 \end{cases}$$

where u_j is a cell-centered quantity. The finite difference equations are linearized about changes in the fundamental variables which are taken to be pressure, liquid and vapor temperatures, and void fraction. These

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manipulations yield a matrix equation for mesh cell(j) that has the following form.

$$\begin{bmatrix} & & \\ & \delta^{P} \\ & \delta^{T} \\ & \delta^{T} \\ & \delta^{T} \\ & \delta^{T} \\ & & \\ & \delta^{T} \\ & & \\ &$$

Because the velocity change is linear in the pressure change, the velocity at the new time level was eliminated from the finite difference equations. Note in this equation that there is no coupling of changes in temperatures or void fraction between cells. This matrix equation can be solved to produce a single linear equation that involves only pressure.

$$a_{j-1} \delta_{j-1} + a_{j} \delta_{j} + a_{j+1} \delta_{j+1} = b_{j},$$
 (2)

where a and b are constants.

Before proceeding, one must subdivide the entire flow network. In TRAC, the network that corresponds to the reactor system is divided so that system components retain their identity, as is shown in Fig. 3. Next the pressure reduction procedure is applied to each cell in a component (such as a pipe) in the manner just described, except at the component boundaries where the momentum equation is temporarily not written. The resulting system of equations appears as

$$\begin{bmatrix} & & & \\$$

where n is the number of mesh cells in the component and δv_R and δv_L are the boundary velocity changes on its right and left sides, respectively. Solving these equations directly by Gauss elimination for the pressure changes inside the pipe in terms of δV_R and δv_r gives

$$\delta P_{i} = c_{i} \delta V_{R} + d_{i} \delta V_{L} + e_{i}, \qquad (4)$$

where c, d, and e are constants.

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Fig. 3. TRAC noding schematic for PWR primary system.

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A momentum equation for the junction between components is next written as

$$\delta V_{i+i_2} = f(\delta P_{i-1}, \delta P_{i+1}) .$$
(5)

Combining Eqs. (4) and (5) leads to a system of equations for the velocity changes in the network.

where m indicates the number of junction velocities. This matrix equation is also solved by Gauss elimination to give the velocity changes, and then the results are back-substituted into Eq. (3) to give the system pressures. The pressures are then back-substituted to solve for void fraction and temperature changes in Eq. (1). Note that the matrix equations are solved directly so no iterations are involved. However, if the system properties change appreciably during this calculation, it might be necessary to linearize again about the latest values and repeat the above process as an outer iteration.

The net effect of the procedure is to reduce a large system of equations to a number of smaller ones that are solved more economically. This procedure is most effective when any given component has a small number of mesh cells, say less than 20. A three-dimensional vessel changes the situation slightly. Normally, a vessel may have hundreds of mesh cells, so a Gauss elimination procedure would be impractical. The pressure equations for the vessel must be solved iteratively. To obtain these equations, the velocities in the pipes are expressed in terms of pressure variations inside the vessel. The vessel calculation can then be done as though the vessel were isolated from the network, since its sources of mass, energy, and momentum from the external network are expressed in terms of internal pressure changes. Once the vessel solution has been found by iteration, the back-substitution is performed and the solution for the entire system, including the vessel, is known.

The stability of the semi-implicit scheme is subject to a material Courant condition of the form

 $\left| \frac{v \delta t}{\Delta x} \right| < 1$.

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A fully implicit scheme that is unconditionally stable is possible with NSM, but the junctions between components still must be treated semi-implicitly. However, the advantage is that if a pipe terminates on a break, the break junction also can be treated fully implicitly. One can use this option if velocities are great enough to limit the time step size severely.

The finite-difference scheme described above is used widely with a great deal of success. However, it does have limitations as regards numerical diffusion¹¹ and a phenomenon often called "water packing."¹² Also, since it is a first-order method in space (and time) it requires a large number of mesh cells to model large gradients adequately. This fact, of course, leads to long problem execution times.

Some new methods being developed for treating the spatial domain seem promising. A weighted residual method developed by Romstadt and Werner¹³ is particularly attractive. It uses polynomial functions defined over a finite space to express the fundamental variables. The polynomials are joined by requiring certain continuity conditions. Through a somewhat novel approximation, the resulting matrix equations have a standard three-point finite difference structure that is readily solved. The method seems to have minimal numerical diffusion properties and no water packing problems. Also, since it is a second-order method it converges to a solution in fewer spatial mesh points than the aforementioned finite difference method. A limitation of this weighted residual method is that it is fully implicit. Coupling to nearest neighbors is through changes in all variables, not just pressures. This is costly, as the additional coupling requires rore computing time. A semi-implicit formulation probably can be developed, but it has not been demonstrated.

One further aspect of LOCA which should be discussed, is the numerical treatment of reflood heat transfer. During reflood, quench fronts can originate at the bottom and top of the core. Those from the bottom are due primarily to the rising pool of water in the core. Those from the top are caused by a film of liquid from the upper plenum falling on the fuel rods. In either case, the axial temperature distribution of the fuel cladding changes pronouncedly at the quench front. Differences of hundreds of degrees within millimeters are not uncommon. Since one must resolve this temperature gradient to predict quench front velocities accorately, a fine vertical mesh in the cladding is required. This is especially costly if a constant fine

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mesh is defined along the entire length of the fuel rod. To avoid this cost, at least one code developer has used a moving mesh whose finest intervals are placed over the quench front. Such a procedure is used in the latest version of RELAP. The logic of moving the mesh is complicated, and treating more than one quench front on a fuel rod presents quite a bookkeeping job. Another approach, used in TRAC, is to superimpose an analytic solution for the quench front velocity on a coarse-mesh solution. Various authors have developed exact one-dimensional and approximate two-dimensional standing wave solutions to the conduction equation for this purpose.^{14,15,16}

Consider a simple case in which only axial conduction in the cladding is considered, the heat transfer coefficient ahead of the quench front is zero, and that behind the quench front is equal to a constant. The quench front location is defined by a rewetting temperature, T_0 . Temperature gradients in the direction normal to the cladding surface are assumed to be zero. The one-dimensional time-independent conduction equation for a quench front moving with a velocity u can be written as

$$\frac{d^2T}{dx^2} + \frac{\alpha cu}{k} \frac{dT}{dX} - \frac{h}{k\varepsilon} (T-T_s) = 0$$

where T is the cladding temperature; k, ρ , c are the conductivity, density, and specific heat of the cladding respectively; and ε is the cladding thickness. The heat transfer coefficient, h, varies as described. The quantity T_g is bulk fluid temperature (sink).

Requiring that the temperature gradient in the cladding be continuous at the point where the temperature is T_{o} provides an equation for the velocity u.

$$u^{-1} = \rho c \left(\frac{\epsilon}{hk}\right)^{\frac{1}{2}} \sqrt{\left(\frac{T_w - T_s}{\sigma}\right) \left(\frac{T_w - T_o}{\sigma}\right)}$$

where ${\rm T}_{\rm W}$ is the initial cladding temperature.

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If two-dimensional effects in the cladding are considered, this equation is modified slightly to obtain an approximate solution.

$$u^{-1} = \frac{\Pi \rho c}{2h} \left(\frac{T_w^{-T} s}{T_o^{-T} s} \right) \left(1 - \frac{4}{\Pi^2} - B_{i} \left(\frac{T_o^{-T} s}{T_w^{-T} s} \right) \right)^{\frac{1}{2}},$$

where Bi is the Biot number, hc/k, which is assumed to be greater than one.

TRAC uses a rather coarse axial mesh in the fuel rod radial conduction calculation.¹⁷ The quench front along the fuel rod is located by searching from the bottom (or the top in instances of falling films) of the core for a coarse mesh temperature that exceeds T_0 . In this mesh cell, a special heat transfer coefficient, \overline{h} , that ensures consistency between the quench front movement and heat removed from the cladding is computed.

$$\bar{h} = Q_{qf} / (\bar{T} - T_s)$$

where

 $Q_{qf} = \rho c u \beta \left(T_w - T_s \right)$

and \overline{T} is the average surface temperature of the cladding and β is the ratio of the cross-sectional area of the cladding to its wetted perimeter. On all other mesh cells, the heat transfer coefficients are computed from standard correlations. The net result of this approach is a direct coupling between quench front propagation and fuel rod stored energy effects. The quench front velocity is used in assessing the heat transfer rate only, not the quench front position.

Additional models are required for anticipated transients without scram (ATWS). ATWS analyses have received less attention than LOCA analyses for many years, but they are beginning to regain some of their earlier importance. Most of the models needed for LOCA analyses, with the possible exception of some reflood models, are used to analyze ATWS transients. An important addition, however, is a detailed neutronics treatment. Neutronics effects must be treated in much more detail in ATWS calculations than in LOCA calculations which require only a rudimentary treatment. ATWS transients demand at least a point reactor kinetics model that accounts for moderator and

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fuel temperature reactivity feedback effects. More sophisticated calculations attempt to account for detailed spatial effects by solving the one-, two-, or three-dimensional space-time neutron kinetics equations. Neutronics feedback is provided in these calculations by correlating the neutron cross sections as functions of important engineering parameters such as temperatures, void fraction, and boron concentration.

Three-dimensional calculations are needed for many of the ATWS transients, such as withdrawal of a single control assembly or dropping of a partial control rod. These calculations are expensive since the neutronics mesh points can number tens of thousands for each neutron energy group if standard finite-difference techniques are used. Fortunately, only two energy groups are needed for thermal reactors.

There have been attempts to reduce the number of neutronic mesh points by considering higher order spatial methods. The more successful have been nodal methods that attempt to express the neutron flux in polynomial representations over a limited region in the reactor core. Special coupling procedures are used to put the polynomials together to obtain a global reactor solution. The weighted-residual method for fluid dynamics originally was designed to treat the neutronics calculations.¹⁸ Another method that seems extremely powerful was developed by Henry and his students.¹⁹ They claim to need only 5000 mesh points per energy group for a full-scale, three-dimensional LWR calculation.

This paper presents a flavor of the methods in use today for solving rather complicated nuclear safety problems. By no means should it be assumed that the subject has been covered completely. In the fluid dynamics discussion, for example, nothing was said about other numerical methods and approximations, such as ICE.²⁰ If one could make only one observation about the trends in thermal reactor safety computation, it would be that the field is progressing rapidly. One-dimensional fluid flow calculations with homogeneous flow and thermal equilibrium models are becoming a thing of the past. Three-dimensional calculations of the vessel, along with separate field equations for each phase are becoming more commonplace and are required to resolve certain licensing issues. Also, for ATWS analyses, three-dimensional neutronics methods are needed for some transients calculations.

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