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# A Time-Dependent, Two-Phase, Thermal-Hydraulic Feedback Model for the Nodal Code QUANDRY

by

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## 1. Introduction

The WIGL thermal hydraulic feedback model [1] was originally incorporated in the nodal code QUANDRY to account for nonlinear cross section feedback effects in LWR's in which boiling of the coolant is neglected [2] and in which flow is assumed to be in the axial direction only. Recently, this feedback model was extended to the static boiling case and added to QUANDRY [3]. It was shown that boiling caused significant decreases in $k_{eff}$ and in the rate of convergence of the outer iteration in the neutronic solution. Aside from this slowed convergence, no numerical difficulties were encountered with static boiling problems.

Since it is also important to allow for thermal hydraulic feedback in transient BWR problems, the WIGL model has been further generalized to the transient boiling case. In this paper, a calculational procedure for solving the time-dependent, two-phase, thermal-hydraulic equations is presented. However, this model has not yet been included in QUANDRY, and thus numerical results illustrating the effects of the boiling feedback on the temporal variation of reactor flux and power distributions are not presently available.

## 2. Theory and Model Development

In the WIGL feedback model, the neutronic cross sections are assumed to be linear functions of three quantities: the fuel temperature $T^f$, the moderator (coolant) temperature $T^c$, and the moderator density $\rho^c$. These quantities can be computed as functions of position and time from the simultaneous solution of the energy balance equations for the fuel and moderator and the continuity equation for the coolant. These equations are solved numerically by first subdividing the reactor into a number of nodal regions (as is done in the neutronic solution), with node (i,j,k) defined by

$$x_i \leq x \leq x_{i+1}$$

$$y_j \leq y \leq y_{j+1}$$

$$z_k \leq z \leq z_{k+1}$$

and where i=1, ..., NX; j=1, ..., NY; and k=1, ..., NZ. Similarly, the time variable is discretized using a number of discrete times $t_n$, n=1, ..., NT. The equations are then averaged over each nodal region and integrated over the various time steps $\Delta t_n (\equiv t_{n+1} - t_n)$. The resulting discretized equations can then be solved for the average fuel temperature $\bar{T}^{f,n}_{ijk}$, the average moderator temperature $\bar{T}^{c,n}_{ijk}$, and the average moderator density $\bar{\rho}^{c,n}_{ijk}$ for all nodes (i,j,k) and all times $t_n$. Feedback to the neutronic equations is then obtained by assuming the cross sections to be linear functions of these node-averaged properties. Mathematically, this linear dependence may be expressed as

$$\Sigma_\alpha = \Sigma_{\alpha,0} + \sum_{m=1}^{3} \frac{\partial \Sigma_\alpha}{\partial \bar{X}_m} (\bar{X}_m - X_{m,0}) \tag{1}$$

where $\Sigma_\alpha = \Sigma_t$, $\Sigma_{21}$, or $\Sigma_f$

$$\bar{X}_m = \begin{cases} \bar{T}^f & \text{for } m=1 \\ \bar{T}^c & \text{for } m=2 \\ \bar{\rho}^c & \text{for } m=3 \end{cases}$$

and where the subscripts 0 denote reference quantities.

## 2.1 Calculation of the Average Moderator Temperature

For flow assumed to be only in the axial direction z, the time-dependent energy equation for the coolant may be written as

$$\frac{\partial}{\partial t}(\rho^c H) + \frac{\partial}{\partial z}(GH) = Q \tag{2}$$

where H is the coolant specific enthalpy, G is the coolant mass flux (i.e., the product of its density and velocity), and Q is the volumetric rate of energy addition to the coolant. This equation may be averaged over each node (i,j,k) to obtain

$$\frac{d}{dt}\,\overline{\rho^c H}_{ijk} + \frac{\overline{GH}_{ij}(z_{k+1}) - \overline{GH}_{ij}(z_k)}{\Delta z_k} = \overline{Q}_{ijk} \tag{3}$$

where

$$\overline{\rho^c H}_{ijk} \equiv \frac{1}{\Delta x_i\, \Delta y_j\, \Delta z_k} \int_{x_i}^{x_{i+1}} dx \int_{y_j}^{y_{j+1}} dy \int_{z_k}^{z_{k+1}} dz\, \rho^c H$$

$$\overline{GH}_{ij}(z) \equiv \frac{1}{\Delta x_i\, \Delta y_j} \int_{x_i}^{x_{i+1}} dx \int_{y_j}^{y_{j+1}} dy\;\; GH$$

and where $\Delta x_i \equiv x_{i+1} - x_i$, $\Delta y_j \equiv y_{j+1} - y_j$, and $\Delta z_k = z_{k+1} - z_k$. Upon neglecting a number of small contributions to $\overline{Q}_{ijk}$ (e.g., viscous dissipation, diffusive heat transfer, gravitational work, etc.), this quantity may be expressed as

$$\bar{Q}_{ijk} = \eta q'''_{ijk} \frac{V^f_{ijk}}{V^c_{ijk}} + (R_1 + R_2)^{-1} (\bar{T}^f_{ijk} - \bar{T}^c_{ijk}) \tag{4}$$

where $R_1 \equiv (A_h U)^{-1}$

$$R_2 \equiv \left[ A_h h_o (\bar{G}_{ijk} / G_o)^{0.8} \right]^{-1}$$

$$\bar{G}_{ijk} = \frac{1}{2} \left[ \bar{G}_{ij}(z_{k+1}) + \bar{G}_{ij}(z_k) \right] \tag{5}$$

$$\bar{G}_{ij}(z) = \frac{1}{\Delta x_i \, \Delta y_j} \int_{x_i}^{x_{i+1}} dx \int_{y_j}^{y_{j+1}} dy \; G$$

and where the remaining notation is the same as that of Smith [2].

To evaluate the coolant enthalpy (which determines the coolant temperature at a given pressure), it is necessary to consider additionally the continuity equation for the coolant:

$$\frac{\partial \rho^c}{\partial t} + \frac{\partial G}{\partial z} = 0 \tag{6}$$

Averaging this equation over the node (i,j,k) yields

$$\frac{d}{dt} \bar{\rho}^c_{ijk} + \frac{\bar{G}_{ij}(z_{k+1}) - \bar{G}_{ij}(z_k)}{\Delta z_k} = 0 \tag{7}$$

where $$\bar{\rho}^c_{ijk} = \frac{1}{\Delta x_i \, \Delta y_j \, \Delta z_k} \int_{x_i}^{x_{i+1}} dx \int_{y_j}^{y_{j+1}} dy \int_{z_k}^{z_{k+1}} dz \; \rho^c \; .$$

With $\bar{H}_{ij}(z)$ defined as $\overline{GH}_{ij}(z)/\bar{G}_{ij}(z)$, Eq. (7) may be multiplied by

$\frac{1}{2}[\bar{H}_{ij}(z_{kH}) + \bar{H}_{ij}(z_k)]$ and subtracted from Eq. (3) to obtain

$$\frac{d}{dt}\overline{\rho^c H}_{ijk} - \frac{1}{2}\left[\bar{H}_{ij}(z_{k+1}) + \bar{H}_{ij}(z_k)\right]\frac{d}{dt}\bar{\rho}^c_{ijk}$$

$$+ \frac{[\bar{G}_{ij}(z_{k+1}) + \bar{G}_{ij}(z_k)][\bar{H}_{ij}(z_{k+1}) - \bar{H}_{ij}(z_k)]}{2\Delta z_k} = \bar{Q}_{ijk} \,. \qquad (8)$$

The first two terms are commonly approximated by

$$\frac{d}{dt}\overline{\rho^c H}_{ijk} - \frac{1}{2}\left[\bar{H}_{ij}(z_{k+1}) + \bar{H}_{ij}(z_k)\right]\frac{d}{dt}\bar{\rho}^c_{ijk} \approx \bar{\rho}^c_{ijk}\frac{d}{dt}\bar{H}_{ij}(z_{k+1}) \,.$$

Substitution of this expression into Eq. (8) and use of Eq. (5) yields

$$\bar{\rho}^c_{ijk}\frac{d}{dt}\bar{H}_{ij}(z_{kH}) + \bar{G}_{ijk}\frac{[\bar{H}_{ij}(z_{k+1}) - \bar{H}_{ij}(z_k)]}{\Delta z_k} = \bar{Q}_{ijk} \,. \qquad (9)$$

Approximation of the time derivative by a forward difference and solution for the coolant enthalpy at the advanced time $t_{n+1}$ gives

$$\bar{H}_{ij}^{n+1}(z_{k+1}) = \bar{H}_{ij}^{n}(z_{k+1}) + \frac{\Delta t_n}{\bar{\rho}_{ijk}^{c,n}}\left[\bar{Q}_{ijk}^{n} - \bar{G}_{ijk}^{n}\frac{\bar{H}_{ij}^{n}(z_{k+1}) - \bar{H}_{ij}^{n}(z_k)}{\Delta z_k}\right] . \tag{10}$$

Equation (10) may be used to compute the enthalpy at any point $z_k$ (k>1) for successive values of $t_n$. Clearly, however, the values of $\bar{Q}_{ijk}$, $\bar{\rho}_{ijk}^{c}$, $\bar{G}_{ijk}$, and $\bar{H}_{ij}$ must be known for the previous time step (and are fixed at the beginning of the transient calculation by initial conditions). In addition, for k=1, $\bar{H}_{ij}^{n}(z_k)$ must be specified for all $t_n$ by a boundary condition giving the time-dependent inlet coolant enthalpy.

If the coolant enthalpy is assumed to vary linarly with axial position z in each node, the node-averaged enthalpy $\bar{H}_{ijk}$ is simply given by

$$\bar{H}_{ijk}^{n+1} = \frac{1}{2}\left[\bar{H}_{ij}^{n+1}(z_{k+1}) + \bar{H}_{ij}^{n+1}(z_k)\right] . \tag{11}$$

The average coolant temperature may then be evaluated from

$$\bar{\bar{T}}_{ijk}^{c,n+1} = T_{sat} - (H_f - \bar{H}_{ijk}^{n+1})/C^c \qquad (\text{when } \bar{H}_{ijk}^{n+1} < H_f) \tag{12a}$$

or

$$\bar{\bar{T}}_{ijk}^{c,n+1} = T_{sat} \qquad (\text{when } \bar{H}_{ijk}^{n+1} \geq H_f) \tag{12b}$$

where $T_{sat}$ is the saturation temperature, $H_f$ is the enthalpy of the saturated liquid, and $C^c$ is the coolant heat capacity at constant pressure.

### 2.2 Calculation of the Average Moderator Density

At any time $t_n$, the moderator density $\rho^c$ is assumed to decrease linearly with enthalpy H for $H < H_{sat}$, whereas its specific volume $1/\rho^c$ is assumed to increase linearly with H for $H > H_{sat}$. Thus the densities at the various axial positions $z_k$ at time $t_{n+1}$ are given by

$$\bar{\rho}_{ij}^{c,n+1}(z_{k+1}) = \bar{\rho}_{ij}^{c,n+1}(z_k) + \frac{\rho_f - \bar{\rho}_{ij}^{c,n+1}(z_k)}{H_f - \bar{H}_{ij}^{n+1}(z_k)} \left[ \bar{H}_{ij}^{n+1}(z_{k+1}) - \bar{H}_{ij}^{n+1}(z_k) \right] \quad (13a)$$

[use for $\bar{H}_{ij}^{n+1}(z_{k+1}) \leq H_f$]

or $$\bar{\rho}_{ij}^{c,n+1}(z_{k+1}) = \left\{ \frac{1}{\rho_f} + \frac{1/\rho_g - 1/\rho_f}{H_g - H_f} \left[ \bar{H}_{ij}^{n+1}(z_{k+1}) - H_f \right] \right\}^{-1} \quad (13b)$$

[use for $H_f < \bar{H}_{ij}^{n+1}(z_{k+1}) \leq H_g$]

where $H_g$ is the enthalpy of the saturated vapor, and $\rho_f$ and $\rho_g$ are the densities of the saturated liquid and saturated vapor. It should be noted that equation (13b) is not applicable when $\bar{H}_{ij}^{n+1}(z_{k+1}) > H_g$ and therefore does not account for possible superheating of the coolant.

In the WIGL model, the average coolant density in each node must be calculated, and thus $\bar{\rho}^{c}_{ij}(z)$ must be averaged over z within the nodes. Again, the assumption of a linear variation of the enthalpy with z in a given node is made, and the node-averaged density $\bar{\rho}^{c,n+1}_{ijk}$ becomes

$$\bar{\rho}^{c,n+1}_{ijk} = \int_{\bar{H}^{n+1}_{ij}(z_k)}^{\bar{H}^{n+1}_{ij}(z_{k+1})} \bar{\rho}^{c}_{ij}(H)\, dH$$

When expressing $\bar{\rho}^{c}_{ij}$ as a function of H in this equation, three physically distinct cases must be considered: (1) Both $\bar{H}_{ij}(z_{k+1})$ and $\bar{H}_{ij}(z_k) \leq H_f$ (i.e., the coolant in the entire node is subcooled), (2) both $\bar{H}_{ij}(z_{k+1})$ and $\bar{H}_{ij}(z_k) \leq H_f$ (i.e., boiling occurs throughout the node), and (3) the saturation enthalpy $H_f$ falls between $\bar{H}_{ij}(z_{k+1})$ and $\bar{H}_{ij}(z_k)$. Expressions for $\bar{\rho}^{c}_{ijk}$ for all of these cases are derived in reference 3 for the static case and are trivially generalized to the transient case below.

<u>Case (1)</u>

$$\bar{\rho}^{c,n+1}_{ijk} = \frac{1}{2}\left[\bar{\rho}^{c,n+1}_{ij}(z_{k+1}) + \bar{\rho}^{c,n+1}_{ij}(z_k)\right] \tag{14}$$

<u>Case (2)</u>

$$\bar{\rho}^{c,n+1}_{ijk} = \frac{\ln\left[\bar{\rho}^{c,n+1}_{ij}(z_k)/\bar{\rho}^{c,n+1}_{ij}(z_{k+1})\right]}{\left[\bar{\rho}^{c,n+1}_{ij}(z_{k+1})\right]^{-1} - \left[\bar{\rho}^{c,n+1}_{ij}(z_k)\right]^{-1}} \tag{15}$$

Case (3)

$$\left.\begin{aligned}
\bar{\rho}_{ijk}^{c,n+1} &= \frac{\alpha_1}{2}\left[\bar{\rho}_{ijk}^{c,n+1}(z_k) + \rho_f\right] \\
&\quad + (1-\alpha_1)\,\frac{\ln\left[\rho_f / \bar{\rho}_{ij}^{c,n+1}(z_{k+1})\right]}{\left[\bar{\rho}_{ij}^{c,n+1}(z_{k+1})\right]^{-1} - \dfrac{1}{\rho_f}} \\
\alpha_1 &\equiv \frac{H_f - \bar{H}_{ij}^{n+1}(z_k)}{\bar{H}_{ij}^{n+1}(z_{k+1}) - \bar{H}_{ij}^{n+1}(z_k)}
\end{aligned}\right\} \quad \bar{H}_{ij}^{n+1}(z_k) \le H_f \le \bar{H}_{ij}^{n+1}(z_{k+1}) \tag{16a}$$

or

$$\left.\begin{aligned}
\bar{\rho}_{ijk}^{c,n+1} &= \frac{\alpha_2}{2}\left[\bar{\rho}_{ij}^{c,n+1}(z_{k+1}) + \rho_f\right] \\
&\quad + (1-\alpha_2)\,\frac{\ln\left[\rho_f / \bar{\rho}_{ij}^{c,n+1}(z_k)\right]}{\left[\bar{\rho}_{ij}^{c,n+1}(z_k)\right]^{-1} - \dfrac{1}{\rho_f}} \\
\alpha_2 &\equiv \frac{H_f - \bar{H}_{ij}^{n+1}(z_{k+1})}{\bar{H}_{ij}^{n+1}(z_k) - \bar{H}_{ij}^{n+1}(z_{k+1})} \; .
\end{aligned}\right\} \quad \bar{H}_{ij}^{n+1}(z_{k+1}) \le H_f \le \bar{H}_{ij}^{n+1}(z_k) \tag{16b}$$

It should be noted that in case 3, two different expressions are used to compute $\bar{\rho}_{ijk}$, depending on the magnitudes of $\bar{H}_{ij}(z_{k+1})$ and $\bar{H}_{ij}(z_k)$ relative to $H_f$.

From Eqs. (13) - (16), it is seen that a knowledge of the enthalpy distribution at the advanced time step and the saturation properties of the coolant allows calculation of the corresponding average coolant density distribution.

## 2.3 Calculation of the Average Coolant Mass Flux

Solution of the coolant energy equation, Eq. (9), requires re-evaluation of the node-averaged coolant mass flux $\overline{G}_{ijk}$ at each time step. For the first time step (i.e. n=1), $\overline{G}^{1}_{ijk}$ is known if the inlet mass flux is specified, since the initial mass flux distribution must be independent of axial position in the reactor (provided the transient is initiated from steady-state operation). For subsequent time steps (n>1), $\overline{G}_{ijk}$ is calculated by solving the coolant continuity equation. Upon replacing the time derivative in the node-averaged continuity equation [Eq. (7)] by a backward difference, Eq. (7) becomes

$$\frac{\overline{\rho}^{c,n+1}_{ijk} - \overline{\rho}^{c,n}_{ijk}}{\Delta t_n} + \frac{\overline{G}^{n+1}_{ij}(z_{k+1}) - \overline{G}^{n+1}_{ij}(z_k)}{\Delta z_k} = 0 . \qquad (17)$$

Solving for $\overline{G}^{n+1}_{ij}(z_{k+1})$ yields

$$\overline{G}^{n+1}_{ij}(z_{k+1}) = \overline{G}^{n+1}_{ij}(z_k) - \frac{\Delta z_k}{\Delta t_n}\left(\overline{\rho}^{c,n+1}_{ijk} - \overline{\rho}^{c,n}_{ijk}\right) . \qquad (18)$$

This relation may be used to compute the coolant mass flux at successive values of $z_k$ for all $t_n$, provided the inlet mass flux $\overline{G}^{n}_{ij}(z_1)$ is specified. The node-averaged mass flux is then calculated from [cf Eq. (5)]

$$\bar{G}^{n+1}_{ijk} = \frac{1}{2}\left[\bar{G}^{n+1}_{ij}(z_{k+1}) + \bar{G}^{n+1}_{ij}(z_k)\right] . \qquad (19)$$

2.4 Calculation of the Average Fuel Temperature

The time-dependent energy balance on the fuel in node (i,j,k) may be written [2]

$$\rho^f C^f \frac{d\bar{T}^f_{ijk}}{dt} = (1-n)\,q'''_{ijk} - \frac{V^c_{ijk}}{V^f_{ijk}}\,\frac{\bar{T}^f_{ijk}-\hat{T}}{R} \qquad (20)$$

where $R = R_1+R_2$ and $\hat{T} = \bar{T}^c_{ijk}$ if $(R_1+R_2)^{-1}(\bar{T}^f_{ijk}-\bar{T}^c_{ijk}) > R_1^{-1}(\bar{T}^f_{ijk}-T_{sat})$

$R = R_1$ and $\hat{T} = T_{sat}$, otherwise

Replacing the time derivative by a backward difference and solving for the node-averaged fuel temperature at the advanced time step yields

$$\bar{T}^{f,n+1}_{ijk} = \left(\frac{\rho^f C^f}{\Delta t_n} + \frac{V^c_{ijk}}{RV^f_{ijk}}\right)^{-1}\left[\frac{\rho^f C^f}{\Delta t_n}\bar{T}^{f,n}_{ijk} + \frac{V^c_{ijk}}{V^f_{ijk}}\frac{\hat{T}^{n+1}}{R} + (1-n)\,q'''^{\,n+1}_{ijk}\right] . \qquad (21)$$

From this equation, it is seen that calculation of the fuel temperature requires values for the coolant temperature (or the saturation temperature) at the same time step and the fuel temperature at the previous time step.

3. Summary of Solution Procedure

The overall solution procedure for the transient WIGL boiling model may be summarized in the following steps:

1. Given the initial enthalpy distribution of the coolant in the reactor, the corresponding initial coolant density distribution $\bar{\rho}^{c,1}_{ijk}$ can be calculated using Eqs. (13) - (16). The initial coolant mass flux distribution $\bar{G}^{1}_{ijk}$ is constant and equal to the specified inlet value. If the initial fuel temperature profile is given, then the initial volumetric rate of energy addition to the coolant $\bar{Q}^{1}_{ijk}$ [cf. Eq. (4)] is also known (since the initial coolant temperature is fixed by its enthalpy, and $q^{''',1}$ is supplied by the neutronic solution).

2. With these initial values of $\bar{H}^{n}_{ij}(z_k)$, $\bar{\rho}^{n}_{ijk}$, $\bar{G}^{n}_{ijk}$, and $\bar{Q}^{n}_{ijk}$, the advanced time enthalpy $\bar{H}^{n+1}_{ij}(z_k)$ is computed for all $z_k$ (k>1) using Eq. (10). For k=1, the enthalpy must be specified as a boundary condition for all times $t_n$. Equation (11) is then used to calculate the average coolant enthalpy $\bar{H}^{n+1}_{ijk}$ in each node at the advanced time step. From these average enthalpies, the average coolant temperature distribution $\bar{T}^{c}_{ijk}$ can be evaluated using Eq. (12).

3. The average coolant density distribution at the advanced time step $\bar{\rho}^{c,n+1}_{ijk}$ is determined using Eqs. (13) - (16).

4. The quantity $\bar{G}^{n+1}_{ijk}$ is updated with the aid of Eqs. (18) and (19). The inlet coolant mass flux $\bar{G}_{ij}(z_1)$ must be specified as a boundary condition for all $t_n$.

5. The average fuel temperature at the advanced time step $\bar{T}^{f,n+1}_{ijk}$ is evaluated directly from Eq. (21)

6. The advanced-time values of $\bar{T}^{f}_{ijk}$, $\bar{T}^{c}_{ijk}$, and $\bar{\rho}^{c}_{ijk}$ are used to update the neutronic cross sections using Eq. (1).

7. Steps 2-6 are repeated for successive time steps for the duration of the transient calculation (i.e., for n=1, ..., NT).

## 4. Limitations of the Model

The basic limitations of the thermal-hydraulic model developed in this paper are a consequence of the simplifying assumptions made in its derivation. For example, by neglecting the coolant momentum equation, we have effectively assumed that pressure is uniform, and that body forces and shear stress are negligible. These same assumptions simplify greatly the term Q in the coolant energy balance, since the work and viscous dissipation terms vanish. Furthermore, the use of a homogeneous, one-dimensional model for the two-phase coolant flow does not allow for possible cross-flow and slip between the two phases. It is also apparent from the development of the equations that pressure is taken to be independent of time (or is at most a slowly varying function of time, so that the term $\frac{dp}{dt}$ can be omitted from the coolant energy equation). Therefore, a rapid de-pressurization problem cannot be treated adequately using the present transient boiling model. For a pressure slowly varying with time, the saturation properties of the coolant (i.e., $T_{sat}$, $\rho_g$, $\rho_f$, $H_g$, and $H_f$) also vary with time and must be re-evaluated at each time step in the numerical solution. Finally, small errors are expected as a result of assuming the fuel and coolant properties (e.g., heat capacity and thermal conductivity) to be independent of temperature, and by assuming the density (or specific volume) of the coolant to be a linear function of enthalpy.

In addition to these inherent limitations of the model, two additional factors must be considered when actually performing the required numerical calculations. First, it is recalled that the time derivative in the coolant energy balance [Eq. (9)] was approximated by a forward time difference. The resulting explicit scheme for computing the advanced-time enthalpy is prone to numerical instability for large time steps, and therefore problems characterized by rapid transients (in which the enthalpy varies sharply with time) require the use of small time increments, which increases the total computational effort. Secondly, the assumption of a linear variation of enthalpy with axial position in each node is likely to introduce some error for very coarse spatial grids. Accordingly, the spatial nodes must be made sufficiently small in the axial direction to insure convergence of the solution with respect to spatial discretization. However, experience with static boiling problems indicates that accurate solutions of the static thermal-hydraulic equations could be obtained using roughly the same spatial grid needed to insure convergence of the neutronic solution. Therefore, it is expected that, at any fixed time during a transient calculation, an acceptable accuracy can be achieved with a relatively coarse axial mesh.

In conclusion, to the extent that the momentum equations can be neglected, that the two phases of the coolant can be treated homogeneously, and that time variations of the thermal-hydraulic parameters are slow, the transient boiling model presented in this paper is expected to be quite valid. In particular, if the coolant flow is purely in the axial direction, and if superheating of the coolant does not occur, the model provides an accurate and inexpensive means of simulating the strong cross section feedback associated with boiling of the coolant under transient conditions in LWR's.