Chapter 4
NUMERICAL SOLUTION

4.1. Explicit and Implicit Schemes

Exact solutions of differential equations introduced in Chapter 2 present many difficulties. Thus, we will use approximate integration methods that are easily generalized for the space discrete equations [7]. The differential equations can be written in matrix notation as:

$$\frac{d}{dt}[x] = [R][x] \tag{4.1.1}$$

where $[x]$ - the eigenvector whose elements $\{x_i\}$, may be power, precursor concentrations, mass, flow, enthalpy, pressure, etc., and

$[R]$ - the matrix whose elements $\{\alpha_{ij}\}$ are the eigenvalues of $[x]$.

In general, equation (4.1.1) is nonlinear, since $[R]$ varies in a complicated fashion as a function of time. We will suppose that the operator $[R]$ is constant during a given transient from time t to t+Δt.

The time derivative in (4.1.1) is replaced by:

$$\frac{d}{dt}[x] \cong \frac{1}{\Delta t}([x^{t+\Delta t}] - [x^t]).$$

Explicit Scheme:

In the *explicit* method, the right hand side of (4.1.1) is replaced by $[R][x^t]$. In this case, (4.1.1) becomes:

$$[x^{t+\Delta t}] = ([I] + [R]\Delta t)[x^t] \tag{4.1.2}$$

where $[I]$ is the unit matrix.

Formally, the exact solution of differential equation (4.1.1) is an exponential of the matrix $[R]$ as

$$[x^{t+\Delta t}] = \exp([R]\Delta t)[x^t].$$

The truncation error is the difference between an approximate solution and the exact solution. Consequently, the truncation error ET of the explicit method is given by:

$$ET = \{[I] + [R]\Delta t - \exp([R]\Delta t)\}[x^t]$$

Expanding the matrix exponential gives

$$ET = ([I] + [R]\Delta t - [I] - [R]\Delta t - \frac{1}{2}[R]^2\Delta t^2 - ...)[x^t] \quad \approx -\frac{1}{2}[R]^2\Delta t^2[x^t].$$

Therefore, the truncation error of the explicit method is of order $\frac{1}{2}\Delta t^2$.

The row i of (4.1.2) in the actual form is:

$$x_i^{t+\Delta t} = (1+\alpha_{ii}\Delta t)x_i^t + \sum_{\ell \neq i}^{N} (1+\alpha_{i\ell}\Delta t)x_\ell^t \qquad (4.1.3)$$

It can be noted that, for negative eigenvalues, at some value of Δt the factor $(1+\alpha_{ii}\Delta t)$ can go negative, causing each subsequent evaluation of $x_i^{t+\Delta t}$ to oscillate in sign and go unstable. Therefore, the choice of Δt must be restricted to give a stable solution. Otherwise, spurious oscillations of quickly increasing amplitudes will overtake the solution.

The explicit scheme is simple and easy to implement.

Implicit Scheme:

In the *implicit* method, the right hand side of (4.1.1) is replaced by $[R][x^{t+\Delta t}]$. After regrouping the terms in $[x^{t+\Delta t}]$, we have

$$[x^{t+\Delta t}] = \{[I] - [R]\Delta t\}^{-1}[x^t] \qquad (4.1.4)$$

The truncation error is obtained from the difference between the approximat solution and the exact solution:

$$ET = \{([I] - [R]\Delta t)^{-1} - \exp([R]\Delta t)\}[x^t]$$

$$\approx \{([I] + [R]\Delta t +[R]^2\Delta t^2 + ...) - ([I] + [R]\Delta t +\frac{1}{2}[R]^2\Delta t^2 + ...)\}[x^t]$$

$$= \frac{1}{2}[R]^2\Delta t^2 [x^t].$$

Thus, the truncation error of the implicit method is of order $\frac{1}{2}\Delta t^2$, the same as that of the explicit method.

Similarly, the row i of (4.1.4) can be written in the following form:

$$x_i^{t+\Delta t} = \frac{x_i^t + \Delta t\sum_{\ell \neq i}\alpha_{i\ell}x_\ell^{t+\Delta t}}{1-\alpha_{ii}\Delta t} \qquad (4.1.5)$$

The eigenvalues can often be large and negative. Consequently, the contributions due to large negative eigenvalues, $\dfrac{1}{1-\alpha_{ii}\Delta t}$, decay away as $\Delta t \to \infty$. Thus, the implicit scheme tends to behave very well at large time steps. Positive eigenvalues pose a threat to the

implicit form. However, this is not a practical problem because the products of an eigenvalue by Δt is kept much less than 1, $\alpha_{ii}\Delta t \ll 1$, for accuracy reasons [5].

The implicit method requires the matrix inversion in order to have the solution at the next time step. This matrix can change at each time interval, so the matrix inversion will have to be performed at each time interval. It requires more calculation effort and time than the explicit method.

Although the explicit method is very easy to implement, the need to have a very small time step will result in the total computation time required for a transient to be much more than for the implicit scheme. It is therefore preferable to apply the implicit scheme. However, for large size matrices, it is quite costly to perform the addition and multiplication of matrices as well as to do a matrix inversion. To avoid this, we prefer to use an iteration technique for solving the system of algebraic equations into which (4.1.5) can be transformed. The system of algebraic equations can be written in matrix notation as:

$$[A][x] = [b] \tag{4.1.6}$$

Jacobi method:

The matrix [A] is split in the following way:

$$[A] = [L] + [D] + [U]$$

where [D]   diagonal matrix, containing only diagonal elements of [A],

[L]   lower triangular matrix, containing those elements of [A] that are bellow the diagonal of [A],

[U]   upper triangular matrix, containing those elements of [A] that are above the diagonal of [A].

The Jacobi method is obtained by sending to the right hand side all the terms that are not on the diagonal:

$$[D][x]^{(k+1)} = -([L] + [U])[x]^{(k)} + [b], \tag{4.1.7}$$

consequently,

$$[x]^{(k+1)} = -[D]^{-1}([L] + [U])[x]^{(k)} + [D]^{-1}[b] \tag{4.1.8}$$

where the index k is denoted to the k-th iteration.

Substituting $[M] = -[D]^{-1}([L] + [U])$ and $[g] = [D]^{-1}[b]$, we get

$$[x]^{(k+1)} = [M][x]^{(k)} + [g] \tag{4.1.9}$$

The vector $[x]^{(k+1)}$ does not replace the vector $[x]^{(k)}$ until the end of iteration k. The matrix $[M]$ is said to be convergent if

$$\lim_{k \to \infty} [M]^k = 0 \text{ , here k is an exponent.}$$

If $[M]$ is convergent, at some iteration K we will find that

$$[x]^{(K+1)} \approx [x]^{(K)} \text{ and } [x] = [x]^{(K+1)}.$$

Jacobi's method is rarely used in practice because of two reasons. First, the two vectors $[x]^{(k)}$ and $[x]^{(k+1)}$ are kept in memory at the same time. Other, it has a poor rate of convergence as compared to other methods.

Gauss-Seidel Method:

Gauss-Seidel method resembles the Jacobi method. However, it uses in the calculation sequence the new elements of $[x]^{(k+1)}$ as soon as they are available. Only one vector has to be kept in memory, and it contains both old and new elements.

In terms of the decomposition of the matrix $[A]$ we have

$$[D][x]^{(k+1)} = -[L][x]^{(k+1)} - [U][x]^{(k)} + [b], \qquad (4.1.10)$$

consequently,

$$[x]^{k+1} = -[D]^{-1}[L][x]^{(k+1)} - [D]^{-1}[U][x]^{(k)} + [D]^{-1}[b] \qquad (4.1.11)$$

Gauss-Seidel has a better rate of convergence than the Jacobi method. It can be proved that if the matrix $[A]$ is diagonally dominant, i.e. each diagonal element is larger in modulus than the sum of the moduli of other elements in its row, then Gauss-Seidel method will converge [8].

4.2. Point Kinetics

If the explicit scheme is applied to the point kinetics equations, the stability condition is rather restrictive: time steps must be smaller than $2\frac{\Lambda}{\beta}$ [7]. Thus, for the DNRR,

$$\Delta t < 2\frac{\Lambda}{\beta} \approx 2 \times 5.10^{-5}/0.0081 = 12 \text{ msec.}$$

In the implicit scheme, from (2.1.5) we have

$$\frac{1}{\Delta t}[\zeta_i^{t+\Delta t} - \zeta_i^t] = -\lambda_i \zeta_i^{t+\Delta t} + \frac{\beta_i}{\Lambda}p^{t+\Delta t}$$

$$\therefore \quad \zeta_i^{t+\Delta t} = \frac{\zeta_i^t + \frac{\beta_i}{\Lambda}\Delta t p^{t+\Delta t}}{1+\lambda_i \Delta t}. \qquad (4.2.1)$$

Assuming that the source term is known or constant, we can rewrite equation (2.1.4) as

$$\frac{1}{\Delta t}[p^{t+\Delta t} - p^t] = \frac{\rho-\beta}{\Lambda}p^{t+\Delta t} + \sum_{i=1}^{N}\lambda_i \zeta_i^{t+\Delta t} + s.$$

Substituting $\zeta_i^{t+\Delta t}$ from (4.2.1), we get

$$\frac{1}{\Delta t}[p^{t+\Delta t} - p^t] = \frac{\rho-\beta}{\Lambda}p^{t+\Delta t} + \sum_{i=1}^{N}\frac{\lambda_i}{1+\lambda_i \Delta t}\zeta_i^t + \sum_{i=1}^{N}\frac{\lambda_i \Delta t}{1+\lambda_i \Delta t}\frac{\beta_i}{\Lambda}p^{t+\Delta t} + s.$$

Regrouping the terms of $p^{t+\Delta t}$ and noting that $\beta = \sum_{i=1}^{N}\beta_i$, we obtain

$$p^{t+\Delta t} = \frac{p^t + \sum_{i=1}^{N}\frac{\lambda_i \Delta t}{1+\lambda_i \Delta t}\zeta_i^t + s\Delta t}{1+\frac{\Delta t}{\Lambda}\left(\sum_{i=1}^{N}\frac{\beta_i}{1+\lambda_i \Delta t}-\rho\right)} \qquad (4.2.2)$$

The power level at the next time step is calculated by (4.2.2) and then substituted into (4.2.1) to have the precursor concentrations of next time step.

For $\rho < \beta$ as in most practical cases, the implicit method gives stable solution with any Δt. However, if $\rho \geq \beta$, as it is the prompt critical case, the power level changes drastically. Therefore, the time step must be of order $\frac{\Lambda}{\beta}$ to avoid spurious oscillations of the power level as well as to have an accurate solution.

The initial steady-state conditions for a critical reactor are:

$$\rho(0) = 0,$$

$$\zeta_i(0) = p_0 \frac{\beta_i}{\lambda_i}, \qquad\qquad (4.2.3)$$

$$s(0) = 0,$$

and a for subcritical reactor:

$$\rho(0) = \rho_0 < 0,$$

$$\zeta_i(0) = p_0 \frac{\beta_i}{\lambda_i}, \qquad\qquad (4.2.4)$$

$$s(0) = -\rho_0 p_0.$$

It should be noted that the solution of the point kinetics is obtained implicitly in power and precursor concentrations, but explicitly in dynamic reactivity. If we treated the reactivity implicitly, it would be very complicated, because the reactivity feedback must be calculated from the known power level.

4.3. Dynamic Reactivity

Although the dynamic reactivity is calculated from the power level obtained from the point kinetics at the current time step, it will only be used in the next time step.

Control Reactivity:

The reactivity inserted by all control elements is calculated by (2.1.10). However, in order to have fast transients, we can introduce any desired reactivity change with time. This is quite useful when initial conditions for the critical reactor are considered, as the initial net reactivity is zero, $\rho(0) = 0$, so the net reactivity is:

$$\rho(t) = \rho_{intr}(t) + \rho_{Xe}(t) + \rho_{temp}(t) + \rho_{void}(t) \tag{4.3.1}$$

where $\rho_{intr}(t)$ is introduced reactivity with time, and

$$\rho_{intr}(0) = -[\rho_{Xe}(0) + \rho_{temp}(0) + \rho_{void}(0)].$$

Thus, $\rho_{intr}(t)$ is given as an input with time to represent any external insertion of positive or negative reactivity into the system.

Xenon Poisoning:

As the neutron power is calculated from the point kinetics, the xenon feedback for the next time step is easy to compute. The implicit scheme applied to the I-135 and Xe-135 build-up equations gives

$$N_I^{t+\Delta t} = \frac{N_I^t + \gamma_I p^t \Delta t}{1 + \lambda_I \Delta t}, \tag{4.3.2}$$

and

$$N_{Xe}^{t+\Delta t} = \frac{N_{Xe}^t + [\gamma_{Xe} p^t + \lambda_I N_I^{t+\Delta t}]\Delta t}{1 + (\lambda_{Xe} + \sigma_{Xe}\Phi)\Delta t}, \tag{4.3.3}$$

where $\Phi = p(t)\Phi^{FP}$.

The equilibrium xenon concentration at full power can be found as

$$N_{Xe}^{FP} = \frac{\gamma_I + \gamma_{Xe}}{\lambda_{Xe} + \sigma_{Xe}\Phi^{FP}} \tag{4.3.4}$$

Knowing the equilibrium xenon poisoning at full power, ρ_{Xe}^{FP}, we can find the xenon reactivity feedback

$$\rho_{Xe}^{t+\Delta t} = \rho_{Xe}^{FP} \frac{N_{Xe}^{t+\Delta t}}{N_{Xe}^{FP}} \tag{4.3.5}$$

The initial steady-state conditions are:

$$p(0) = p_0,$$

$$N_I(0) = \frac{\gamma_I}{\lambda_I} p_0,$$

$$N_{Xe}(0) = \frac{\gamma_I + \gamma_{Xe}}{\lambda_{Xe} + \sigma_{Xe} p_0 \Phi^{FP}} p_0. \tag{4.3.6}$$

Temperature Reactivity:

Temperature reactivity feedback is due to changes in fuel temperature and coolant/moderator, i.e. water, temperature as in (2.1.13). Thus,

$$\rho_{temp} = \overline{\alpha}_f (T_f - T_0) + \overline{\alpha}_w (T_w - T_0) \tag{4.3.7}$$

where the average temperature reactivity coefficients are determined as

$$\overline{\alpha}_f = \frac{1}{T_f - T_0} \int_{T_0}^{T_f} \alpha_f \, dT_f \qquad \text{for fuel, and}$$

$$\overline{\alpha}_w = \frac{1}{T_w - T_0} \int_{T_0}^{T_w} \alpha_w \, dT_w \qquad \text{for coolant/moderator.}$$

The average fuel and water temperatures of the core are:

$$T_f = \frac{\sum_{i=0}^{N_{core}} T_{fi}}{N_{core}} \tag{4.3.8}$$

$$T_w = \frac{\sum_{i=0}^{N_{core}} T_i}{N_{core}} \tag{4.3.9}$$

where T_{fi} average core node fuel temperature,

T_i average core node coolant temperature, and

N_{core} number of average core nodes.

The reference temperature T_0 is usually taken as the initial core temperature at zero power level.

For nuclear reactors with natural convection cooling like the DNRR, it is extremely difficult to determine directly fuel and coolant coefficients, since fuel and coolant temperatures are not independent parameters. Thus, it is nearly impossible to keep one parameter constant while changing the other. In practice, at constant reactor power (p = constant) and inlet core coolant temperature (T_1 = constant), all thermal-hydraulic

parameters in the core are relatively stable after extended operations at a constant power level, and remain stable as long as both p and T_1 are unchanged. Therefore, temperature reactivity change can be expressed in term of those two independent parameters as

$$d\rho_{temp} = \left(\frac{\partial\rho}{\partial T_1}\right)_p dT_1 + \left(\frac{\partial\rho}{\partial p}\right)_{T_1} dp \qquad (4.3.10)$$

or, in more practically integral form, as

$$\rho_{temp} = \overline{\alpha}_{T_1}(T_1 - T_0) + \overline{\alpha}_p p \qquad (4.3.11)$$

where the average reactivity coefficients are determined as

$$\overline{\alpha}_{T_1} = \frac{1}{T_1 - T_0}\int_{T_0}^{T_1}\left(\frac{\partial\rho}{\partial T_1}\right)_p dT_1 \quad \text{for inlet coolant temperature, and}$$

$$\overline{\alpha}_p = \int_0^p\left(\frac{\partial\rho}{\partial p}\right)dp \qquad \text{for power.}$$

As T_1 and p are very easily measured, the most reliable control parameters of the reactor, ρ_{temp} is preferably determined by (4.3.10). Thus, at a constant power level, changing inlet coolant temperature and recording control rod positions, we can find $\rho_{temp} = \rho_T$ at p = const, so

$$\overline{\alpha}_{T_1} = \frac{\rho_T}{T_1 - T_0}, \text{ \$/°C.}$$

Changing the reactor power level, measuring inlet coolant temperature and recording control rod positions, we can find the power coefficient as:

$$\overline{\alpha}_p = \frac{\rho_{temp} - \overline{\alpha}_{T_1}(T_1 - T_0)}{p}, \text{ \$/\%FP.}$$

However, $\overline{\alpha}_{T_1}$ and $\overline{\alpha}_p$ are determined at steady-state conditions, when fuel and coolant temperatures are well stabilized at a given power p and inlet coolant temperature T_1. During transients they could not be used since both coolant and fuel temperatures are still evolving to their stabilized values.

At steady-state conditions, coolant and fuel temperatures can be expressed through power and inlet coolant temperature:

$$T_w = \frac{T_1 + T_2}{2} = T_1 + \frac{T_2 - T_1}{2} = T_1 + \frac{Q_0 p}{2c_p W_c}, \qquad \text{and}$$

$$T_f = T_w + \frac{Q_0 p}{Sh} = T_1 + \frac{Q_0 p}{2c_p W_c} + \frac{Q_0 p}{Sh}$$

where T_2 average core outlet temperature, [°C]

          Q_0 thermal power at p=100% (full power), [W]

          W_c .core mass flow, [kg/s]

          c_p coolant specific heat, [J/kg.K]

          S   core heating surface area, [m²]

          h   heat transfer coefficient, [W/m².K].

Substituting T_w and T_f into (4.3.7), and after regrouping in terms of T_1 and p, we have

$$\rho_{temp} = (\overline{\alpha}_f + \overline{\alpha}_w)(T_1 - T_0) + \left(\frac{\overline{\alpha}_f + \overline{\alpha}_w}{2c_p W_c} + \frac{\overline{\alpha}_f}{Sh}\right)Q_0 p \qquad (4.3.12)$$

Comparing (4.3.12) with (4.3.11), we can have

$$\overline{\alpha}_f + \overline{\alpha}_w = \overline{\alpha}_{T_1} \qquad \text{and} \qquad (4.3.13)$$

$$\left(\frac{\overline{\alpha}_f + \overline{\alpha}_w}{2c_p W_c} + \frac{\overline{\alpha}_f}{Sh}\right)Q_0 = \overline{\alpha}_p \qquad (4.3.14)$$

Solving (4.3.13) and (4.3.14) for $\overline{\alpha}_f$ and $\overline{\alpha}_w$, we finally have

$$\overline{\alpha}_f = \left(\overline{\alpha}_p p - \frac{Q_0 p}{2c_p W_c}\overline{\alpha}_{T_1}\right)\frac{Sh}{Q_0 p}, \quad \text{or more conveniently:}$$

$$\overline{\alpha}_f = \left(\overline{\alpha}_p p - \overline{\alpha}_{T_1}\frac{T_2 - T_1}{2}\right)\frac{1}{T_f - T_w} \qquad (4.3.15)$$

and $\overline{\alpha}_w = \overline{\alpha}_{T_1} - \overline{\alpha}_f,$ or

$$\overline{\alpha}_w = \left(1 - \frac{T_2 - T_1}{2(T_f - T_w)}\right)\overline{\alpha}_{T_1} - \frac{p}{T_f - T_w}\overline{\alpha}_p \qquad (4.3.16)$$

The above provides a method to measure fuel and coolant temperatures for an average channel and to estimate their average values T_f and T_w. First, the fuel assembly in the cell that we consider average, i.e. its radial power factor is $k_r \cong 1$, is removed. Then, an instrumented fuel assembly with thermocouples is inserted into this cell. The core inlet and outlet coolant temperatures (T_1 and T_2) are measured by two thermocouples located on entrance and exit non-fueled parts. The average water temperature T_w is taken as (T_1 + T_2)/2. The fuel temperatures are measured by several thermocouples buried in the fuel cladding along the length of the fuel. To calculate the average fuel temperature T_f, these measured temperature values are fitted by a curve and then averaged.

The secondary loop is switched off during the experiment. The water temperature in the tank is initially low (about ambient temperature). Reactor power is increased in 10%FP steps from 10% to 100%, with the power held constant for a few minutes after each change. At each power level, when the core thermal-hydraulic parameters stabilize, the control rods' position and the core inlet temperature T_1 are recorded, and then the power is moved to the next level. As the heat generated by fission is not discharged, the water temperature in the tank is gradually increasing. When the power level reaches 100%, it is reduced back to 10% and the above process of power increases and taking of measurements is repeated, but with a higher T_1. The experiment is terminated when T_1 has reached the operational limit (about 32^0C for the DNRR). The experimental data are the control rods' position at predetermined power levels with different T_1 and are used to calculate $\overline{\alpha}_{T_1}$ and $\overline{\alpha}_p$ as described above. Simultaneously with recording control rods' position, p and T_1, the core outlet temperature (T_2) as well as fuel temperatures are recorded in order to estimate the core coolant and fuel temperatures (T_w and T_f). Then, the water and fuel temperature coefficients are calculated by (4.3.14) and (4.3.15).

For the DNRR, the temperature coefficients were determined experimentally and are given in Appendix B.

4.4. Heat Generation and Heat Transfer

Heat Generation:

The fission heat deposited in the fuel is given by equation (2.2.23). For a fuel element with known k_r, we subdivide it into an arbitrary number of axial sections and rewrite (2.2.23) for each section, assuming the average heat rate over the section with the section centre at z and length of Δz:

$$q_v(z, t) = q_{v0} \, \alpha \, p(t) \, k_r \, k_z \qquad (4.4.1)$$

where $q_{v0} = \dfrac{FP}{n_{fb} V_{fb}}$, $[W/m^3]$,

n_{fb} = number of fuel assemblies, and

V_{fb} = volume of fuel contained in one fuel assembly,

k_z is ratio of heat generated in the section to total heat generated in fuel:

$$k_z = \frac{\displaystyle\int_{z-\Delta z/2}^{z+\Delta z/2} \varphi(z)dz}{\displaystyle\int_{0}^{Hf} \varphi(z)dz} \qquad (4.4.2)$$

where H_f is the active fuel height.

In addition to this direct fission heat, there is also the heat generated by decay of fission products which are assumed to be distributed proportionally to the neutron flux. Thus,

$$q_v(z, t) = q_{v0} \, [\alpha \, p(t) + p_{fp}(t)] \, k_r \, k_z \qquad (4.4.3)$$

The fission power $p(t)$ is obtained from the point kinetics. The decay power $p_{fp}(t)$, however, is found by solving the build-up equations of fission products (2.2.25). Here, the implicit scheme is applied to get:

$$\varpi_i^{t+\Delta t} = \frac{\varpi_i^t + \gamma_i p^t \Delta t}{1 + \lambda_i \Delta t}, \qquad (4.4.4)$$

$$p_{fp}(t) = \sum_{i=1}^{N} \lambda_i \varpi_i(t)$$

The initial conditions for fresh core are

$$\varpi_i(0) = 0$$

and for equilibrium in fission product inventory at constant power p_0 are

$$\varpi_i(0) = \frac{\gamma_i}{\lambda_i} p_0. \qquad (4.4.5)$$

For U-235 fuel, the residual heat due to decay of fission products after the reactor has been shut down can be calculated by [6]:

$$\frac{p_s(t)}{p_0} = \left[\frac{0.1}{(t_s + 10)^{0.2}} - \frac{0.087}{(t_s + 2.10^7)^{0.2}}\right] - \left[\frac{0.1}{(t_s + t_0 + 10)^{0.2}} - \frac{0.087}{(t_s + t_0 + 2.10^7)^{0.2}}\right]$$

(4.4.6)

where t   time after shutdown, s

      t_0 time of operation at power p_0 before shutdown, s.

We will use (4.4.6) to estimate the fission yields and decay constants of the pseudo-fission product groups as follows. At the moment of shutdown after a long time of operation at power p_0, with $t_0 \to \infty$ in (4.4.6), we have

$$p_{fp}(t_0) = \sum_{i=1}^{N} \gamma_i\, p_0 = p_s(0) = p_0 f(t=0, t_0 \to \infty)$$

$$\therefore \quad \sum_{i=1}^{N} \gamma_i = f(t=0, t_0 \to \infty) = 0.0608$$

where $f(t, t_0)$ is the right hand side in (4.4.6). It means that the decay heat could add up to 6% more to the fission heat. After the shutdown, there is no more production term in the build-up equations and each pseudo-fission product group will decay by exponential law. Therefore,

$$p_{fp}(t) = \sum_{i=1}^{N} \gamma_i \varpi_i(t) = \sum_{i=1}^{N} \gamma_i\, p_0 \exp(-\lambda_i t) = p_0\, f(t)$$

$$\therefore \quad \sum_{i=1}^{N} \gamma_i e^{-\lambda_i t} = f(t)$$

(4.4.7)

It is an expansion of the function $f(t)$ in the exponential series. The values of constants γ_i and λ_i are given in Appendix B.

Heat Transfer:

One-dimensional heat conduction in the radial direction of a fuel element is considered. For general heat conduction in each axial fuel section Δz, we discretize the spatial temperature T by choosing *N* radial discrete points, so that there must be a point at any interface surface between fuel and cladding as well as between cladding and fluid.
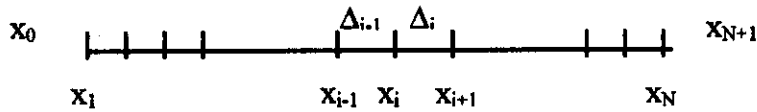
By denoting $T_i^t = T(x_i, t)$, and $\Delta_i = (x_{i+1} - x_i)$ as shown, the conduction equation can be written [9, 10]:

$$\frac{C_i}{\Delta t}(T_i^{t+\Delta t} - T_i^t) = Q_i + \frac{1}{R_{i-1}}(T_{i-1}^{t+s\Delta t} - T_i^{t+s\Delta t}) + \frac{1}{R_i}(T_{i+1}^{t+s\Delta t} - T_i^{t+s\Delta t}). \quad (4.4.8)$$

In (4.4.8), C_i is the heat capacity, [J/K], of the volume around the point i:

$$C_i = \frac{1}{2}([c\rho V]_{i-1} + [c\rho V]_i) \quad (4.4.9)$$

where c   specific heat, [J/kg.K],

ρ density, [kg/m^3],

V   volume, [m^3].

Also, Q_i is the amount of heat deposited around the point i, [W],

$$Q_i = \frac{1}{2}([q_v V]_{i-1} + [q_v V]_i) \quad (4.4.10)$$

where q_v is obtained from (4.4.3).

R_i is the heat resistance over all the heat transfer area, [K/W]. For solids,

$$R_i = \frac{\Delta_i}{k_i \overline{S_i}} \quad (4.4.11)$$

where $\overline{S_i}$ average heat transfer area, [m^2], between points i and $i+1$

k_i heat conductance, [W/m.K].

Generally, c, ρ and k are temperature dependent. Also, c and ρ are taken at temperature T_i, while k is taken at an average temperature $(T_i + T_{i+1})/2$.

We can use (4.4.8) for the edge points with the boundary conditions of Newton's law of cooling by changing the heat resistance of the interface as

$$R_N = \frac{1}{hS} \quad \text{and} \quad \Delta_N = 0$$

where S   heat transfer surface, [m^2],

h   heat transfer coefficient, [W/m^{2}K].

To the above system of N points we now add two more points, the fluid temperatures T_0 and T_{N+1}.

Similarly, the symmetric condition $q = \left(\dfrac{\partial T}{\partial x}\right)_0 = 0$ can also be considered, simply set

$$\frac{1}{R_0} = 0$$

in (4.4.8).

For the explicit scheme, s = 0, and, for the implicit scheme, s = 1. If the explicit scheme is applied, (4.4.8) can be rewritten:

$$T_i^{t+\Delta t} = \left[1 - \left(\frac{1}{R_{i-1}} + \frac{1}{R_i}\right)\frac{\Delta t}{C_i}\right]T_i^t + \left(\frac{T_{i-1}^t}{R_{i-1}} + \frac{T_{i+1}^t}{R_i} + Q_i\right)\frac{\Delta t}{C_i} \qquad (4.4.12)$$

The stability condition for the explicit method is

$$1 - \left(\frac{1}{R_{i-1}} + \frac{1}{R_i}\right)\frac{\Delta t}{C_i} \geq 0.$$

Assuming a constant heat transfer area, material properties and interval length Δ, this condition takes the form

$$\Delta t \leq \frac{1}{2}\frac{c\rho}{k}\Delta^2.$$

For U-Al alloy, $c\rho \approx 2.10^6$ J/m^3, $k \approx 158$ W/mK [11], even if we only take the minimum two points of the whole fuel thickness $\Delta = 0.7\times10^{-3}$ m, then

$$\Delta t \leq \frac{1}{2}2.10^6(0.7\times10^{-3})^2/158 \approx 3 \text{ msec.}$$

For the implicit scheme, i.e. s = 1, after regrouping in terms of $T_i^{t+\Delta t}$ we can obtain

$$T_i^{t+\Delta t} = \frac{T_i^t + \left(\dfrac{T_{i-1}^{t+\Delta t}}{R_{i-1}} + \dfrac{T_{i+1}^{t+\Delta t}}{R_i} + Q_i\right)\dfrac{\Delta t}{C_i}}{1 + \left(\dfrac{1}{R_{i-1}} + \dfrac{1}{R_i}\right)\dfrac{\Delta t}{C_i}} \qquad (4.4.13)$$

The Gauss-Seidel method can be used to solve (4.4.13). The temperatures of the previous time step T_i^t are the best values to be guessed for the first iteration $[T_i^{t+\Delta t}]^{(1)} = [T_i^t]$. For each subsequent iteration, the most recent values of $[T_i^{t+\Delta t}]^{(k)}$ are used to recalculate C_i and R_i and other $[T_i^{t+\Delta t}]^{(k)}$. Instead of verifying the convergence of temperatures, we verify the convergence of the heat flux from surface to fluid flow $q = h(T_c - T_w)$, because the heat flux is more important and will be used in the hydrodynamic calculations.

The above described method for calculating heat conduction can be avoided in some cases by using the lumped method. If we consider the fuel and the cladding as a hot

object with a constant temperature T immersed in the fluid flow with temperature T_w, then we can write the heat balance for fuel as:

$$C \frac{dT}{dt} = - hS(T-T_w) + Q \qquad (4.4.14)$$

Heat capacity, C, [J/K], and heat generated, Q, are

$$C = [c\rho V]_f + [c\rho V]_c$$

$$Q = q_v V_f \qquad (4.4.15)$$

with notation f referring to 'fuel' and c to 'cladding'.

Applying the implicit scheme, we find

$$T^{t+\Delta t} = \frac{T^t + (hST_w + Q)\dfrac{\Delta t}{C}}{1 + hS\dfrac{\Delta t}{C}} \qquad (4.4.16).$$

The lumped method can be used with little error, if the criterion for its use is appropriate, i.e. when Biot number, Bi, is less than 0.1 [10].

$$Bi = \frac{hV}{kS} < 0.1$$

It is recommended that the lumped method should be used when it is appropriate, because it is extremely simple. As the heat transfer coefficient is calculated by empirical correlation with a typical error of 20% or more, the calculation of temperature distribution in solids does not need to be very accurate.

For the DNRR, typical value of h ~ 10^3 W/m²K for subcooled fluid flow, half fuel thickness is 1.25×10^{-3} m, and k = 158 W/m.K, then

$$Bi \sim 10^3 \times 1.25 \times 10^{-3}/158 = 0.008 \ll 0.1.$$

Thus, the lumped method can be applied for most cases until fully-developed nucleate boiling takes place, when the heat transfer coefficient may reach more than 10^4 W/m²K

4.5. Hydrodynamics

For the thermal hydraulic system of the nodes and links as described in Chapter 3, the flow equation (2.2.11) for a link with index j is:

$$\frac{dW_j}{dt} = \frac{A_j}{L_j}[(P_u - P_d) - K_j|W_j|W_j - \rho_j g L_j \sin\theta] \qquad (4.5.1)$$

where $K_j = \dfrac{f_j \dfrac{L_j}{D_j} + k_j}{2\rho_j A_j^2}$.

In (4.5.1), indexes u and d refer respectively to upstream node and downstream node of the link. If $W_j > 0$, then the flow is actually from the upstream node to the downstream node. Otherwise reverse flow takes place.

Omitting index j of the coefficients for simplification, we can transform (4.5.1) in implicit form into:

$$\Delta W_j = \frac{A}{L}\Delta t \left[(P_u^{t+\Delta t} - P_d^{t+\Delta t}) - K|W_j^{t+\Delta t}|W_j^{t+\Delta t} - \rho g L \sin\theta\right], \text{ and}$$

$$W_j^{t+\Delta t} = W_j^t + \Delta W_j. \qquad (4.5.2)$$

For the node i, the equations (2.2.7) and (2.2.17) are rewritten for changes in mass and enthalpy as:

$$\Delta M_i = (\sum_{j\in i=d} W_j - \sum_{j\in i=u} W_j)\Delta t, \text{ and}$$

$$M_i^{t+\Delta t} = M_i^t + \Delta M_i \qquad (4.5.3)$$

$$\Delta H_i = (\sum_{j\in i=d} W_j h_j - \sum_{j\in i=u} W_j h_j + Q_i)\,\Delta t, \text{ and}$$

$$H_i^{t+\Delta t} = H_i^t + \Delta H_i \qquad (4.5.4)$$

The notation $j \in i=u$ means that i is the upstream node of the link j, and $j \in i=d$ means that it is the downstream node of the link j. Link enthalpy h_j is of the upstream node if flow is positive, otherwise, of the downstream node.

The heat term Q_i consists of heat flux to the node fluid volume and heat generated within the node volume. Thus, for the core nodes

$$Q_i = qS + (1 - \alpha)q_v V_f \qquad (4.5.5)$$

where $q = h(T_c - T_w)$ is the heat flux obtained from heat transfer calculations, and the last term is heat due to neutron thermalization in water.

The equation of state for close nodes, i.e. V_i = constant, has a form

$$\Delta P_i = \frac{F_{1P}\Delta M_i + F_{2P}\Delta H_i}{F_{4P}M_g + F_{5P}M_f}, \text{ and}$$

$$P_i^{t+\Delta t} = P_i^t + \Delta P_i \qquad (4.5.6)$$

as well as

$$\Delta T_i = \frac{F_{1T}\Delta M_i + F_{2T}\Delta H_i}{F_{4T}M_g + F_{5T}M_f}, \text{ and}$$

$$T_i^{t+\Delta t} = T_i^t + \Delta T_i \qquad (4.5.7)$$

For the open node exposed to the atmosphere as the upper pool node of the DNRR, we can calculate the node pressure directly

$$P_{up} = B + \frac{1}{2}\rho g H_{up} = B + \frac{1}{2}\rho g \frac{V_{up}}{A_{up}},$$

where B is barometric pressure, H_{up}, A_{up} and V_{up} are the node height, cross-section area and volume. Since $\rho V = M$, generally, we have

$$P_{up}^{t+\Delta t} = B + C(M_{up}^t + \Delta M_{up}), \text{ and}$$

$$\Delta P_{up} = C \Delta M_{up} \qquad (4.5.8)$$

where the constant C depends on where the node centre is chosen. If the node centre is at the middle of the node volume, then $C = \frac{1}{2}g/A_{up}$. Then, we can find the change in volume

$$\Delta V_{up} = \frac{\Delta P_{up}(F_{4P}M_g + F_{5P}M_f) - F_{1P}\Delta M_{up} - F_{2P}\Delta H_{up}}{F_{3P}} \qquad (4.5.9)$$

and, consequently, temperature

$$\Delta T_{up} = \frac{F_{1T}\Delta M_{up} + F_{2T}\Delta H_{up} + F_{3T}\Delta V_{up}}{F_{4T}M_g + F_{5T}M_f}, \text{ and}$$

$$T_{up}^{t+\Delta t} = T_{up}^t + \Delta T_{up} \qquad (4.5.10)$$

It is easy to derive the equations for steady-state conditions. Thus, in the above equations, setting all changes of flow, mass, enthalpy and pressure to zero, we have:

Mass: $$\sum_{j\in i=d} W_j = \sum_{j\in i=u} W_j, \qquad (4.5.11)$$

or $W = W_{in} = W_{out}$ for nodes with one inflow and one outflow;

Enthalpy: $$\sum_{j\in i=d} W_j h_j + Q_i = \sum_{j\in i=u} W_j h_j, \qquad (4.5.12)$$

or $\quad h_{out} = h_{in} + \dfrac{Q_i}{W}$ for nodes with one inflow and one outflow;

Flow: $\qquad P_u - P_d - \rho g L \sin\theta = K|W|W \qquad\qquad (4.5.13)$

Equation (4.5.13) is the balance of buoyancy to friction pressure drop across any link between two nodes at steady-state conditions. For close circuits like the DNRR without pump flows in and out, if we write (4.5.13) for every node and sum their left hand sides and right hand sides, we have:

$$\sum_j g \rho_j L_j \sin\theta = \sum_j K_j |W|W \qquad\qquad (4.5.14)$$

Equation (4.5.14) is a traditional equation used for flow calculations under steady-state conditions.

If the flow is known, equations (4.5.3) - (4.5.10) are quite easy to solve. However, equation (4.5.2) causes some difficulties as it contains both pressure and flow of the next time step as unknowns. The friction term could be replaced with

$$K|W^{t+\Delta t}| \, W^{t+\Delta t} \cong K| \, W^t|(\, W^t + 2\Delta W).$$

For a node with one link in and one link out, (4.5.6) can be transformed further using mass and enthalpy equations (4.5.3) and (4.5.4) as

$$\Delta P_i = C_{1i}\Delta M_i + C_{2i}\Delta H_i$$
$$= C_{1i}(W_{j-1} - W_j)\Delta t + C_{2i}(W_{j-1}h_{j-1} - W_j h_j + Q_i)\Delta t$$
$$= \chi_{i,j-1}W_{j-1}\Delta t + \chi_{i,j}W_j\Delta t + C_{2i}Q_i\Delta t,$$

with $\quad C_1 = \dfrac{F_{1P}}{F_{4P}M_g + F_{5P}M_f}$,

$\qquad C_2 = \dfrac{F_{2P}}{F_{4P}M_g + F_{5P}M_f}$ and

$\chi_{i,j} = C_{1i} + C_{2i}h_j.$

So, the pressure difference in (4.5.2) can be replaced with

$$P_u^{t+\Delta t} - P_d^{t+\Delta t} = P_u^t - P_d^t + \Delta P_u - \Delta P_d$$

$$= (P_u^t - P_d^t) + [\chi_{u,j-1} W_{j-1}^{t+\Delta t} - (\chi_{u,j} + \chi_{d,j})W_j^{t+\Delta t} + \chi_{d,j+1}W_{j+1}^{t+\Delta t} + C_{2u}Q_u - C_{2d}Q_d]\Delta t.$$

After collecting terms in (4.5.2) and solving for flow change, we have

$$W_j^{t+\Delta t} = \frac{W_j^t + \frac{A}{L}\Delta t\left[(P_u^t - P_d^t) + K|W_j^t|W_j^t + b + c_Q + (\chi_{u,j-1}W_{j-1}^{t+\Delta t} + \chi_{u,j+1}W_{j+1}^{t+\Delta t})\Delta t\right]}{1 + 2K|W_j^t|\frac{A}{L}\Delta t + (\chi_{uj} + \chi_{dj})\frac{A}{L}\Delta t^2}$$

$$(4.5.15)$$

with b = - ρgLsinθ and c_Q = ($C_{2u}Q_u$- $C_{2d}Q_d$)Δt. Gauss-Seidel method can be used to solve (4.5.15) for flows of all links.

Note that the calculation accuracy is also dependent on the size of the time step Δt. With large Δt, the pressure change may be rather large, so that the node pressure may not remain under the lower bound of the pressure fit curve. Therefore, Δt should be carefully chosen not to be either too large or too small. With some optimized value of Δt, which can be determined from running the code, we can neglect the flow changes of W_{j-1} and W_{j+1} in calculating $W_j^{t+\Delta t}$ by (4.5.15). This is very useful as the iteration is no longer needed to solve (4.5.15). In this case, we have

$$\Delta W_j = \frac{\frac{A}{L}\Delta t\left[(P_u^t - P_d^t) - K|W_j^t|W_j^t + b + c_Q - (\chi_{uj} + \chi_{dj})W_j^t\Delta t + (\chi_{u,j-1}W_{j-1}^t + \chi_{u,j+1}W_{j+1}^t)\Delta t\right]}{1 + 2K|W_j^t|\frac{A}{L}\Delta t + (\chi_{uj} + \chi_{dj})\frac{A}{L}\Delta t^2}$$

$$(4.5.16)$$

All terms in the left hand side of (4.5.16) are know from the previous time step.

4.6. Safety Limits

Maximum Wall Temperature:

To avoid excessive corrosion of the aluminium cladding of the fuel for long operations, the maximum wall temperature is recommended as

$$T_c^{max} = 105°C.$$

Onset of Nucleate Boiling:

Bergles-Rhosenow correlation (2.2.32) is used to predict the ONB. The ONB could take place if the wall overheating were:

$$\Delta T_{sat} = \left(\frac{q}{15.6 P^{1.156}}\right)^{\frac{1}{n}}, \quad n = 2.3\, P^{-0.0234} \qquad (4.6.1)$$

where   q   the local heat flux, $[Btu/ft^2\text{-}hr] = 3.155 q[W/m^2]$

       P   pressure, $[psia] = 145.04 P[MPa]$

     ΔT_{sat} wall overheating, $[°F]$.

The wall temperature at the predicted ONB would be:

$$T_{cONB} = T_{sat} + \frac{5}{9}\Delta T_{sat}, \quad [°C], \qquad (4.6.2)$$

where T_{sat} is fluid saturation temperature at the local pressure, $[°C]$.

The ONB heat flux, on the other hand, is determined by Newton's law of cooling with the convective heat transfer coefficient h as

$$q_{ONB} = h(T_{cONB} - T_b), \quad [W/m^2] \qquad (4.6.3)$$

The margin to ONB is, therefore,

$$\text{Margin to ONB} = \frac{T_{cONB} - T_b}{T_c - T_b} \qquad (4.6.4)$$

Critical Heat Flux and Departure from Nucleate Boiling:

The critical heat flux (CHF) is estimated by the Mishak correlation (2.2.34) and the margin to the departure from nucleate boiling (DNB) is calculated as:

$$\text{Margin to DNB} = \frac{q_{CHF}}{q}.$$