

THE POINT KINETICS ALGORITHM FOR FX2

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ABSTRACT

The two-dimensional space-time kinetics code FX2 is based on the factorization approach to solving the time-dependent diffusion equations. As such, it contains a three-level time step structure. The largest step is the interval between shape function recalculations. Within this interval are the time points at which coefficients of the amplitude function equations are recalculated. Finally, there are time points used for integration of the amplitude function equations, i.e., the point kinetics equations.

In this memorandum the algorithm used to integrate the point kinetics equations is described. This algorithm, an undetermined parameter (weighted residual) method, uses subdomain weighting and piecewise quadratic trial functions. The method is used in conjunction with an automatic time-step-selection scheme, which is also described.

INTRODUCTION

The two-dimensional space-time kinetics code FX2 is based on the factorization¹⁻³ (quasistatic) approach to solving the time-dependent multigroup diffusion equations. That is, it is assumed that the flux shape changes much more slowly in time than does its amplitude. Hence, very few shape function recalculations are needed relative to the number of amplitude function recalculations. The shape function calculations are done by a two-dimensional inhomogeneous multigroup diffusion theory calculation. The amplitude function calculations are done by the point kinetics algorithm to be described in this memorandum. The algorithm is an extension of a method devised by Kaganove⁴ to solve the conventional point kinetics equations. Modification of Kaganove's method is necessary in order to account for the effects of fuel motion that might occur during disassembly or slumping accidents. Since the hydrodynamic effects during disassembly are described on a moving mesh the modifications to the point kinetics equations take the form of corrections to account for moving precursors.

The derivation of the algorithm will be described first, followed by a discussion of the input and output information required. Finally, the computational logic involved in the solution will be described.

THE POINT KINETICS ALGORITHM

Solution Method

The point kinetics equations for FX2 are (using the definitions and notation of reference 3):

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The derivation of the algorithm will be described first, followed by a discussion of the input and output information required. Finally, the computational logic involved in the solution will be described.

THE POINT KINETICS ALGORITHM

Solution Method

The point kinetics equations for EX2 are (using the definitions and

notation of reference 2):

$$\dot{N} = \left(\frac{\rho - \beta}{\Lambda} + \frac{k_0 - 1}{\Lambda k_0} \right) N + \sum_{s=1}^m \lambda_s \eta_s + \sum_{s=1}^m \lambda_s \xi_s + Q' \quad (1)$$

$$\dot{\eta}_s = \frac{\beta'_s}{\Lambda} N - (\lambda_s + \kappa_s) \eta_s, \quad 1 \leq s \leq m \quad (2)$$

where

N = amplitude function,

ρ = reactivity,

β = effective delayed neutron fraction,

k_0 = eigenvalue of source-free adjoint equation (unity unless the reactor is initially subcritical),

Λ = generation time,

Q' = external source,

λ_s = decay constant for sth precursor family,

η_s = weighted integral concentration of sth precursor family,

ξ_s = correction to concentration of the sth precursor family due to fuel motion,

κ_s = loss coefficient for sth precursor family,

β'_s = effective delayed neutron fraction for the sth family as calculated on the moving mesh.

The first step toward obtaining a solution is to formally integrate Eqs. (2) over the time interval $t_{j-1} \leq t \leq t_j$. The result is

$$\begin{aligned} \eta_s(t) = & \eta_s(t_{j-1}) \exp \left[- \int_{t_{j-1}}^t (\lambda_s + \kappa_s(\tau)) d\tau \right] \\ & + \int_{t_{j-1}}^t \exp \left[- \int_{t'}^t (\lambda_s + \kappa_s(\tau)) d\tau \right] \frac{\beta'_s}{\Lambda} (t') N(t') dt' \end{aligned} \quad (3)$$

$$(1) \quad \rho' + \sum_{s=1}^m \lambda_s \rho_s + \sum_{s=1}^m \beta_s \rho_s + N \left(\frac{\rho_0 - \rho}{\Lambda} + \frac{\rho_0}{\Lambda} \right) = N \rho$$

$$(2) \quad \rho_s = \rho_0 \exp(-\lambda_s t) + \int_0^t \exp(-\lambda_s(t-\tau)) \left(\beta_s \rho_s + \lambda_s \rho \right) d\tau$$

where

- N = magnitude function,
- λ_s = reactivity,
- β_s = effective delayed neutron fraction,
- ρ_0 = eigenvalue of source-free adjoint equation (only unless the reactor is initially subcritical),
- Λ = generation time,
- ρ' = external source,
- λ_s = decay constant for s th precursor family,
- ρ_s = weighted integral concentration of s th precursor family,
- β_s = correction to concentration of the s th precursor family due to fission reaction,
- λ_s = loss coefficient for s th precursor family,
- β_s = effective delayed neutron fraction for the s th family as calculated on the moving mesh.

The first step toward obtaining a solution is to formally integrate (1) over the time interval $t - \Delta t \leq t \leq t$. The result is

$$(3) \quad \rho_s(t) = \rho_s(t - \Delta t) \exp(-\lambda_s \Delta t) + \int_{t-\Delta t}^t \exp(-\lambda_s(t-\tau)) \left(\beta_s \rho_s(\tau) + \lambda_s \rho(\tau) \right) d\tau$$

If Eq. (3) is substituted into Eq. (1), then

$$\begin{aligned} \dot{N} = & \left(\frac{\rho - \beta}{\Lambda} + \frac{k_0 - 1}{\Lambda k_0} \right) N(t) + \sum_{s=1}^m \lambda_s \left\{ \eta_s(t_{j-1}) \exp \left[- \int_{t_{j-1}}^t (\lambda_s + \kappa_s(\tau)) d\tau \right] \right. \\ & + \int_{t_{j-1}}^t \exp \left[- \int_{t'}^t (\lambda_s + \kappa_s(\tau)) d\tau \right] \frac{\beta'_s}{\Lambda} (t') N(t') dt' \\ & \left. + \xi_s(t) \right\} + Q' \end{aligned} \quad (4)$$

Next, assume the following trial solution for $N(t)$ over the interval

$t_{j-1} \leq t \leq t_j$:

$$N_K(t) = \sum_{k=0}^K A_k (t - t_{j-1})^k \quad (5)$$

$$\frac{dN_K}{dt} = \sum_{k=1}^K k A_k (t - t_{j-1})^{k-1} \quad (6)$$

The following residual is formed when the approximate solution is put into

Eq. (4):

$$\begin{aligned} R_N(t) = & \frac{dN_K}{dt} - \left[\frac{\rho - \beta}{\Lambda} + \frac{k_0 - 1}{\Lambda k_0} \right] N_K(t) \\ & - \sum_{s=1}^m \lambda_s \left\{ \eta_s(t_{j-1}) \exp \left[- \int_{t_{j-1}}^t (\lambda_s + \kappa_s(\tau)) d\tau \right] \right. \\ & + \int_{t_{j-1}}^t \exp \left[- \int_{t'}^t (\lambda_s + \kappa_s(\tau)) d\tau \right] \frac{\beta'_s}{\Lambda} (t') N_K(t') dt' \\ & \left. + \xi_s(t) \right\} - Q'(t) \end{aligned} \quad (7)$$

The parameters A_k are evaluated by the method of undetermined parameters, with subdomain weighting.⁵ The time-step selection technique developed by Kaganove⁴ is used to ensure a stable, accurate solution.

It is obvious that $A_0 = N_K(t_{j-1})$, so that only A_1, \dots, A_K , need to be evaluated over the time interval. Nested subdomains are chosen, such that each begins at t_{j-1} . The largest is the full interval, the next largest the half-interval then the quarter interval, etc., until K intervals are chosen. Unit step functions over each subdomain are the weighting functions. Mathematically, the weighting functions are written as

$$V_r(t) = U(t) - U(t-t_r), \quad r = 1, \dots, K, \quad (8)$$

where

$$t_r = t_{j-1} + \frac{(t_j - t_{j-1})}{2^{r-1}} = t_{j-1} + \frac{\Delta t_j}{2^{r-1}} \quad (9)$$

(thus defining $\Delta t_j \equiv t_j - t_{j-1}$). The method of undetermined parameters, concisely written as

$$\int_{t_{j-1}}^{t_j} V_r(t) R_N(t) dt = 0, \quad r = 1, \dots, K, \quad (10)$$

can then be used to obtain K algebraic equations to solve for A_1, \dots, A_K .

The parameters ρ , β , Λ , ξ_s , Q' , β'_s and κ_s are, in general, functions of time. Since their functional dependencies cannot, in general, be pre-specified, they shall be approximated by fitting to quadratic functions

The parameters A_k are evaluated by the method of undetermined parameters with subdomain weighting.² The time-step selection technique developed by Lagrove¹ is used to ensure a stable, accurate solution.

It is obvious that $A_0 = \dot{X}(t_{j-1})$, so that only A_1, \dots, A_K need to be evaluated over the time interval. Nested subdomains are chosen such that each begins at t_{j-1} . The largest is the full interval, the next largest the half-interval then the quarter interval, etc., until K intervals are chosen. Third step functions over each subdomain are the weighting functions. Mathematically, the weighting functions are written as

$$V_k(t) = U(t - t_{j-1}) - U(t - t_{j-1} - \Delta t_k) \quad k = 1, \dots, K \quad (8)$$

where

$$t_{j-1} - \Delta t_k = t_{j-1} - \frac{t_j - t_{j-1}}{2^k} \quad k = 1, \dots, K \quad (9)$$

(this defining $\Delta t_0 = t_j - t_{j-1}$). The method of undetermined parameters, concisely written as

$$\int_{t_{j-1}}^{t_j} V_k(t) \dot{X}(t) dt = 0 \quad k = 1, \dots, K \quad (10)$$

can then be used to obtain K algebraic equations to solve for A_1, \dots, A_K . The parameters $c_1, c_2, A, \epsilon_1, \epsilon_2, Q^1, Q^2$ and κ_1, κ_2 are, in general, functions of time. Since their functional dependencies cannot, in general, be prescribed, they shall be approximated by fitting to polynomial functions

over time intervals - called reactivity time steps - that are, in general, quite a bit larger than the point kinetics intervals. The functional behavior of the parameters can be written as

$$p(t) = p(t_{j-1}) + (t-t_{j-1})(a_1+2a_2 t_{j-1}) + a_2(t-t_{j-1})^2 \quad (11)$$

where

$$p = \frac{\rho - \beta + (k_0-1)/k_0}{\Lambda}, \quad (12)$$

$$\xi_s(t) = \xi_s(t_{j-1}) + (t-t_{j-1})(c_{1s}+2c_{2s} t_{j-1}) + c_{2s}(t-t_{j-1})^2, \quad (13)$$

$$\frac{\beta'_s}{\Lambda}(t) = \frac{\beta'_s}{\Lambda}(t_{j-1}) + (t-t_{j-1})(b_{1s}+2b_{2s} t_{j-1}) + b_{2s}(t-t_{j-1})^2$$

$$s = 1, \dots, m. \quad (14)$$

$$Q'(t) = Q'(t_{j-1}) + (t-t_{j-1})(q_1+2q_2 t_{j-1}) + q_2(t-t_{j-1})^2. \quad (15)$$

where the coefficients have been evaluated at an earlier time t_{i-1} which is in turn set to zero, so that all times are those that have elapsed since t_{i-1} . Since κ_s is a crude function, it is approximated as the initial value over the time interval (i.e., $\bar{\kappa}_s$) to simplify evaluation of the integrals that appear in Eq. (7). When Eqs. (5), (6), and (11) - (15) are substituted into Eq. (10), with the weighting functions given by Eqs. (8) and (9), the result is

$$\sum_{k=1}^K R_{rk} A_k = S_{rk}, \quad r = 1, \dots, K \quad (16)$$

over time intervals - called reactivity-time steps - that are, in general, quite a bit larger than the point kinetics intervals. The functional behavior of the parameters can be written as

$$p(z) = p_0(z) + (z - z_1) p_1(z) + (z - z_1)(z - z_2) p_2(z) \quad (11)$$

where

$$p_0(z) = \frac{a_0 + a_1 z + a_2 z^2}{\lambda} \quad (12)$$

$$p_1(z) = \frac{b_1(z - z_1) + b_2(z - z_1)(z - z_2)}{(z - z_1)^2} \quad (13)$$

$$\frac{a_0}{\lambda} = \frac{a_1}{\lambda} z_1 + \frac{a_2}{\lambda} z_1 z_2 \quad (14)$$

$$z = 1, \dots, m \quad (15)$$

$$p_2(z) = \frac{c_1(z - z_1)(z - z_2) + c_2(z - z_1)^2}{(z - z_1)^2(z - z_2)} \quad (16)$$

where the coefficients have been evaluated at an earlier time t_{i-1} which is in turn set to zero, so that all times are those that have elapsed since t_{i-1} . Since p_2 is a crude function, it is approximated as the initial value over the time interval (t_{i-1}, t_i) to simplify evaluation of the integrals that appear in Eq. (9). When Eqs. (11), (12), (13) and (14) are substituted into Eq. (10), with the weighting functions given by Eqs. (8) and

(9), the result is

$$\frac{d}{dt} \sum_{k=1}^K X_k = S X_k \quad (17)$$

where

$$\begin{aligned}
 R_{rk} = & \Delta t_r^k - \left[\frac{p(t_{j-1})\Delta t_r^{k+1}}{k+1} + \frac{(a_1+2a_2t_{j-1})\Delta t_r^{k+2}}{k+2} + \frac{a_2\Delta t_r^{k+3}}{k+3} \right] \\
 & + \sum_{s=1}^m \left\{ \frac{\beta'_s}{\Lambda} (t_{j-1}) \frac{[\Delta t_r^{k+1} - (k+1)I_{s,k}(\Delta t_r)]}{k+1} \right. \\
 & + (b_{1s}+2b_{2s}t_{j-1}) \frac{[\Delta t_r^{k+2} - (k+2)I_{s,k+1}(\Delta t_r)]}{k+2} \\
 & \left. + b_{2s} \frac{[\Delta t_r^{k+3} - (k+3)I_{s,k+2}(\Delta t_r)]}{k+3} \right\} \quad (17)
 \end{aligned}$$

$$\begin{aligned}
 S_{rk} = & \left(p(t_{j-1})\Delta t_r + (a_1+2a_2t_{j-1}) \frac{\Delta t_r^2}{2} + a_2 \frac{\Delta t_r^3}{3} \right. \\
 & + \sum_{s=1}^m \left\{ \frac{\beta'_s}{\Lambda} (t_{j-1}) [\Delta t_r - I_{s,o}(\Delta t_r)] + (b_{1s}+2b_{2s}t_{j-1}) \left[\frac{\Delta t_r^2}{2} - I_{s,1}(\Delta t_r) \right] \right. \\
 & \left. + b_{2s} \left[\frac{\Delta t_r^3}{3} - I_{s,2}(\Delta t_r) \right] \right\} A_o + \sum_{s=1}^m \left\{ \lambda_s \left[\eta_s(t_{j-1})I_{s,o}(\Delta t_r) \right. \right. \\
 & \left. \left. + \xi_s(t_{j-1})\Delta t_r + (c_{1s}+2c_{2s}t_{j-1}) \frac{\Delta t_r^2}{2} + c_{2s} \frac{\Delta t_r^3}{3} \right] \right\} \\
 & + \left[Q'(t_{j-1})\Delta t_r + (q_1+2q_2t_{j-1}) \frac{\Delta t_r^2}{2} + q_2 \frac{\Delta t_r^3}{3} \right], \quad (18)
 \end{aligned}$$

and

$$\begin{aligned}
 I_{s,k}(\Delta t) = & \int_{t_{j-1}}^t \exp[-(\lambda_s + \bar{\kappa}_s)(t-t')] (t'-t_{j-1})^k dt' \\
 (\Delta t = t - t_{j-1}). \quad (19)
 \end{aligned}$$

Some important features of the I-functions are described in the Appendix.

The set of algebraic equations represented by Eq. (16) can then be solved

for the parameters A_k , which are in turn substituted into Eq. (5) to obtain the amplitude function at t_j .

Piecewise quadratic functions ($K=2$) are used in FX2 because they have worked very well in QX1. And, they are very well suited to be used in conjunction with Kaganove's time-step-halving-and-doubling scheme for automatically selecting the time step size. This time-step-selection technique will now be described.

Time Step Selection

Suppose that a solution has been obtained at t_{j-1} and that Δt_j has been selected. Then, two independent solutions (sets of parameters) of the point kinetics equations are found at t_j . The first of these integrates over the whole time step, yielding a solution directly at t_j . The second solution is for only half the step, yielding a solution at $t_{j-1} + \frac{\Delta t_j}{2}$. The half-step solution is then extrapolated to t_j . It will not be the same as that determined directly, but it should be close. The degree of closeness determines whether or not the solution is acceptable.

The two values are compared by forming the error norm

$$\epsilon = \frac{|N_{\text{ext}}(t_j) - N(t_j)|}{N_{\text{ext}}(t_j)}, \quad (20)$$

and comparing it with a preselected tolerable error ϵ_1 . If $\epsilon < \epsilon_1$, then the amplitude function $N(t_j)$ is acceptable and the solution can be found for the next step. If, in addition, $\epsilon < C \epsilon_1$ where C is a preselected parameter less than unity (usually set to 0.1), then the next time step is estimated to be $2\Delta t_j$. Otherwise, $\Delta t_{j+1} = \Delta t_j$.

If, on the other hand, $\epsilon > \epsilon_1$, the solution at t_j is not acceptable, and the time step is halved. Two independent solutions to the point kinetics equations are again found, this time for $t = t_{j-1} + \frac{\Delta t_j}{2}$ and $t = t_{j-1} + \frac{\Delta t_j}{4}$. Note that the first of these has already been made for the original comparison and hence need not be repeated. The solutions are again compared as described above. If an acceptable value of $N(t_{j-1} + \frac{\Delta t_j}{2})$ is found, the solution for t_j will again be attempted in the same manner. This time, however, $t = t_{j-1} + \frac{\Delta t_j}{2}$ at the lower end of the time step, so that independent solutions are formed for $t = t_{j-1} + \frac{3}{4} \Delta t_j$ and $t = t_j$.

If the value $N(t_{j-1} + \frac{\Delta t_j}{2})$ is not acceptable the time step is halved again and the calculation is repeated for the quarter step. Calculation continues until an acceptable solution has been obtained for $t = t_j$. The procedure then begins anew to determine $N(t_{j+1})$, etc., until the end of the reactivity step is reached.

REQUIRED INPUT AND OUTPUT INFORMATION

The following information is needed upon entry to the point kinetics algorithm: the amplitude function $N(t_{i-1})$, the coefficients $p(t_{i-1})$, a_1 , a_2 , $\xi_s(t_{i-1})$, c_{1s} , c_{2s} , $\frac{\beta'_s}{\Lambda}(t_{i-1})$, b_{1s} , b_{2s} , $Q'(t_{i-1})$, b_{1s} , b_{2s} , $Q(t_{i-1})$, q_1 , q_2 , $\bar{k}_s(t_{i-1})$, and the time interval (called the reactivity step) over which these are to be used (i.e., t_{i-1} to t_i). These coefficients are evaluated by fitting the inner products for reactivity, etc., from the previous two i -intervals to parabolas. The functions are

If, on the other hand, $e > \epsilon$, the solution at t_j is not acceptable and the time step is halved. Two independent solutions to the point kinetics equations are again found, this time for $t = t_{j-1} + \frac{\Delta t}{2}$ and $t = t_{j-1} + \frac{\Delta t}{2}$. Note that the first of these has already been made for the original comparison and hence need not be repeated. The solutions are again computed as described above. If an acceptable value of $N(t_{j-1} + \frac{\Delta t}{2})$ is found, the solution for t_j will again be attempted in the same manner. This time, however, $t = t_{j-1} + \frac{\Delta t}{2}$ at the lower end of the time step, so that independent solutions are found for $t = t_{j-1} + \frac{\Delta t}{4}$ and $t = t_{j-1} + \frac{3\Delta t}{4}$. If the value $N(t_{j-1} + \frac{\Delta t}{4})$ is not acceptable the time step is halved again and the calculation is repeated for the quarter step. Calculation continues until an acceptable solution has been obtained for $t = t_j$. The procedure then begins anew to determine $N(t_{j+1})$, etc., until the end of the reactivity step is reached.

REQUIRED INPUT AND OTHER INFORMATION

The following information is needed upon entry to the point kinetics algorithm: the magnitude function $N(t_{j-1})$, the coefficients $\beta(t_{j-1})$, $\beta_1(t_{j-1})$, $\beta_2(t_{j-1})$, $\beta_3(t_{j-1})$, $\beta_4(t_{j-1})$, $\beta_5(t_{j-1})$, $\beta_6(t_{j-1})$, $\beta_7(t_{j-1})$, $\beta_8(t_{j-1})$, $\beta_9(t_{j-1})$, $\beta_{10}(t_{j-1})$, $\beta_{11}(t_{j-1})$, $\beta_{12}(t_{j-1})$, $\beta_{13}(t_{j-1})$, $\beta_{14}(t_{j-1})$, $\beta_{15}(t_{j-1})$, $\beta_{16}(t_{j-1})$, $\beta_{17}(t_{j-1})$, $\beta_{18}(t_{j-1})$, $\beta_{19}(t_{j-1})$, $\beta_{20}(t_{j-1})$, $\beta_{21}(t_{j-1})$, $\beta_{22}(t_{j-1})$, $\beta_{23}(t_{j-1})$, $\beta_{24}(t_{j-1})$, $\beta_{25}(t_{j-1})$, $\beta_{26}(t_{j-1})$, $\beta_{27}(t_{j-1})$, $\beta_{28}(t_{j-1})$, $\beta_{29}(t_{j-1})$, $\beta_{30}(t_{j-1})$, $\beta_{31}(t_{j-1})$, $\beta_{32}(t_{j-1})$, $\beta_{33}(t_{j-1})$, $\beta_{34}(t_{j-1})$, $\beta_{35}(t_{j-1})$, $\beta_{36}(t_{j-1})$, $\beta_{37}(t_{j-1})$, $\beta_{38}(t_{j-1})$, $\beta_{39}(t_{j-1})$, $\beta_{40}(t_{j-1})$, $\beta_{41}(t_{j-1})$, $\beta_{42}(t_{j-1})$, $\beta_{43}(t_{j-1})$, $\beta_{44}(t_{j-1})$, $\beta_{45}(t_{j-1})$, $\beta_{46}(t_{j-1})$, $\beta_{47}(t_{j-1})$, $\beta_{48}(t_{j-1})$, $\beta_{49}(t_{j-1})$, $\beta_{50}(t_{j-1})$, $\beta_{51}(t_{j-1})$, $\beta_{52}(t_{j-1})$, $\beta_{53}(t_{j-1})$, $\beta_{54}(t_{j-1})$, $\beta_{55}(t_{j-1})$, $\beta_{56}(t_{j-1})$, $\beta_{57}(t_{j-1})$, $\beta_{58}(t_{j-1})$, $\beta_{59}(t_{j-1})$, $\beta_{60}(t_{j-1})$, $\beta_{61}(t_{j-1})$, $\beta_{62}(t_{j-1})$, $\beta_{63}(t_{j-1})$, $\beta_{64}(t_{j-1})$, $\beta_{65}(t_{j-1})$, $\beta_{66}(t_{j-1})$, $\beta_{67}(t_{j-1})$, $\beta_{68}(t_{j-1})$, $\beta_{69}(t_{j-1})$, $\beta_{70}(t_{j-1})$, $\beta_{71}(t_{j-1})$, $\beta_{72}(t_{j-1})$, $\beta_{73}(t_{j-1})$, $\beta_{74}(t_{j-1})$, $\beta_{75}(t_{j-1})$, $\beta_{76}(t_{j-1})$, $\beta_{77}(t_{j-1})$, $\beta_{78}(t_{j-1})$, $\beta_{79}(t_{j-1})$, $\beta_{80}(t_{j-1})$, $\beta_{81}(t_{j-1})$, $\beta_{82}(t_{j-1})$, $\beta_{83}(t_{j-1})$, $\beta_{84}(t_{j-1})$, $\beta_{85}(t_{j-1})$, $\beta_{86}(t_{j-1})$, $\beta_{87}(t_{j-1})$, $\beta_{88}(t_{j-1})$, $\beta_{89}(t_{j-1})$, $\beta_{90}(t_{j-1})$, $\beta_{91}(t_{j-1})$, $\beta_{92}(t_{j-1})$, $\beta_{93}(t_{j-1})$, $\beta_{94}(t_{j-1})$, $\beta_{95}(t_{j-1})$, $\beta_{96}(t_{j-1})$, $\beta_{97}(t_{j-1})$, $\beta_{98}(t_{j-1})$, $\beta_{99}(t_{j-1})$, $\beta_{100}(t_{j-1})$. These coefficients are evaluated by fitting the inner products for reactivity, etc., from the previous two Δt -intervals to parabolae. The functions are

then extrapolated to $t = t_i$. The inner products are recalculated at $t = t_i$ after $N(t_i)$ has been found. The recomputed values are compared with the extrapolated values, and the necessary corrections are made.

Once the amplitude function is evaluated at $t = t_i$, it is used, along with $N(t_{i-1})$ and $N(t_{i-2})$ to evaluate n_1 , n_2 , and n_3 for use in the expression

$$\ln N(t_{i+1}) = n_1 + n_2(t_{i+1} - t_i) + n_3(t_{i+1} - t_i)^2. \quad (21)$$

This extrapolation, which takes place once an estimate of t_{i+1} has been determined, is necessary to compute the energy generated over the $i+1$ st interval from the increase in fuel temperature. The estimate of $N(t_{i+1})$ obtained from Eq. (21) is, of course, later corrected by carrying out a point kinetics calculation over the interval $[t_i, t_{i+1}]$.

In addition to the amplitude function information, the quantities \hat{a}_S^i and \hat{b}_S^i , as defined in Eq. (19) of reference 3, are available from the point kinetics calculation. These quantities, needed to properly update the concentrations of delayed neutron precursors, are given by the expressions

$$\hat{a}_S^i = \frac{1}{\Delta t_i} \int_{t_{i-1}}^{t_i} \exp \left[- \int_t^{t_i} (\lambda_S + \kappa_S(\tau)) d\tau \right] (t - t_{i-1}) N(t) dt \quad (22)$$

$$\hat{b}_S^i = \frac{1}{\Delta t_i} \int_{t_{i-1}}^{t_i} \exp \left[- \int_t^{t_i} (\lambda_S + \kappa_S(\tau)) d\tau \right] (t_i - t) N(t) dt. \quad (23)$$

We shall now outline the method of evaluating these quantities.

then extrapolated to $t = t_{i+1}$. The inner products are recalculated at $t = t_{i+1}$ after $N(t_i)$ has been found. The computed values are compared with the extrapolated values, and the necessary corrections are made.

Once the amplitude function is evaluated at $t = t_{i+1}$, it is used, along with $N(t_{i-1})$ and $N(t_{i-2})$ to evaluate $n_1, n_2, n_3,$ and n_4 for use in the expression

$$(21) \quad n_1 N(t_{i+1}) = n_1 + n_2(t_{i+1} - t_i) + n_3(t_{i+1} - t_i)^2 + n_4(t_{i+1} - t_i)^3$$

This extrapolation, which takes place once an estimate of t_{i+1} has been determined, is necessary to compute the energy generated over the $i+1$ st interval from the increase in fuel temperature. The estimate of $N(t_{i+1})$ obtained from Eq. (21) is, of course, later corrected by carrying out a

point kinetics calculation over the interval $[t_i, t_{i+1}]$.

In addition to the amplitude function information, the quantities β_2^{-1} and β_2^{-2} as defined in Eq. (19) or reference 1, are available from the point kinetics calculation. These quantities, needed to properly update the concentrations of delayed neutron precursors, are given by the ex-

pressions

$$(22) \quad \beta_2^{-1} = \frac{1}{\Delta t} \int_{t_{i-1}}^{t_i} \exp \left[\lambda_2 (t - t_{i-1}) \right] \lambda_2^{-1} N(t) dt$$

$$(23) \quad \beta_2^{-2} = \frac{1}{\Delta t} \int_{t_{i-1}}^{t_i} \exp \left[\lambda_2 (t - t_{i-1}) \right] \lambda_2^{-2} N(t) dt$$

We shall now outline the method of evaluating these quantities.

Within the time interval $[t_{i-1}, t_i]$ there are J point kinetics steps ($t_0 = t_{i-1}$, and $t_J = t_i$). Let us, therefore, evaluate the integrals by summing the components of each point kinetics step; specifically,

$$\hat{a}_S^i = \frac{1}{\Delta t_i} \sum_{j=1}^J \int_{t_{j-1}}^{t_j} \exp [- (\lambda_S + \bar{\kappa}_S)(t_i - t)] (t - t_{i-1}) \sum_{k=0}^K A_k (t - t_{j-1})^k dt \quad (24)$$

$$\hat{b}_S^i = \frac{1}{\Delta t_i} \sum_{j=1}^J \int_{t_{j-1}}^{t_j} \exp [- (\lambda_S + \bar{\kappa}_S)(t_i - t)] (t_i - t) \sum_{k=0}^K A_k (t - t_{j-1})^k dt \quad (25)$$

This is necessary because $N(t)$ is a piecewise polynomial function over the interval $[t_{i-1}, t_i]$, such that its coefficients differ over each point kinetics interval. Finally, after some manipulations, it can be shown that

$$\hat{a}_S^i = \frac{1}{\Delta t_i} \sum_{j=1}^J \{ \exp [- (\lambda_S + \bar{\kappa}_S)(t_i - t_j)] \sum_{k=0}^K A_k [I_{S,k+1}(\Delta t_j) + (t_{j-1} - t_{i-1}) I_{S,k}(\Delta t_j)] \} \quad (26)$$

$$\hat{b}_S^i = \frac{1}{\Delta t_i} \sum_{j=1}^J \{ \exp [- (\lambda_S + \bar{\kappa}_S)(t_i - t_j)] \sum_{k=0}^K A_k [(t_i - t_{j-1}) I_{S,k}(\Delta t_j) - I_{S,k+1}(\Delta t_j)] \} \quad (27)$$

COMPUTATIONAL LOGIC

The logical sequence of the point kinetics solution is shown in Fig. 1. The first step is to calculate the coefficients that appear in Eqs. (11) - (15). Then, the time values are initialized, the convergence criteria are set, and the

starting values of the point kinetics parameters are calculated. These parameters will be updated later according to Eqs. (11) - (15). We are now ready to solve for the A_k for the first time step.

We begin by calculating the I-functions needed for Δt_1 and $\Delta t_1/2$ (see Appendix). Then, we can find the coefficients R_{rk} and S_{rk} of Eq. (16) for the full step and for the half step. The determinant of coefficients is formed for each step, and solved to obtain the values of A_k for t_1 and $t_1/2$. These, in turn, are used to find $N(t_1)$ and $N_{ext}(t_1)$. If they are not close enough to each other, then the time step is halved and a solution at $t_1/2$ is attempted. If I-functions for the half-step are needed they are calculated. Otherwise, the determinants of coefficients for both the half step and the quarter step are formed and solved for the A_k .

When $\epsilon < \epsilon_1$ the solution is considered to be converged, and the next time step is selected. This next step is double the previous one if $\epsilon < 0.1 \epsilon_1$. Otherwise, the step length remains the same. In either case the point kinetics parameters are updated to the latest time step, as are the precursor concentrations. An edit of the current information can also be made at this time. If more I-functions need to be calculated for the next time step they are so calculated; otherwise, the determinants of coefficients are formed and solved for the half step and the full step.

When a converged solution has been found at $t = t_i$ (the end of the reactivity step), the parabolic coefficients for $\ln N$, needed to estimate the amplitude function behavior over the next reactivity step are calculated. Then, the information is taken from the module to be used in other parts of the program.

starting values of the point kinetics parameters are calculated. These parameters will be updated later according to Eqs. (11) - (13). We are now ready to solve for the A_k for the first time step.

We begin by calculating the λ -functions needed for A_1 and A_2 (see Appendix). Then, we can find the coefficients R_{k1} and S_{k1} of Eq. (16) for the full step and for the half step. The determinant of coefficients is formed for each step, and solved to obtain the values of A_k for t_1 and $t_1/2$. These, in turn, are used to find $N(t_1)$ and $N(t_1/2)$. If they are not close enough to each other, then the time step is halved and a solution at $t_1/2$ is attempted. If λ -functions for the half-step are needed they are calculated. Otherwise, the determinants of coefficients for both the half step and the quarter step are formed and solved for the A_k .

When $\epsilon < \epsilon_1$ the solution is considered to be converged, and the next time step is selected. This next step is double the previous one if $\epsilon < 0.1 \epsilon_1$. Otherwise, the step length remains the same. In either case the point kinetics parameters are updated to the latest time step, as are the precursor concentrations. An edit of the current information can also be made at this time. If more λ -functions need to be calculated for the next time step they are so calculated; otherwise, the determinants of coefficients are formed and solved for the half step and the full step.

When a converged solution has been found at $t = t_1$ (the end of the reactivity step), the parabolic coefficients for β in M needed to estimate the magnitude function behavior over the next reactivity step are calculated. Then, the information is taken from the module to be used in other parts of the program.

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APPENDIX

The $I_{S,m}(\Delta t)$ Functions

The I-functions are defined as

$$I_{S,m}(\Delta t) = \int_{t_{j-1}}^t e^{-(\lambda_S + \bar{\kappa}_S)(t-t')} (t'-t_{j-1})^m dt' \quad , \quad \Delta t = t - t_{j-1}. \quad (A1)$$

From the definition, it is evident that

$$I_{S,0}(\Delta t) = \frac{1}{\lambda_S + \bar{\kappa}_S} \left[1 - e^{-(\lambda_S + \bar{\kappa}_S) \Delta t} \right] \quad (A2)$$

Using Eqs. (A1) and (A2), the following recursion relationship can easily be derived:

$$I_{S,m}(\Delta t) = \frac{1}{\lambda_S + \bar{\kappa}_S} [\Delta t^m - m I_{S,m-1}(\Delta t)], \quad m \geq 1 \quad (A3)$$

Finally, using Eqs. (A1), (A2), and (A3), a very useful expression for the integral of the I-function is found:

$$\int_{t_{j-1}}^{t_r} I_{S,m}(\Delta t) dt = \frac{1}{m+1} I_{S,m+1}(\Delta t_r) \quad , \quad (A4)$$

where

$$\Delta t_r = t_r - t_{j-1} .$$

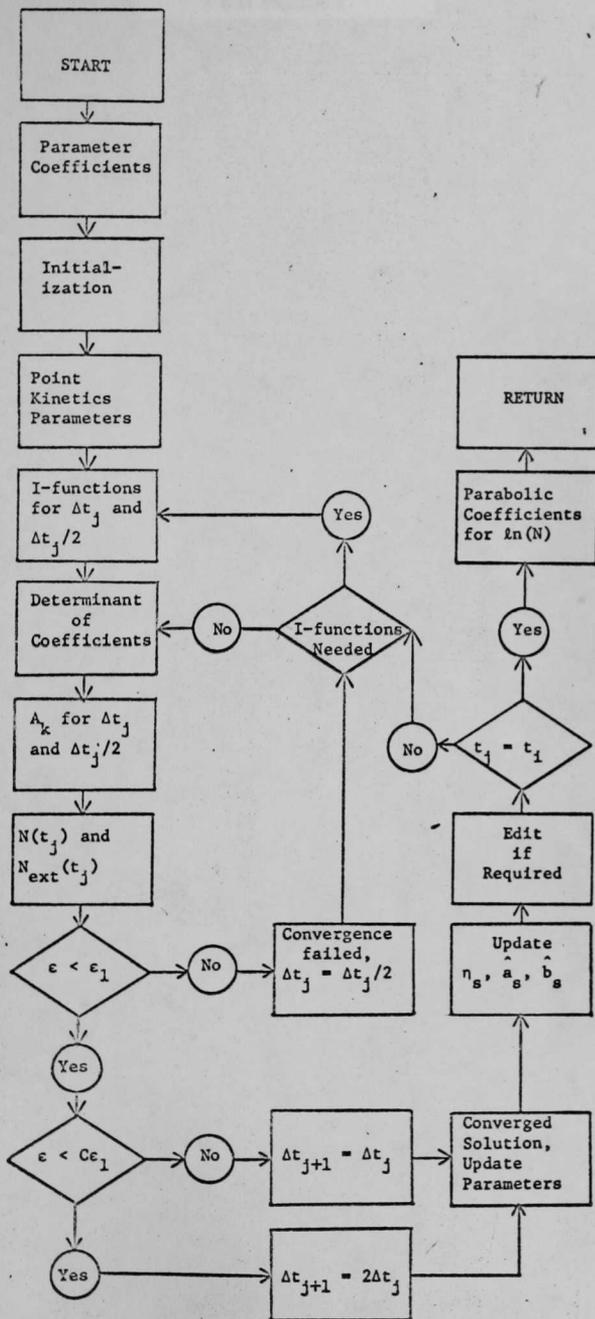


Figure 1. Logical Sequence of Point Kinetics Solution

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