Three Level Space-Time Kinetics Based on Super Nodal Analysis

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ABSTRACT

In order to reduce the computing costs of the time-dependent diffusion calculations without introducing unacceptable inaccuracies in the solution, a three level space-time kinetics procedure which is a combination of NET (Nodal Equivalence Theory) and QS (Quasi-Static method) is being developed. The time scales are divided into a three level hierarchy. On the smaller time step, the point kinetics equations are solved. At intermediate time steps, a coarse representation of the reactor core is solved using NET. Finally, full fine mesh calculation are performed over a large time scale. This scheme appears to have the potential of simulating demanding transients with lower computational cost than conventional methods. Detailed investigation are being carried out to reproduce the total power and flux distribution in coarse level calculations.

1. Introduction

The accurate calculation of the power produced throughout a nuclear reactor core during transient operation is essential to both the design and safe operation of the reactor. These transients cover a wide range of events from fuel depletion to catastrophic accident excursions. Practically, the extension of sophisticated numerical methods developed to solve transport equations to time-dependent problems which need thousands of calculations is very expensive from the point of the view of the computational resources required. Hence, time-dependent diffusion equations are normally considered as the starting point for transient calculations. The time-dependent diffusion equations (also known as space-time kinetics equations) are[1]:

$$[v]^{-1}\frac{\partial}{\partial t}[\Phi] = \vec{\nabla}\cdot[D]\,\vec{\nabla}[\Phi] - [\Sigma][\Phi] + (1-\beta)\left[\chi_p\right]\left[\upsilon\Sigma_f\right]^{\mathrm{T}}[\Phi] + \sum_{n=1}^{D}\left[\chi_{dn}\right]\lambda_n C_n \ , \qquad (1)$$

$$\frac{\partial}{\partial t}C_n = \beta_n\left[\upsilon\Sigma_f\right]^{\mathrm{T}}[\Phi] - \lambda_n C_n \ , \qquad (2)$$

Despite the substantial increase in speed and memory of computer hardware in the recent years, the numerical solution of these equations is still far from being practical for regular calculations. The cost of the calculations is normally due to the three-dimensional nature of the power distribution through a large and often geometrically complicated core. Since for a CANDU reactor, a typical transient calculation requires about 10000 mesh points, the corresponding transient calculations are

[1] Notations are fairly standard.

very time consuming. Consequently, developing efficient methods for treating both the spatial and temporal variables at a lower computational cost is of major importance.

The spatial methods can be categorized as follows: direct methods, space-time factorization methods, and modal and synthesis methods. In direct methods such as finite difference and nodal methods, both space and time are directly discretized to produce a set of linear algebraic equations. Space-time factorization methods such as point kinetics, quasi-static methods are based on the factorization of the space and time dependent flux into two parts. One part is only time dependent and the other part is space- and weakly time-dependent. Finally, synthesis and modal methods are based on approximation of the flux by a linear combination of predetermined time-dependent spatial distributions. Time integration methods involve many methods such as θ-method, ADI (alternating direction implicit) method, stiffness confinement method, and the family of Runge-Kutta methods.

2. Nodal Equivalence Theory

Equivalence theory[1],[2] was initially developed to solve the assembly homogenization problem. The assembly homogenization problem is to determine the equivalent diffusion theory parameters for each localized heterogeneous region (fuel pins, control rods, etc.) of a nuclear reactor during a static calculation. Equivalence theory can theoretically reproduce the heterogeneous solution of the nodes in a reactor. In equivalence theory, the major assumption is that the heterogeneous solution of the reactor calculation is known a priori. However, the goal of spatial homogenization is to be able to accurately predict the solution for the heterogeneous reactor without actually solving the heterogeneous problem. Therefore, by applying a set of approximations[3], the heterogeneous solution of an assembly in static calculations can be reproduced with an acceptable degree of error. The basic idea of nodal equivalence theory is to use modified interface flux continuity condition (defined by discontinuity factors) in order to preserve the group surface currents, all group reaction rates and the reactor eigenvalue. For transient calculations, a complete derivation of NET would start with the time-dependent diffusion equation for a model of the heterogeneous reactor. In recent years some applications of nodal equivalence theory to time-dependent problems have been reported[4], [5],[6]. However, in these works the discontinuity factors are obtained from a set of static calculations or approximated to allow for control rod motions or other material change.

3. Description of the Method

The basis of the method is the space-time factorization which is the decomposition of the time-dependent neutron flux into the product of two functions: an amplitude function that depends only on time and a shape function that depends on space and energy as well as time:

$$[\Phi(\vec{r},t)] = [S(\vec{r},t)]\,T(t), \tag{3}$$

where $S(\vec{r},t)$ is shape function and $T(t)$ is amplitude function. Normally, it is considered that the shape function is weakly time dependent, and as result it does not need to be computed at every time

step. By applying this relationship to time-dependent diffusion equations, two sets of equations can be obtained[7] :

- the point kinetics equations for amplitude function,
- and space-time equations for the shape function.

In the classical improved quasi-static method [8] , the point kinetics equations are solved on a smaller time scale than the shape function. This is normally acceptable because the amplitude varies much faster than the shape function. In the cases where fast local shape distortions occur, the full core shape equations must be solved often during a transient. In this situation even the QS method becomes computationally expensive. In order to reduce the computational costs, the quasi-static shape function can be calculated in different node size levels where each node size level corresponds to a time step hierarchy. It is supposed that the shape function in the coarser node size varies faster than those of the finer nodes. Therefore the shape function in the coarser node should be calculated more often. By using nodal equivalence theory the preservation of the reactor eigenvalue, all group reaction rates and surface currents for each coarse mesh is guaranteed. Based on this approach and considering just one intermediate coarse level between the fine mesh calculation and the point kinetics, a three time step hierarchy has been proposed[9] (Figure 1 and 2). At the smallest time step, the point kinetics equations are solved. The coarse mesh shape function is calculated by solving the multigroup diffusion equations over coarse regions. Finally, after many coarse mesh calculations, the full core fine mesh shape function is recalculated using the full multigroup diffusion equations. The solution of the fine mesh level is considered as the heterogeneous solution of the reactor and is used to update average cross sections, diffusion coefficients and discontinuity factors for coarse regions.

4. Code Development

As previously mentioned the method consists of three time steps: fine mesh, coarse mesh and point kinetics step. A new computer code named NDF which implements the aforementioned solution scheme is under development. This code consists of three major modules: fine and coarse level modules (including both spatial and time integration), and point kinetics equation solver (including time integration scheme). Furthermore, development of additional drivers for performing three-level quasi-static type of calculations is underway.

4.1 fine step module

In this module, by using an appropriate nodal method the heterogeneous or exact solution of a model of a real CANDU-6 reactor can be calculated. Later, reproducing this exact solution at a lower computational cost is the ultimate motivation behind of any nodal-coarse solution method. It has been proven that, among many available nodal methods, the mesh-centered finite difference method which is the lowest order of all nodal approximation, is sufficient for the study of CANDU reactors with one mesh per cell unit[10] . The higher order approximations in the nodal method

would only produce a marginal improvement of the flux solution. In the MCFD method, the net surface currents are approximated by assuming that the flux varies linearly between the node centerpoint and the midpoint of any surface of the node. Eliminating the surface fluxes by enforcing continuity of the net current and flux across each interface leads to equations involving only the node-averaged fluxes. All diffusion parameters for the unit cells (fine level) are precalculated by using the transport code DRAGON[11] . Furthermore, by taking advantage of a full representation of all moving devices in the computer codes XSIMUL/DONJON[12] , NDF modules are able to perform complicated static and dynamic calculations related to control and safety devices in CANDU reactors.

4.2 Coarse step module

For coarse calculations, the Generalized Equivalence Theory(GET) formulation of NET is chosen because no iterative process is needed to calculate the discontinuity factors[2] . According to GET, discontinuity factors are defined as ratios of the heterogeneous fluxes and coarse mesh homogeneous fluxes over coarse mesh interface:

$$f^{-}_{gu,I,J,K}(u_l,t)=\frac{\Phi^{\text{het}}_{gu,I,J,K}(u_l,t)}{\Phi^{\text{hom}}_{gu,I,J,K}(u_l,t)}\ ,\ f^{+}_{gu,I,J,K}(u_{l+1},t)=\frac{\Phi^{\text{het}}_{gu,I,J,K}(u_{l+1},t)}{\Phi^{\text{hom}}_{gu,I,J,K}(u_{l+1},t)}\ , \tag{4}$$

where $f^{-}_{gu,I,J,K}(u_l,t)$ and $f^{+}_{gu,I,J,K}(u_{l+1},t)$ are discontinuity factors in the u direction. In the NDF coarse module, a mesh-centered finite difference scheme is chosen and applied over coarse regions of the reactor allowing discontinuity of surface fluxes for all the nodes. Once more, the mesh centered finite difference scheme is the fastest to calculate because of its simple nature, having only one unknown per node per energy group. Also, the coupling terms are not dependent on fluxes or currents, and, therefore, do not require any further iteration. By using this scheme on the coarse mesh, the discontinuity factors are defined by:

$$f^{-}_{gu,I,J,K}(u_l,t)=\frac{\bar{\Phi}_{gu,I,J,K}(u_l,t)}{\bar{\Phi}_{gu,I,J,K}(t)+\frac{H^l_u}{2}\bar{D}^{-1}_{gu,I,J,K}\bar{J}_{gu,I,J,K}(u_l,t)}\ ,$$

$$f^{+}_{gu,I,J,K}(u_{l+1},t)=\frac{\bar{\Phi}_{gu,I,J,K}(u_{l+1},t)}{\bar{\Phi}_{gu,I,J,K}(t)-\frac{H^l_u}{2}\bar{D}^{-1}_{gu,I,J,K}\bar{J}_{gu,I,J,K}(u_{l+1},t)}\ , \tag{5}$$

where $\bar{\Phi}_{gu,I,J,K}(u_l,t)$ and $\bar{J}_{gu,I,J,K}(u_l,t)$ are the average nodal heterogeneous surface flux and current, and $\bar{\Phi}_{gu,I,J,K}(t)$ is the average nodal heterogeneous flux. Close examination of relationship (5) shows that the discontinuity factors depend only on the local spatial flux shape. Hence, we would expect that the discontinuity factors change slightly during mild transients. This would probably allow the use of constant discontinuity factors available from the initial criticality calculations. However, transients involving larger spatial flux changes (resulting perhaps, from control rod motions) are expected to require updating of the discontinuity factors. Also, it seems that updating discontinuity factors in the mesh-centered finite-difference method is of more importance than the other transverse-integrated nodal methods, since all information due to an important large spatial flux will be transferred to the coarse mesh level only by the average fluxes and surfaces. A potential advantage of the three level method is that one can adjust the time interval between the updating of the discontinuity factors by considering the nature of the transient, without introducing

any nonlinear iteration procedure. For transients involving small spatial flux changes, the time interval between two fine mesh calculations can be chosen very long, while for a transient involving more important spatial changes, the updating must be carried out more frequently.

4.3 Point kinetics module

The major difficulty in this step comes from the stiffness of the point reactor kinetics equations. Thus, the generalized Runge-Kutta (GRK4A) method of the Kaps-Rentrop family[13] is used. Since the point kinetics parameters $\rho(t)$, $\beta(t)$, $\Lambda(t)$, and $\beta_n(t)$ are time dependent and defined by weighted integrals of the flux and cross sections, these parameters must be updated at the end of each coarse mesh calculation. Since the number of coarse regions is small, these calculations are not time consuming. In this step the time dependent cross sections and time dependent flux represent the effects of perturbations to the core during the transient. Since the coarse shape function is assumed to be constant between two coarse mesh calculations, the point kinetics parameters are not exact, and result in a certain amount of error being introduced into the solution.

4.4 Boundary Condition Treatment

The usual treatment of boundary conditions for the large nodes on the exterior boundary of the core is simply to fill in the empty nodes with extra reflector materials. However, by applying equivalence theory, boundary condition on the outside surfaces of the large nodes can be determined. By applying these equivalent boundary conditions in NDF, coarse mesh static diffusion calculations reproduce the fine mesh solution extremely well.

4.5 Time integration method

Any type of spatial approximation leads to an initial value problem for a coupled system of ordinary differential equations:

$$\frac{d}{dt}\begin{bmatrix}\Phi\\ C\end{bmatrix}=\begin{bmatrix}H_{11} & H_{12}\\ H_{21} & H_{22}\end{bmatrix}\begin{bmatrix}\Phi\\ C\end{bmatrix}. \tag{6}$$

In order to manage stability and convergence of the time-dependent solution, the θ finite difference scheme is one of the most well-established procedures. Therefore a full implementation of the θ-method on both the fine and coarse levels is prepared. In the present version of the NDF, the values of θ can be different for flux and delayed neutron precursors, and are independent of space.

5. Code Validation

We present some validation results in both static and space-time kinetics calculations.

5.1 Static Calculations

As is expected, using the exact values of the equivalence parameters in the coarse mesh calculations leads to an almost perfect reproduction of the reactor eigenvalue and collapsed nodal average fluxes.

A typical example is illustrated in Figure 3. A CANDU-6 reactor is modelled in 3D Cartesian geometry with (26 x 26 x 12) fine nodes and three coarse mesh configurations: (3 x 3 x 2) coarse nodes, (5 x 5 x 2) coarse nodes, and (10 x 10 x 2) coarse nodes. The adjuster bank #1 (including the center rod and the 4 corner rods) is set into 11 different position from 0% to 100% of full insertion. For each bank position a full fine calculation is performed. Applying the equivalence theory, the reactor eigenvalue as well as the coarse flux distribution are calculated. Comparison between the results shows that the reactor eigenvalue and average fluxes are extremely well predicted. However the maximum average flux error for the case with a (10 x 10 x 2) coarse mesh is almost 3 times less than those from (3 x 3 x 2) coarse mesh.

Additional tests prove that using a set of reference values for the equivalence parameters causes relatively small errors in the reactor eigenvalue and average fluxes. In the following examples, the coarse mesh flux distributions are calculated using the reference values of the equivalence parameters. In the first example (Figure 4), the adjuster rod bank#1 is set to a reference position (100% of insertion), then a full fine calculations is performed and this flux distribution is used to calculate the reference equivalence parameters (diffusion coefficients, cross sections, and discontinuity factors). It can be observed that using these reference equivalence parameters for different positions of bank#1 results in an almost negligible error in k_{eff} and average fluxes.

In a typical CANDU-6 reactor, the liquid zone control system is designed to perform two main functions, first control of gross power output and second spatial control, i.e., the control of flux/power shape. This means that the zone control system is maintaining the desired global power level of the reactor by counteracting any power distortion or oscillation caused by a reactivity perturbation. In the next example (Figure 5), the effect of using "reference equivalence parameters" in static calculations for different levels of liquid zone controllers is studied. In this example all liquid zone controllers are set to a reference level. The fine flux distribution of the reference level is, then used to calculate the reference equivalence parameters (diffusion coefficients, cross sections, and discontinuity factors). It can be observed that using these reference equivalence parameters for different levels of liquid zone controllers results in small errors in k_{eff} and average fluxes.

5.2 Dynamic calculations[2]

A numerical scheme is stable if a small perturbation in boundary conditions or computer round-off errors do not lead to a significant changes in the solution. One way to study stability of a numerical scheme is to perform a *Do Nothing* transient. In this transient, the space and time integrators are initiated by a steady state solution. The solution advances in time with no perturbation. Evidently after many seconds no significant change in the solution must be observed. Figures(6) and (7) show the results of this kind of analysis. The coarse mesh discretisation consists of (5 x 5 x 4) nodes. Detailed studies demonstrate that much coarser nodes can lead to substantial errors in the

[2] All the transients are initiated by perturbing a steady-state situation. It is assumed in the moment that this perturbations occurs, the flux and precursors concentrations are at their steady-state values. These steady-state conditions are obtained from an initial static calculation. Since, obtaining the static eigenvalue equal to unity is unlikely, the fission cross section values in both the diffusion and precursor equations are divided by the initial static eigenvalue.

calculations. These errors are possibly due to classical iterative error in flux calculations which are amplified in homogenized cross sections in the large volume of the reactor.

In the next example (Figures 8 and 9), the response of Reactor Regulating System (RRS) to a very substantial perturbation is simulated. In the initial steady-state conditions all the reactivity devices are set to the nominal positions. In the beginning of the reactor power transition, the bank#1 (including the center rod and the 4 corner rods) is instantaneously extracted from the core. It can be observed that the RRS is reasonably able to maintain the reactor power level at its initial reference value. Also using exact values of homogenization parameters leads to almost perfect reproduction of average fluxes and dynamic reactivity.

6. Future work

In the transient calculations it is not practical to perform fine mesh calculations uniquely to update the equivalence parameters. To deal with this problem different solutions have been considered. The first is to establish an equivalence parameter database. All devices are initially set to a reference position (0% of insertion for control absorber rods, 100% of insertion for adjuster rods and 50% of full level for liquid zone controllers). Each device is then moved and set to a new position independently. Based on the resulting fine mesh calculation, all equivalence parameters are then calculated and saved in the database. This database will hopefully permit fewer fine mesh calculations on long transients such as those involving Xenon. Ongoing tests show that when many devices are present in the core, simple superposition or linear interpolation of the tabulated values of cross sections and discontinuity factors result in large errors. These errors are mostly due to device interference effects that are not considered in the database generation. Another proposed solution is to define the correction terms which are the differences between the exact values of the equivalence parameters at the end of the fine mesh calculation and those which are tabulated. These correction terms would then be added to tabulated values of the equivalence parameters during the next fine time step. Another method is to consider the variation of the dynamic reactivity calculated in the point kinetics level as a criterion for switching between different time hierarchies. Further examination is ongoing to choose the best way of dealing with device interference effects. In the near future, the NDF three-level driver will permit complicated transient calculations with interesting application in safety analysis to be perfomed. The results will be compared to those of classical improved quasi-static and direct fine mesh solutions obtained from NDF.

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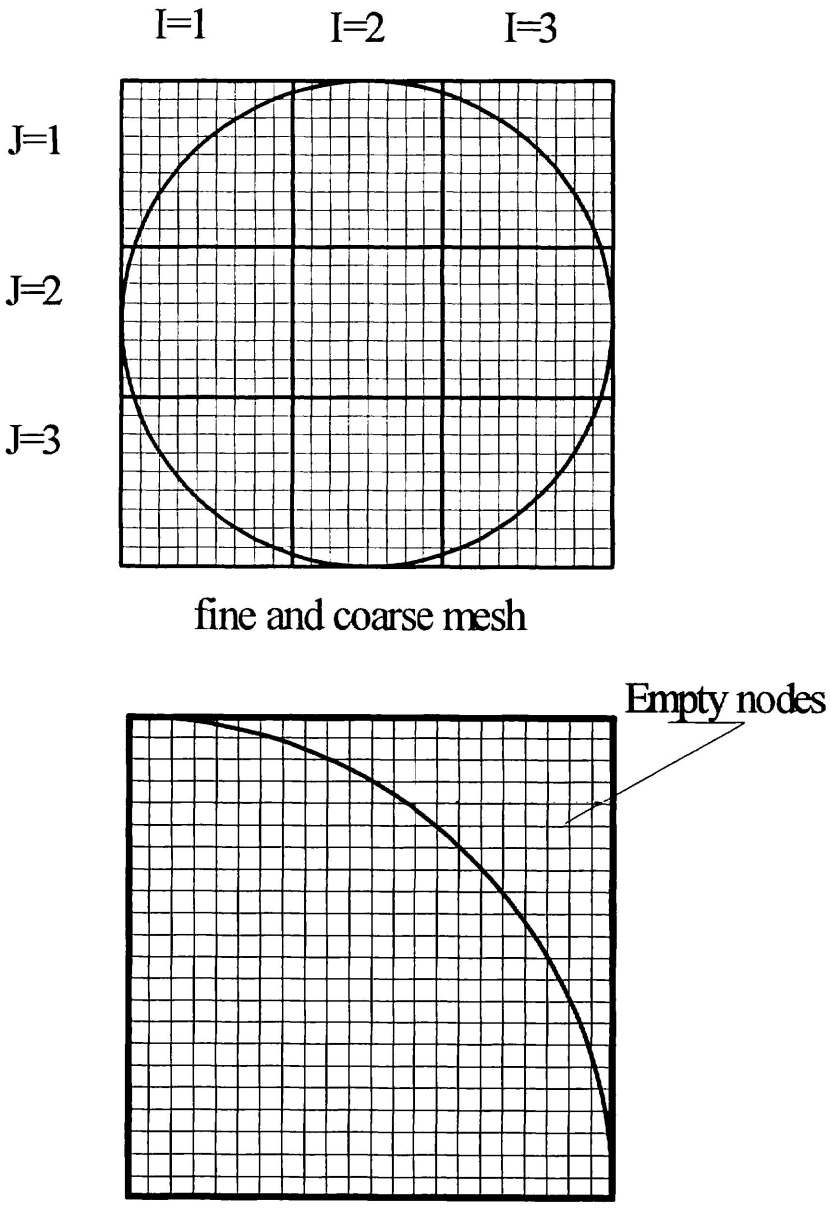

Figure 1: Fine and coarse representation of a CANDU reactor

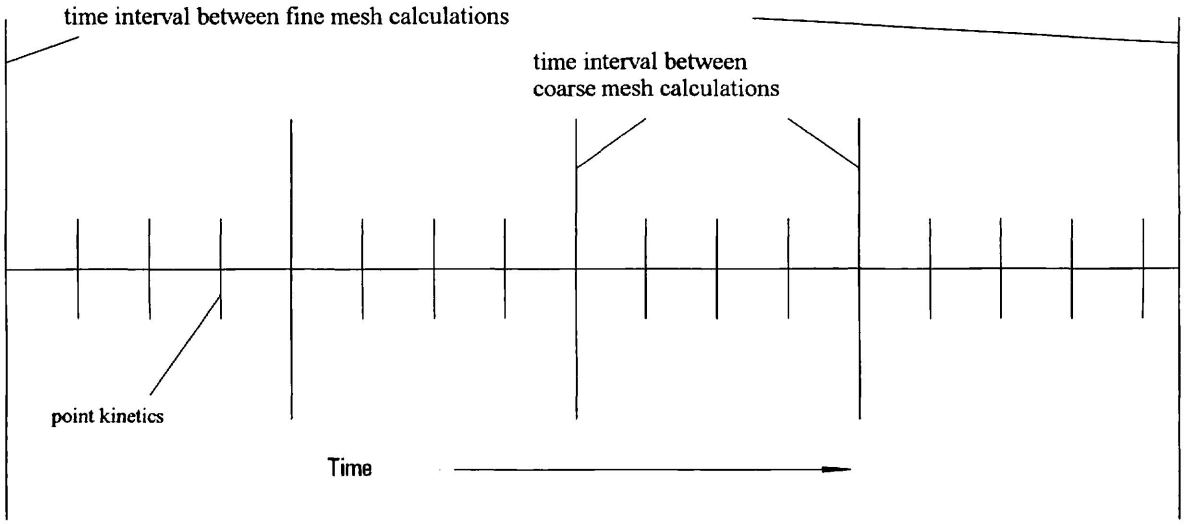

Figure 2: Three time step hierarchy

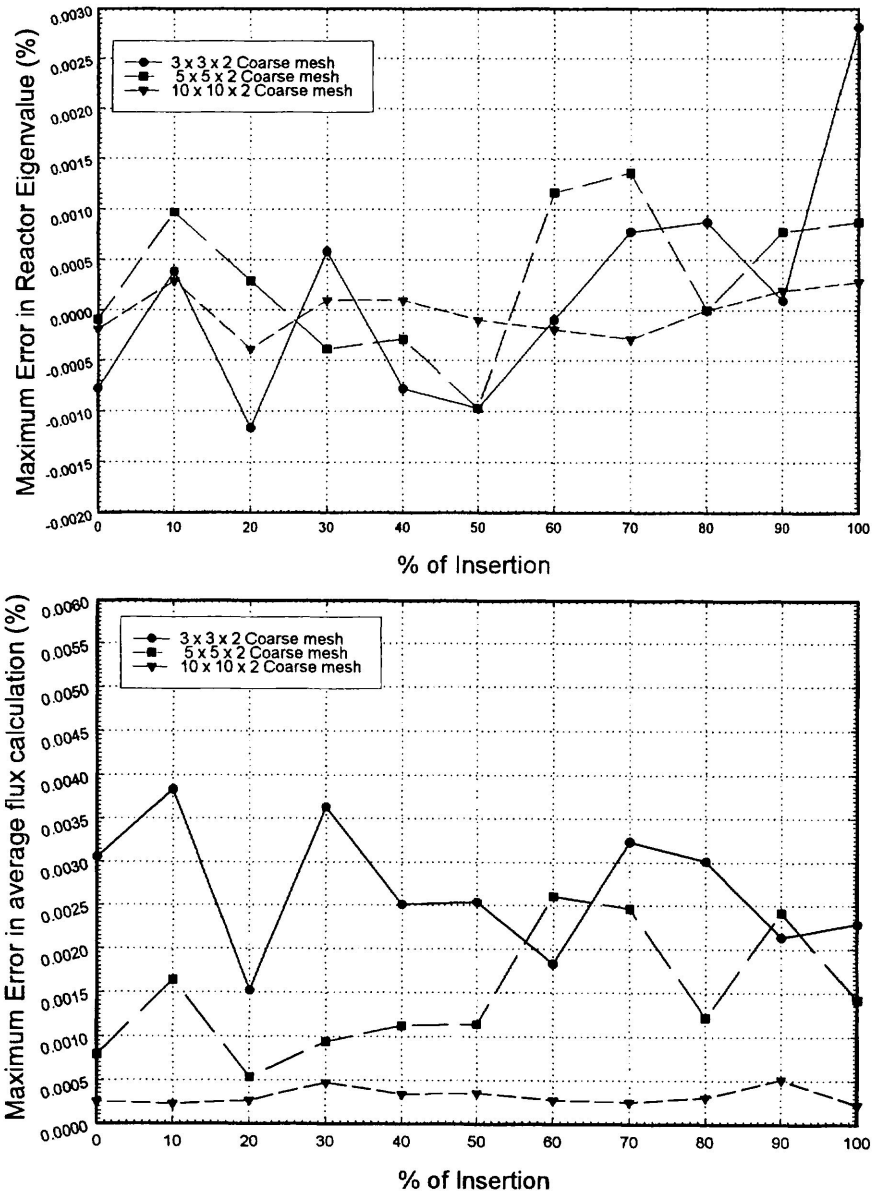

Figure 3: Static calculations using exact values of the equivalence parameters

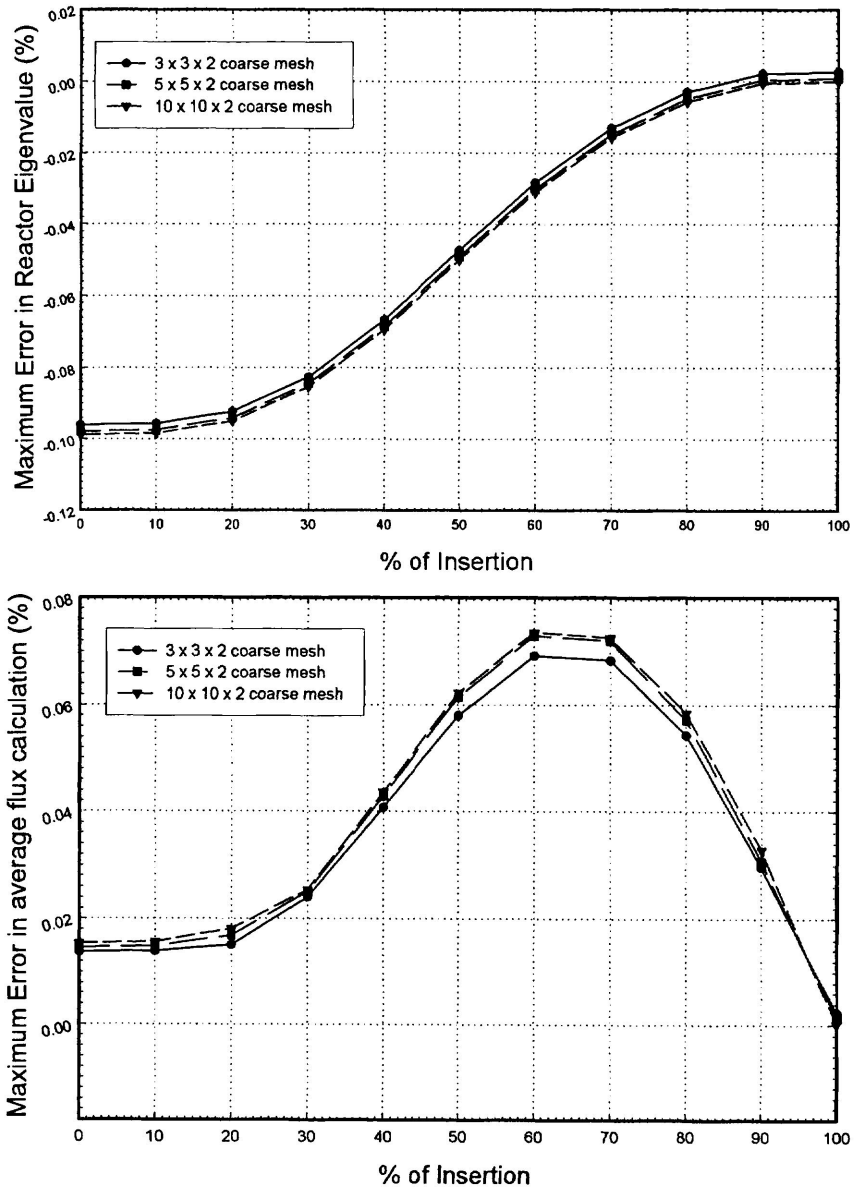

Figure 4: Static calculations using reference equivalence parameters(Adjuster Bank #1)

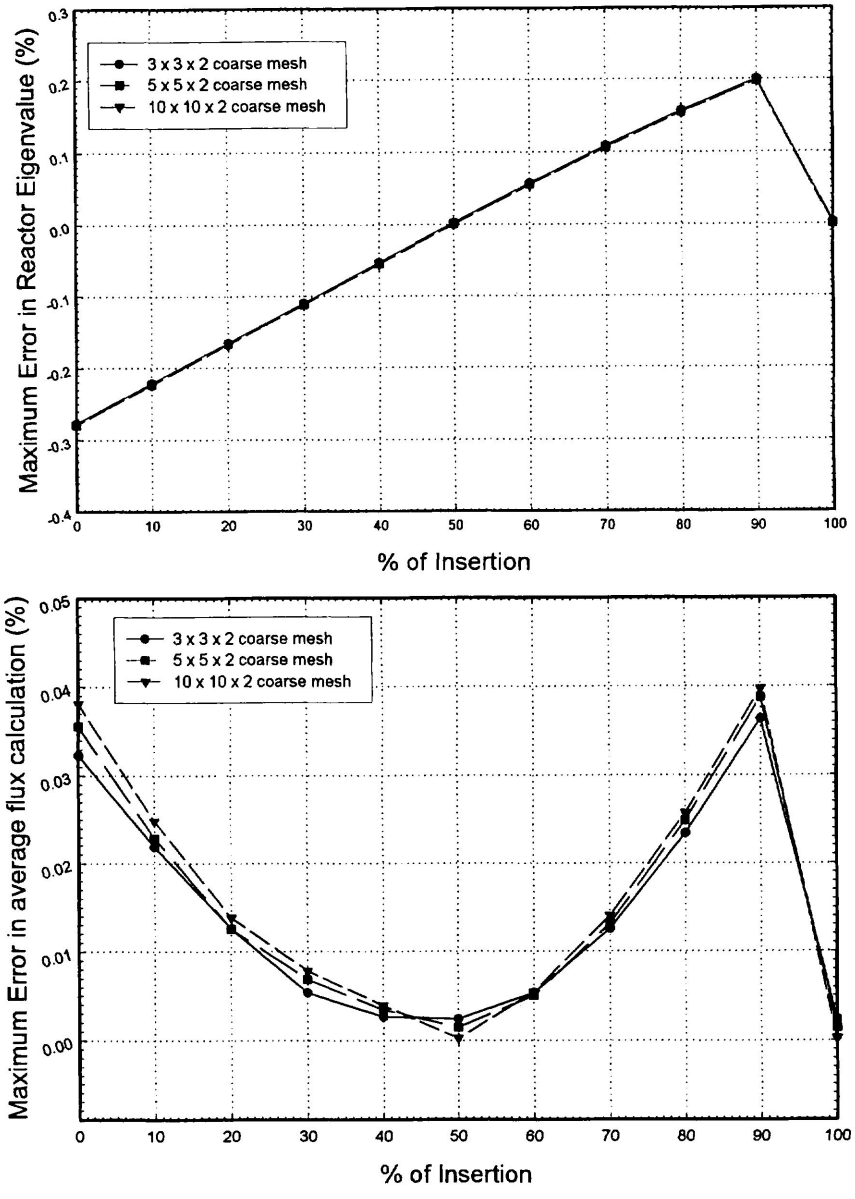

Figure 5: Static calculations using reference equivalence parameters (Liquid Zone Controllers)

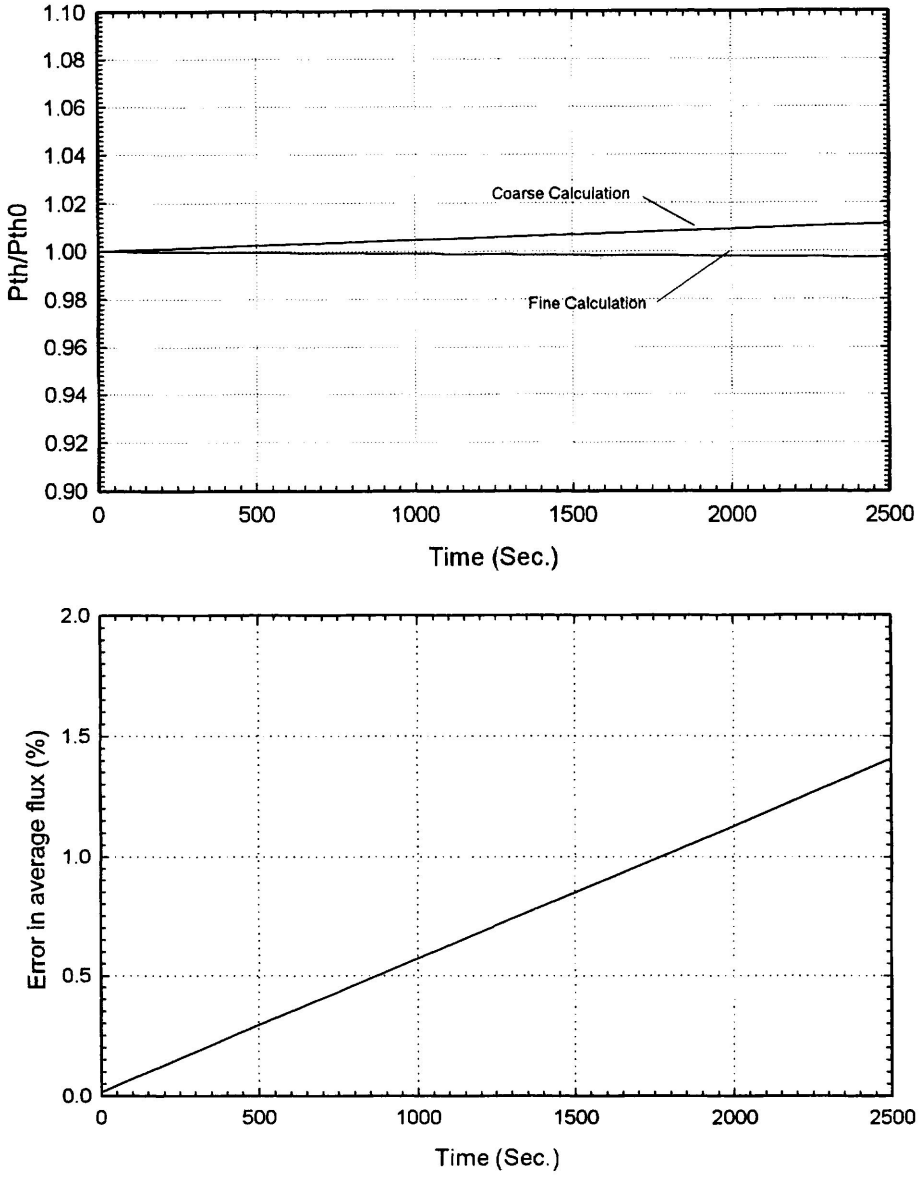

Figure 6: Do Nothing transient without SSR

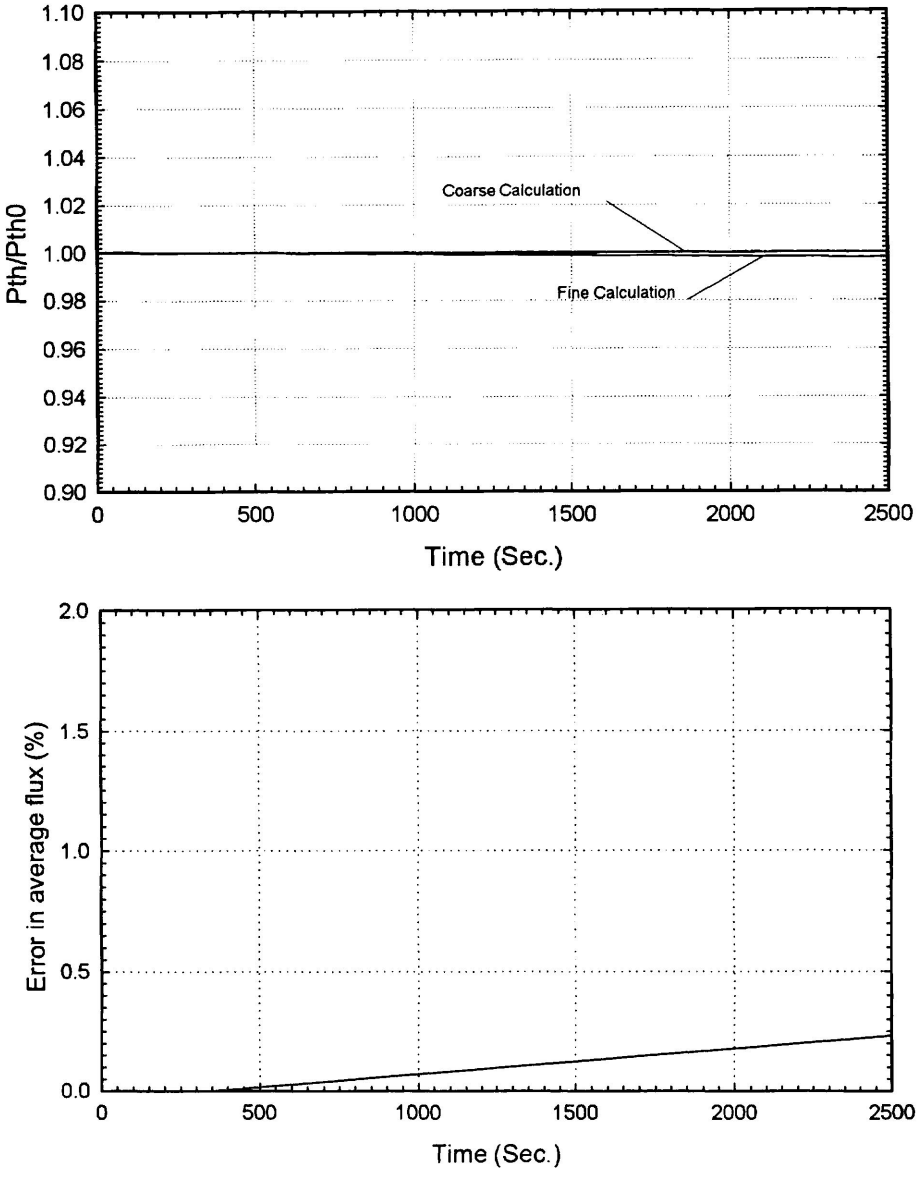

Figure 7: Do Nothing transient with SRR

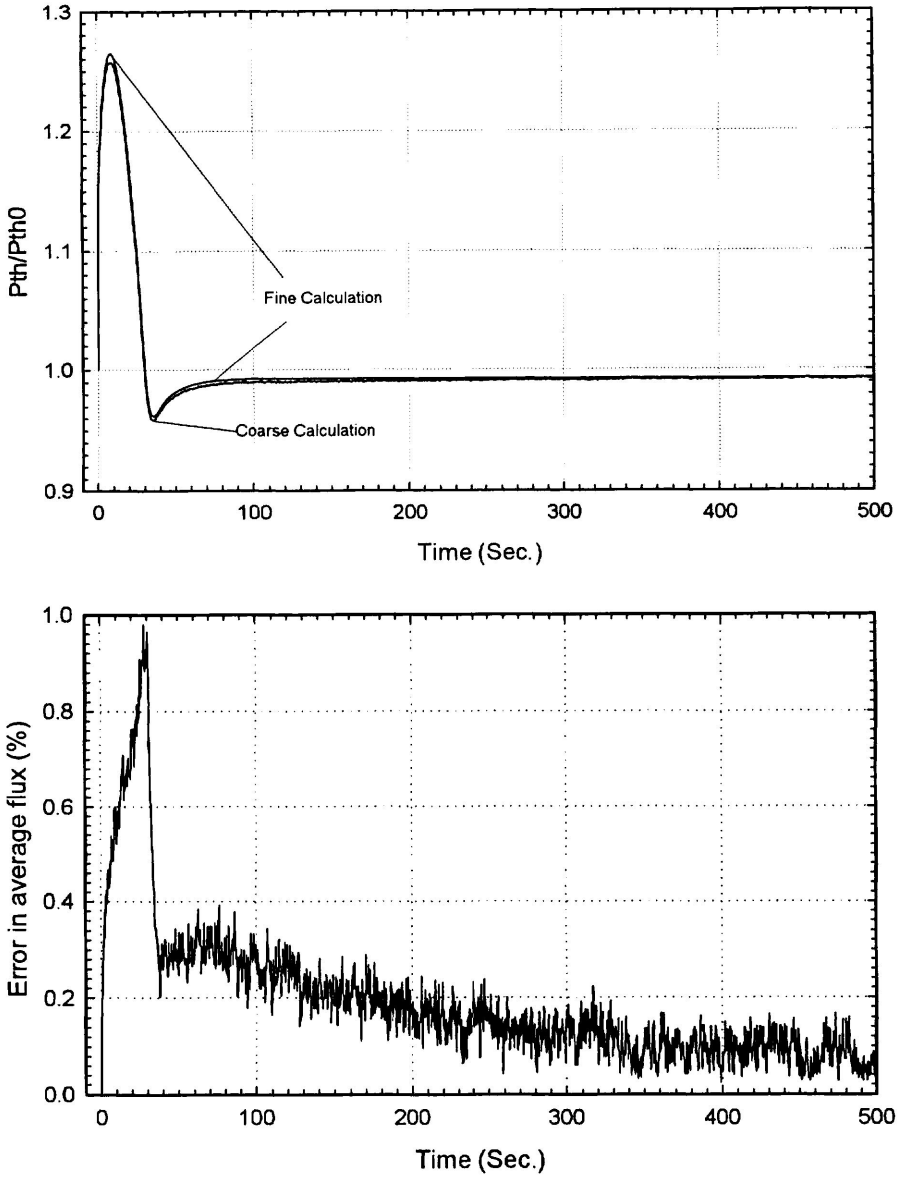

Figure 8: Dynamic calculations using exact values of equivalence parameters

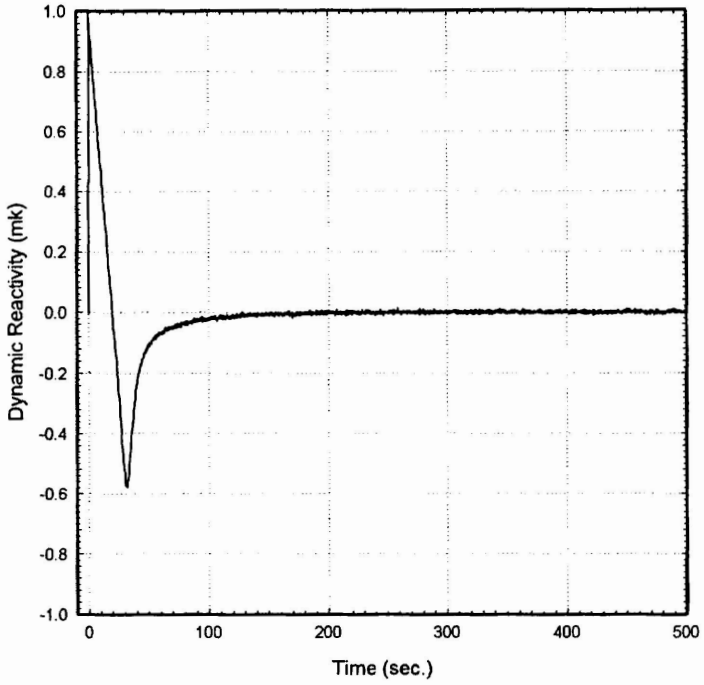

Figure 9: Dynamic reactivity (fine and coarse calculations)