PHYSOR 2002, Seoul, Korea, October 7-10, 2002

REACTIVITY ESTIMATION FOR SOURCE-DRIVEN SYSTEMS USING FIRST-ORDER PERTURBATION THEORY

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ABSTRACT

Applicability of the first-order perturbation (FOP) theory method to reactivity estimation for source-driven systems is examined in this paper. First, the formally exact point kinetics equations have been derived from the space-dependent kinetics equations and the kinetics parameters including the dynamic reactivity have been defined. For the dynamic reactivity, exact and first-order perturbation theory expressions for the reactivity change have been formulated for source-driven systems. It has been also shown that the external source perturbation itself does not change the reactivity if the initial λ-mode adjoint flux is used as the weight function. Using two source-driven benchmark problems, the reactivity change has been estimated with the FOP theory method for various perturbations. By comparing the resulting reactivity changes with the exact dynamic reactivity changes determined from the space-dependent kinetics solutions, it has been shown that the accuracy of the FOP theory method for the accelerator-driven system (ADS) is reasonably good and comparable to that for the critical reactors. The adiabatic assumption has also been shown to be a good approximation for the ADS kinetics analyses.

I. INTRODUCTION

Accelerator-driven systems are currently being proposed for the transmutation of nuclear wastes.[1] The determination of the safety characteristics of ADSs would require the application of system analysis codes such as SAS4A/SASSYS[2]. These codes typically use the point kinetics approximation for solving the neutron kinetics equations. In addition, the point kinetics analyses are often utilized for the scoping evaluation of the source-driven systems. An issue that arises in the point kinetics approach is the need to provide appropriate reactivity coefficients that are typically derived from first-order perturbation (FOP) theory.

In the conventional source-free reactor systems, two concepts of reactivities are used. These are the static and dynamic reactivities. The static reactivity indicates the off-criticality of a physical state, i.e., a distance from the critical state. On the other hand, the dynamic reactivity is related to an actual transient, thus it is a time-dependent quantity. In a similar way, both static and dynamic reactivities could be consistently defined for the source-driven system, as discussed in Ref. 3.

The concept of reactivity is required only in lumped parameter models such as the point kinetics equations. In a point kinetics model for a source-free system, the dynamic reactivity is the primary driving function that determines the system response during a transient. On the other hand, the

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dynamic response of a source-driven system is governed by both the associated dynamic reactivity and the external source. The neutronic behavior of a subcritical core is usually rather sensitive to the source characteristics such as energy spectrum, spatial distribution, etc. Previously, concerning the reactivity of source-driven systems, Gandini[4] proposed a special concept of reactivity, the so-called generalized reactivity, which incorporates both the conventional dynamic reactivity and the external source. However, the suitability of a dynamic reactivity definition generally depends on its consistency.[3] Thus, the conventional definition of the dynamic reactivity is utilized in this paper.

The objective of this paper is to address the validity of the FOP theory for predicting the change of the dynamic reactivity in the source-driven system. In Section II, a consistent reactivity expression is derived for the exact point kinetics equations and the perturbation theory expressions for the reactivity are presented in Section III. Section IV contains the numerical test results for benchmark problems. Lastly, conclusions and future works are provided in Section V.

II. POINT KINETICS EQUATIONS FOR SOURCE-DRIVEN SYSTEMS

For a source-driven system with an independent source S, the space-energy-dependent dynamics equations for the neutron flux Φ and delayed neutron precursors C_k can be written in an operator form [3] as

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} = (F_p - M)\Phi + \sum_k \chi_{dk}\lambda_k C_k + S, \tag{1a}$$

$$\frac{\partial C_k}{\partial t} = -\lambda_k C_k + \int_E F_{dk}\Phi dE, \tag{1b}$$

where v is the neutron velocity, F_p is the prompt fission source operator, F_{dk} are the delayed fission source operators, M is the neutron migration and loss operator, λ_k is the decay constant for the *k*-th group delayed neutron precursors, and χ_{dk} is the emission spectrum of the *k*-th delayed neutron group. The flux can be factorized without any approximation into an amplitude function $p(t)$ and a space-, energy-, and time-dependent shape function $\Psi(r,E,t)$ such that

$$\Phi(r,E,t) = p(t)\cdot\Psi(r,E,t), \tag{2}$$

with a constraint on the shape function

$$\iint \frac{1}{v} w(r,E)\Psi(r,E,t)\,dE\,dV = K_0, \tag{3}$$

where w is a weighting function and K_0 is a constant.

The formally exact point kinetics equations can consistently be derived by inserting the flux factorization into Eq. (1) and integrating over space and energy with a weighting function. In this model, a dynamic reactivity is defined in terms of the weighting function and time-dependent shape function. The weighting function should be chosen such that the reactivity is insensitive to errors in the shape function.[3] For an initially critical reactor, the initial adjoint flux fulfils this requirement. However, for a subcritical reactor with an independent source, the adjoint function is not uniquely defined, and thus the reactivity can be defined in various ways, depending on the weighting function. Typically, the λ–mode adjoint function of the initial state has been used as the weighting function, since it leads to a formulation that eliminates the first-order flux errors. The λ–mode adjoint function of the initial state $\Phi^*_{\lambda_0}$ can be obtained by solving the following adjoint equation

$$(M_0^* - \lambda_0 F_0^*)\Phi_{\lambda_0}^* = 0, \tag{4}$$

where F^* and M^* are the adjoint operators of F (= $F_p + \sum_k F_{dk}$) and M, respectively, and subscript 0 means the initial state.

Inserting the factorization in Eq. (2) into Eq. (1), integrating over space and energy with the weighting function $\Phi_{\lambda_0}^*$, and dividing the resulting expression by

$$F_\lambda(t) = (\Phi_{\lambda_0}, F\Psi), \tag{5}$$

the point kinetics equations for an initially subcritical system can be obtained as:

$$\frac{dp}{dt} = \frac{\rho(t) - \beta(t)}{\Lambda(t)} p(t) + \frac{1}{\Lambda_0} \sum_k \lambda_k \zeta_k(t) + \frac{s(t)}{\Lambda(t)}, \tag{6a}$$

$$\frac{d\zeta}{dt} = -\lambda_k \zeta_k(t) + \frac{F_\lambda(t)}{F_{\lambda 0}} \beta_k(t) p(t), \tag{6b}$$

where

$$\rho(t) = (\Phi_{\lambda_0}^*, [F - M]\Psi) / F_\lambda(t), \tag{6c}$$

$$\zeta_k(t) = (\Phi_{\lambda_0}^*, \chi_{dk} C_k) / F_{\lambda 0}, \tag{6d}$$

$$s(t) = (\Phi_{\lambda_0}^*, S) / F_\lambda(t). \tag{6e}$$

and the other notations are standard.[3] In Eq. (6), the precursors and independent source are represented in the "reduced" form rather than in simple adjoint-weighted integrals employed in more conventional point kinetics equations. These reduced quantities represent the relative values of these integrals to the adjoint-weighted quasi-stationary fission source, and provide a simpler and more direct physical interpretation than the conventional ones.

The reactivity defined in Eq. (6c) is called "dynamic reactivity," and it is formed with the time-dependent flux as it physically appears during a transient. It is noteworthy that the dynamic reactivity at $t = 0$ is numerically equal to the static reactivity of the initial stationary state:

$$\rho(0) = 1 - \lambda_0 = 1 - 1/k_{eff}^0 = \rho_0. \tag{7}$$

This is because the dynamic reactivity is defined in the same form as the static one and the initial source-free λ–mode adjoint function is used as the weighting function.

III. PERTURBATION THEORY EXPRESSIONS OF REACTIVITY

The parameters of the exact point kinetics equations can be determined only when the exact solution of the space-energy-dependent problem is known. Thus, some approximations need to be introduced to derive a practical point reactor model. For the practical estimation of reactivity changes, perturbation theory expressions are generally employed. In this section, the exact perturbation theory (EPT) expression is first derived from the dynamic reactivity defined in Eq. (6c). Then, the FOP reactivity expression is approximately obtained from the exact one. The EPT expression based on the adiabatic approximation is also derived for comparison purposes.

The formally exact perturbation formula for the difference between the dynamic reactivity ρ (t) and the initial static reactivity ρ_0 can be expressed by the differences of the operators in the following form:[3]

$$\delta\rho^{EPT} = \rho(t) - \rho_0 = \frac{(\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\Psi)}{(\Phi^*_{\lambda_0}, F\,\Psi)}. \tag{8}$$

where $\Delta F = F - F_0$ and $\Delta M = M - M_0$. This is due to the property of the initial λ–mode adjoint function employed as weight function, and can be easily verified as:

$$\begin{aligned}(\Phi^*_{\lambda_0}, F\Psi)[\rho(t) - \rho_0] &= (\Phi^*_{\lambda_0}, [(1-\rho_0)F - M]\Psi) = (\Phi^*_{\lambda_0}, [\lambda_0 F - M]\Psi) \\ &= (\Phi^*_{\lambda_0}, [(\lambda_0 F - M) - (\lambda_0 F_0 - M_0)]\Psi) = (\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\Psi)\end{aligned} \tag{9}$$

The exact perturbation formula of Eq. (8) shows that the reactivity is changed only when the operators are perturbed. In other words, if the flux is perturbed by some means without changing the core properties, the reactivity is not changed by this flux perturbation. For example, the external source perturbation does not change the reactivity even though it results in a flux perturbation. As mentioned above, in the point kinetics equations derived using the initial λ–mode adjoint flux as the weighting function, the external source change is directly accounted for through the reduced source term. The space and energy dependent effects of the source perturbation are accounted for by the same adjoint weighting function. If a source change occurs in a low-importance phase space (in terms of space and energy), the resulting change of the reduced source would be small. On the other hand, any source change in a high-importance regime would incur significant change in the reduced source.

Representing the time dependent flux in Eq. (8) as $\Psi = \Psi_0 + \Delta\Psi$, where Ψ_0 is the initial flux satisfying the inhomogeneous equation

$$(F_0 - M_0)\Psi_0 = -S_0, \tag{10}$$

the exact perturbation expression of Eq. (8) can be reduced to

$$\delta\rho^{EPT} \cong \frac{(\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\Psi_0) + (\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\Delta\Psi)}{(\Phi^*_{\lambda_0}, F\,\Psi_0)} \left\{ 1 - \frac{(\Phi^*_{\lambda_0}, F\,\Delta\Psi)}{(\Phi^*_{\lambda_0}, F\,\Psi_0)} \right\} \tag{11}$$

If we neglect the second and higher order terms, the FOP expression for the reactivity change is obtained in the form,

$$\delta\rho^{FOP} = \frac{(\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\Psi_0)}{(\Phi^*_{\lambda_0}, F\,\Psi_0)}, \tag{12}$$

Note that Eq. (12) is very similar to the source-free FOP expression for the static reactivity change, except that F_0, instead of F, is used in the latter case.

Eqs. (8) and (12) clearly demonstrate the advantage of using the initial λ–mode adjoint function as a weighting function. If a different weighting function is used, the EPT formula cannot be represented by simple differences of the operators, and hence the simple second-order accurate FOP expression of Eq. (12) cannot be obtained. It is also important to note that if we represent the time dependent flux shape by a perturbation of initial λ–mode flux as:

$$\Psi = \Psi_{\lambda 0} + \Delta\Psi_\lambda, \tag{13}$$

then $(\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\Delta\Psi)$ of Eq. (11) becomes $(\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\Delta\Psi_\lambda)$, and might not be second order any more. Since $\Delta\Psi_\lambda$ represents the deviation of the source-driven flux shape from the fundamental eigenmode, it is not zero at the initial state and might be comparable to either Ψ_0 or $\Psi_{\lambda 0}$. Therefore, $(\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\Delta\Psi_\lambda)$ cannot be neglected in general without compromising the accuracy of the FOP expression.

The flux shape in a source-driven system is predominantly governed by the external source when the system is not close to being critical. Rydin and Woosley[5] have shown that when the ADS is sufficiently subcritical, the effects of delayed neutrons on the system dynamics are negligibly small. This suggests that the adiabatic assumption[3,6] could be a good approximation in a source-driven system. In the adiabatic approximation, the time-dependent flux shape can be determined by the stationary equation

$$(F - M)\varphi = -S\,, \tag{14}$$

Inserting this flux shape into Eqs. (6c) and (8), the adiabatic dynamic reactivity and the corresponding EPT expression for reactivity change are obtained as

$$\tilde{\rho} = \frac{(\Phi^*_{\lambda_0}, [F - M]\varphi)}{(\Phi^*_{\lambda_0}, F\,\varphi)}, \tag{15}$$

$$\delta\tilde{\rho}^{EPT} = \frac{(\Phi^*_{\lambda_0}, [\lambda_0 \Delta F - \Delta M]\varphi)}{(\Phi^*_{\lambda_0}, F\,\varphi)}, \tag{16}$$

IV. NUMERICAL TESTS AND DISCUSSION

Applicability of the FOP expression for reactivity change was tested against two source-driven problems, which were obtained by modifying the TWIGL and SNR-300 benchmark problems[7]. Figures 1 and 2 respectively show the schematic configurations of modified TWIGL and SNR-300 benchmark problems. The original TWIGL problem was modified by introducing a fixed source of strength 1.75812×10^6 n/cm^3 (over all energy groups) in the region 1 and by adjusting the fission cross sections such that k_{eff} = 0.95. The modified SNR-300 problem was obtained by replacing the central three fuel rings with a non-fuel material (control rod follower in the problem) and by adjusting the fission cross sections of the inner and outer cores uniformly such that k_{eff} = 0.98. A distributed external source with a total strength of 5.5267×10^6 n/sec was introduced in the assemblies in the first and second rings in such a way that the relative source densities in the first and second rings be 0.7 and 0.3, respectively. The source spectrum vector in 4-group structure was assumed to be (0.9, 0.1, 0.0, 0.0), which is harder than the specified fission spectrum vector of (0.768, 0.232, 0.0, 0.0).

Two types of perturbations were introduced in the TWIGL problem: first the thermal capture cross section in region 2 was reduced by about 5% (Case T1), and the ν value in region 2 was additionally increased by 0.85% in the second case (Case T2). For the SNR-300 problem, three cross section perturbations were considered. The fission cross sections were first increased by 1% in the inner zone (Case S1), and the capture cross sections of the control rod region were additionally decreased by 8% in the second case (Case S2). In the third case (Case S3), in order to introduce the flux shape

distortion from the initial shape as well as bigger reactivity change, the reduction of capture cross sections in Case S2 was increased to 14% from 8%.

The accuracy of the FOP theory method was first tested for cases T1, S2, and S3 by comparing the FOP theory reactivity with the exact dynamic reactivity determined from the space-energy-dependent kinetics solution. The space-energy-dependent solutions were obtained using the implicit time-differencing option of the DIF3D-K[8] nodal kinetics code. The adiabatic and FOP theory reactivities were also computed using the space-time factorization options of DIF3D-K and were compared with the exact dynamic reactivity. The cross section perturbations were introduced at a constant rate over a time period of 0.2 second. The resulting time-dependent dynamic and FOP theory reactivities are compared in Fig. 3, and their values at 0.5 second are compared in Table I. Note that the initial dynamic reactivity is exactly the same as the conventional static reactivity. These results clearly show that the adiabatic dynamic reactivities are essentially the same as the exact dynamic reactivities. This implies that the adiabatic assumption is an excellent approximation even for the case S3 whose final reactivity is equivalent to $k_{eff} = 0.993$. The results also show that the FOP theory method consistently underpredicts the reactivity change. However, the estimation errors are only 3.5%, 1.2%, and 2.6% for the cases T1, S2, and S3, respectively. Taking into account the magnitude of the reactivity change, it can be said that the FOP theory method for these perturbations in the source-driven systems is reasonably accurate.

The FOP theory reactivity changes were also estimated for all the cross section perturbations using the finite difference diffusion theory method. Based on the above results of the adiabatic approximation, however, the accuracy of the FOP theory method was tested by comparing the FOP theory reactivity and the adiabatic dynamic reactivity. The real and adjoint fluxes calculations were performed using the finite difference diffusion theory option of the DIF3D code[9]. The resulting adiabatic dynamic reactivities and the FOP theory reactivities are compared in Table II. By comparing the results of Tables I and II, it can be seen that the initial reactivities estimated with the finite difference method deviate from the values determined with the nodal method by 0.2% and 11.6% for the TWIGL and SNR-300 problem, respectively. These differences are due to the mesh error of the finite difference method; the SNR-300 problem shows a larger deviation since only six triangular meshes were used per each hexagonal node, whereas a much finer Cartesian mesh was used in the TWIGL problem. Due to the mesh error, the adiabatic reactivity changes of the cases T1, S2, and S3 are also mispredicted by 0.9%, 2.3%, and 2.6%, respectively. These errors can be removed by refining the computational meshes in the finite difference calculations, but it was not attempted since both the adiabatic dynamic and FOP theory reactivities were consistently calculated using the same mesh structure.

The results in Table II show that the EPT expression estimated with the flux shape at the final perturbed state reproduces the reactivity changes exactly. The FOP theory method underpredicts the reactivity change by about 3.8% in Case T1 and by 4.5% in Case T2. For the SNR-300 problem, the prediction errors of the FOP theory method are even smaller; the error is only 2.8% even for the Case S3 which involves the largest reactivity change (0.0145). These results indicate that the FOP theory expression based on the initial flux of the external source problem is reasonably accurate. However, it is noteworthy that the reactivity changes are consistently underpredicted by the FOP theory method.

The effects of the flux shape function on the FOP theory reactivity were further investigated by applying the initial and final fluxes of the source-free eigenvalue problem to the FOP theory expression of the reactivity change. As shown in Table III, the initial and final flux shapes of the source-free problem result in 7.6% and 9.9% errors, respectively, which are much larger than the errors obtained with the initial flux of the external source problem. On the other hand, they predict the exact reactivity change in the source-free system (0.00935) accurately; the final flux shape reproduces it exactly, and the initial flux shape underpredicts it by 2.1%. These results confirm that the flux shape

used in the perturbation theory expressions should be determined with the consistent neutron balance equation.

V. CONCLUSIONS AND FUTURE WORKS

The applicability of first-order perturbation (FOP) theory to reactivity estimation for source-driven systems was examined. Using the initial λ-mode adjoint flux as the weight function, the formally exact point kinetics equations were derived from the space- and energy-dependent neutron kinetics equations and the kinetics parameters including the dynamic reactivity were defined. Exact and first order perturbation theory expressions for the reactivity change were formulated for source-driven systems. It was shown that the use of the initial λ-mode adjoint flux as the weight function results in simple perturbation expressions similar to those for critical reactors. It was also shown that the external source perturbation itself does not change the reactivity in these formulations.

Using two source-driven problems obtained by modifying the TWIGL and SNR-300 benchmark problems, the prediction accuracy of the FOP theory method for reactivity changes was estimated for various perturbations. The reactivity changes predicted by the FOP method were compared with exact dynamic reactivity changes determined by space-dependent kinetics solutions. The adiabatic dynamic reactivity was also computed and was compared with the exact dynamic reactivity. Numerical results showed that the adiabatic assumption is a good approximation for the ADS dynamics analyses and the accuracy of the FOP theory method for the ADS is reasonably good (less than 5% error for all test cases) and comparable to that for critical reactors.

The flux shape used in the perturbation theory expressions should be determined with the consistent neutron balance equation. In other words, the initial flux shape used in the FOP theory expression for the reactivity change should be determined from the external source problem. It was also found that FOP theory consistently underpredicts the reactivity change. However, it is not clear whether this is an intrinsic property of the subcritical system or an accidental coincidence of the limited set of test problems. It requires further investigation.

In this study, rather simple standard benchmarks for the conventional source-free systems were modified to simulate source-driven systems. In order to make more definite conclusions, further studies need to be performed using more realistic perturbations in source-driven systems.

REFERENCES

1. A Roadmap for Developing Accelerator Transmutation of Waste (ATW) Technology – A Report to Congress," DOE/RW-0519, October (1999).
2. "The SAS4A LMFBR Accident Analysis Code System," ANL/RAS 83-38 Revision 2, February (1988).
3. K. O. Ott and R. J. Neuhold, *Introductory Nuclear Reactor Dynamics*, American Nuclear Society, La Grange Park, Illinois (1985).
4. A. Gandini, "HGPT Based Sensitivity Time-Dependent Methods for the Analysis of Subcritical Systems," Annals of Nuclear Energy, **28**, 1193 (2001).
5. R. A. Rydin and M. L. Woosley, "Evidence of Source Dominance in the Dynamic Behavior of Accelerator-Driven System," Nuclear Science and Engineering, **126**, 341 (1997).
6. D. L. Hetrick, Dynamics of Nuclear Reactor, The University of Chicago Press, Chicago, Illinois, (1971).
7. Argonne Code Center: Benchmark Problem Book, ANL-7416, Supplement 2 (1977).

8. T. A. Taiwo and H. S. Khalil, "An Improved Quasistatic Option for the DIF3D Nodal Kinetics Code," Proceedings of the Topical Meeting on Advances in Reactor Physics, Charleston, South Carolina, p. 2-469, March 1992.
9. K. L. Derstine, "DIF3D: A Code to Solve One-, Two, and Three-Dimensional Finite Difference Diffusion Theory Problems," ANL-82-64, Argonne National Laboratory, April (1984).

Table I. Reactivity Changes Predicted by Spatial Kinetics and FOP Theory Methods

Case		T1	S2	S3
Initial reactivity		-0.05249	-0.02232	-0.02232
Reactivity change	Implicit spatial kinetics	0.00857	0.01024	0.01484
	Adiabatic spatial kinetics	0.00859	0.01024	0.01485
	FOP theory method	0.00827	0.01012	0.01445

Table II. Comparison of Adiabatic Dynamic Reactivity and FOP Theory Reactivity

Case	Adiabatic Dynamic Reactivity		Exact $\delta\rho$	FOP $\delta\rho$
T1	Initial	-0.0526	0.0085	0.0082
	Final	-0.0441		
T2	Initial	-0.0526	0.0133	0.0127
	Final	-0.0393		
S1	Initial	-0.0197	0.0043	0.0043
	Final	-0.0154		
S2	Initial	-0.0197	0.0100	0.0099
	Final	-0.0097		
S3	Initial	-0.0197	0.0145	0.0141
	Final	-0.0053		

Table III. FOP Theory Reactivity Changes of Case T1 Estimated with Source-Free Problem Fluxes

Flux Shape	$\delta\rho$
Initial unperturbed flux shape of source-free eigenvalue problem	0.0092
Final perturbed flux shape of source-free eigenvalue problem	0.0094

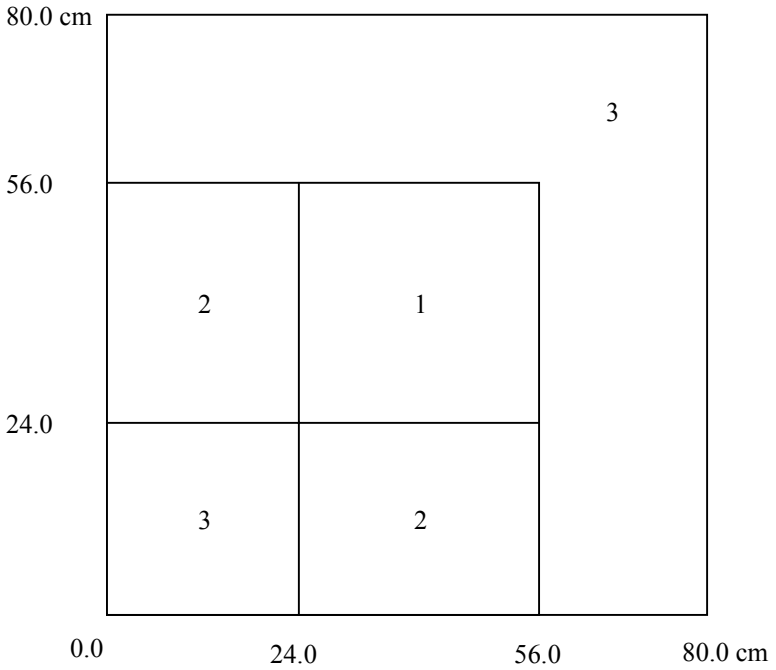

Fig. 1. Quadrant Core of the Modified TWIGL External-Source Problem

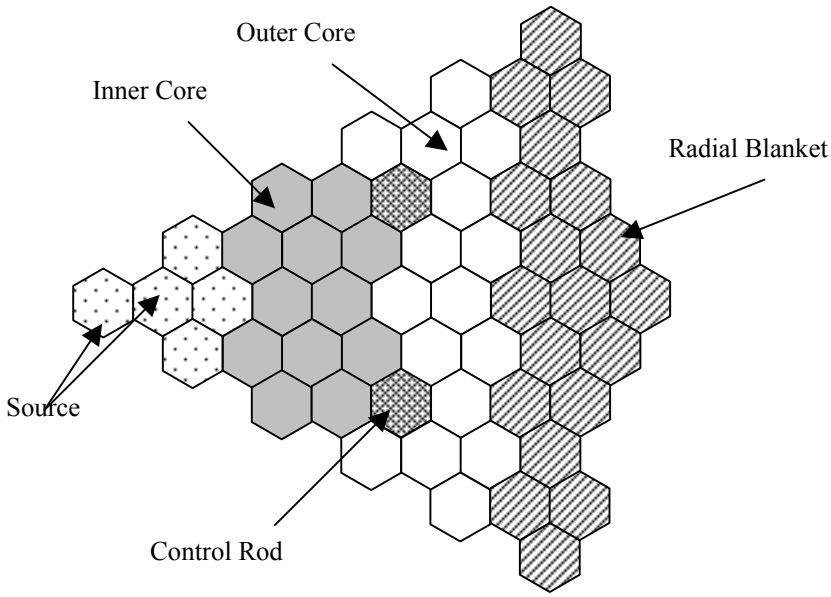

Fig. 2. Schematic Configuration of the Modified SNR300 Benchmark Problem (Sixth Core)

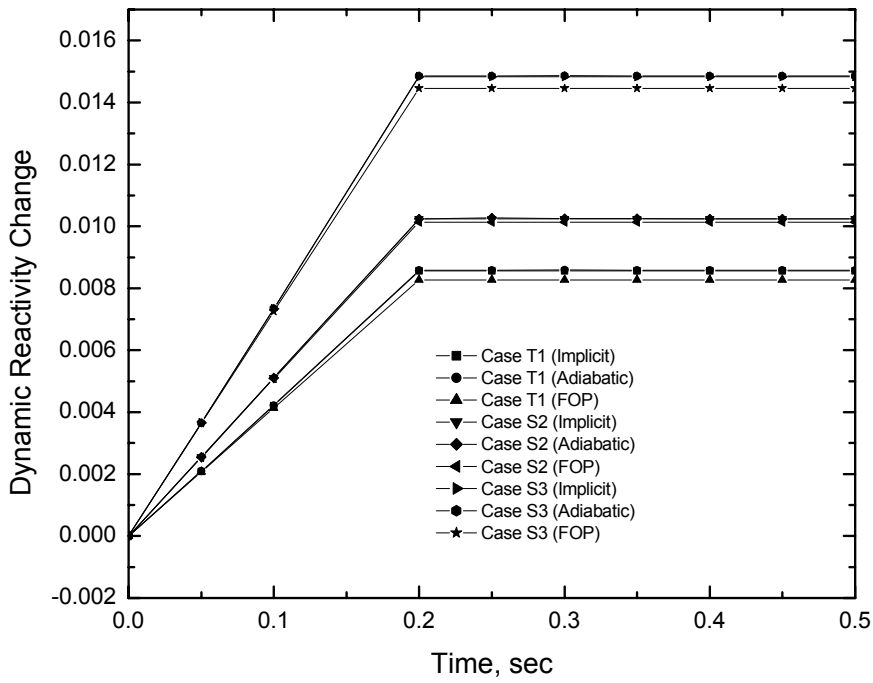

Fig. 3. Comparison of Time-Dependent Reactivity Changes

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