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Time-Step Selection Considerations in the Analysis of Reactor Transients with DIF3D-K*

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INTRODUCTION

The DIF3D-K[1-2] code solves the three-dimensional, time-dependent multigroup neutron diffusion equations by using a nodal approach for spatial discretization and either the theta method or one of three space-time factorization approaches for temporal integration of the nodal equations. The three space-time factorization options (namely, improved quasistatic, adiabatic and conventional point kinetics) were implemented because of their potential efficiency advantage for the analysis of transients in which the flux shape changes more slowly than its amplitude. Here we describe the implementation of DIF3D-K as the neutronics module within the SAS-HWR accident analysis code. We also describe the neutronics-related time-step selection algorithms and their influence on the accuracy and efficiency of the various solution options.

IMPLEMENTATION OF THE SPATIAL KINETICS OPTIONS

For the purpose of interfacing with the SAS-HWR code, a time period called a "time domain" is defined in the DIF3D-K module to correspond to the main thermal-hydraulics (T-H) time step in the SAS-HWR code. It is at the end of this time period that information is passed between the DIF3D-K module and other T-H and material distribution modules of the SAS-HWR code. At the beginning of a main time step, SAS-HWR extrapolates the reactor power across the time-step and performs T-H and material relocation calculations using the extrapolated power. The code then computes cross sections at the end of the time step using pre-determined correlations with respect to independent state variables. The DIF3D-K module assumes a linear depen-

dence for the cross sections within a main time step; this dependence is determined using the end-of-time step values for the current and preceding time steps. Within each time domain (or main step), smaller (theta solution) time-steps are used with the theta scheme for time integration. In the space-time factorization options, three nested time-step intervals are defined. In decreasing order of time-step size, they are the shape interval, the reactivity interval, and the point kinetics solution interval.

The DIF3D-K module internally adjusts these time intervals based on a set of user-specified criteria. For the theta option, the adjustment constrains the time step size (Δt) such that

$$\Delta t = \frac{(\omega \Delta t)_{max}}{|\omega^k_{max}|} \tag{1}$$

where $(\omega \Delta t)_{max}$ is a user specified value, and $|\omega^k_{max}|$ is the maximum value over all nodes k of the transient fission source inverse period. The shape interval for the factorization options (which can be larger than a time domain) is selected based on an input maximum allowable shape change, a maximum allowable number of reactivity steps per shape interval, the requirement that the interval size be less than ten times the previous size, and limitations on the maximum projected shape change over the interval. A shape interval is also terminated at the end of an imbedded reactivity interval if the amplitude function changes by an amount greater than a user-specified criterion. New kinetics parameters (reactivity, beta effective and prompt neutron lifetime) are computed at the end of a reactivity interval, using a shape vector obtained from a linear combination of the two preceding shape vectors. The shape extrapolation scheme can optionally be disabled, in which case the shape and reactivity steps are the same.

The size of a reactivity interval within a shape interval is determined at the end of the preceding interval based on an input maximum allowable reactivity-interval size, the requirement that the interval size be less than twice the previous size, and the requirement that the projected amplitude change over the reactivity interval be less than a user-specified criterion. Across each point kinetics step within a reactivity interval, the point kinetics equations are solved with the modified Kaganove scheme[3] which employs an automated time-step halving and doubling algo-

rithm to compute the time-step size needed to achieve a user-specified precision.

NUMERICAL EXPERIENCE

Effectiveness of Time Step Selection Approach

We have observed that the theta-solution, shape, reactivity and point kinetics time-step adjustment schemes are adequate, and that the default values of the associated user-specified parameters are conservative for most problems. Numerical test cases also indicated that the accuracy and efficiency of the code is strongly dependent on the main time-step size used for coupling the neutronics and T-H calculations. Presently, this size is prescribed by the user and it is determined by a parametric study of the transient. However, it appears that relatively simple algorithms for automatic main time-step adjustment can be developed. One possibility is to automatically reduce the main time step when the number of shape calculations (or theta solution steps) in the previous main time step exceeds a certain number. The selection of the main time-step size can also be tied to the rate of change of material properties and T-H conditions.

Efficiency and Accuracy of Space-time Factorization Options

Results from test problems confirmed that the conventional point kinetics and adiabatic approaches can severely mispredict a transient, and that the improved quasistatic scheme produces very accurate solutions. Sample results for a HWR transient (without feedback) are shown in Table 1. As expected, substantial savings in computational time were achieved with the factorization options for problems involving minor shape changes. The savings in computing time achievable with the improved quasistatic scheme was found to depend on the accuracy relative to the reference (fully implicit) theta solution. The ratio of the computation time for the fully implicit scheme to that for the improved quasistatic scheme appears to decrease as the allowable error in the predicted core power increases.[2] This suggests that the fully implicit method becomes more competitive as the accuracy requirement is relaxed.

In transients involving very significant distortion of the flux shape, and for which there is a strong coupling between neutronics and T-H, the improved quasistatic approach has been found

not to be necessarily more efficient than the fully implicit solution approach. In such a situation the improved quasistatic approach may require more computation time than the fully implicit approach, primarily because of the added calculations needed to evaluate the kinetics parameters and the code logic for solving the amplitude and shape equations on different time scales. This may be true for other time integration schemes which are made efficient by taking large time-step sizes, but also require extensive computation at each solution time point.

REFERENCES

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2. 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.

3. J. J. Kaganove, "Numerical Solution of the One-Group Space-Independent Reactor Kinetics Equations for Neutron Density Given Excess Reactivity," ANL-6132, Argonne National Laboratory (1960).

Table 1. Results for a Super-Prompt-Critical Transient Case Without Feedback

Time (s)	Reference Reactivity[a]	CORE POWER			
		Theta[a]	Improved Quasistatic[b]	Point Kinetics	Adiabatic[b]
0.00	0.00000	1.0000	1.0000	1.0000	1.0000
0.10	0.00908	1.8251	1.8256	1.4801	1.8793
0.20	0.01177	8.9447	8.9558	2.3334	9.8805
0.30	0.01428	60.295	60.615	3.1238	70.024
0.40	0.01715	801.63	810.56	4.0502	999.39
0.50	0.01726	16669.	16981.	5.0256	21918.
No. of shape calcs.		-	78	-	78
No. of time steps		11076	85	9	84
Computation time, s[c]		3616	177	23	288

[a]Reference solution computed with (fully implicit) theta option employing $(\omega\Delta t)_{max} = 10^{-3}$. A description of this transient is presented in Reference 2.

[b]Shape recalculation based on 10% maximum shape change (default value).

[c]On the ANL Cray X-MP/18 computer.

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