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SPQR: A Monte Carlo Reactor Kinetics Code

S. N. Cramer
H. L. Dodds

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SPQR: A Monte Carlo Reactor Kinetics Code

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Date Published - February 1980

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ACKNOWLEDGMENTS

The authors would like to express their appreciation to T. J. Hoffman for his contributions to the Monte Carlo development of the code, and to W. W. Engle, Jr. for obtaining the TDA results.

ABSTRACT

The SPQR Monte Carlo code has been developed to analyze fast reactor core accident problems where conventional methods are considered inadequate. The code is based on the adiabatic approximation of the quasi-static method. This initial version contains no automatic material motion or feedback. An existing Monte Carlo code is used to calculate the shape functions and the integral quantities needed in the kinetics module. Several sample problems have been devised and analyzed. Due to the large statistical uncertainty associated with the calculation of reactivity in accident simulations, the results, especially at later times, differ greatly from deterministic methods. It was also found that in large uncoupled systems, the Monte Carlo method has difficulty in handling asymmetric perturbations.

I. INTRODUCTION

The scenarios of most hypothetical core disruptive accidents (HCDA) lead ultimately to material motion due to the high temperatures and pressures generated. The analysis of these accidents by one- and two-dimensional deterministic methods usually becomes questionable during and after core disassembly because of geometric complexities. The Monte Carlo method is the only calculational technique capable of handling general three-dimensional geometries, and it is for this reason that the SPQR* code has been developed. This code utilizes the quasi-static model in its adiabatic form as the method of solution. The shape function and integral quantities such as reactivity, generation time, etc., are generated by the Monte Carlo portion of the code for use in the kinetics module.

At present there is no automatic feedback in the code. Material motion must be simulated by a series of geometry descriptions or by cross-section changes in specific parts of the reactor system. Several sample problems devised to test SPQR are given in the Appendix. These problems are all one-dimensional, and the critical adjoint solutions necessary for the quasi-static model were obtained from discrete ordinate codes. These one-dimensional problems, with no feedback, were devised to test the feasibility of using Monte Carlo methods in time-dependent supercritical calculations. It was found that a statistical uncertainty of several percent in the calculation of the integral parameters, particularly the reactivity, could produce an uncertainty of several orders of magnitude in the power density for times of less than one second after the accident begins.

II. QUASI-STATIC MODEL

The quasi-static method is well known and well documented. For use in SPQR the development from the transport equation given by Bell and Glasstone¹ is followed. Using the notation of this reference, the flux is divided into a purely time-dependent amplitude and a shape function

*Stochastic Program for Quasi-Static Research

which is slowly varying in time. The amplitude is calculated on a fine time mesh, whereas the shape is calculated much less frequently over a broader time scale.

$$\phi(\bar{r}, \bar{\Omega}, E, t) = P(t)\psi(\bar{r}, \bar{\Omega}, E, t) \quad (1)$$

The use of this definition with the time-dependent forward transport equation and the adjoint steady-state (critical) equation leads to the familiar kinetics equations.

$$\frac{dP(t)}{dt} = \left[\frac{\rho(t) - \beta(t)}{\Lambda(t)} \right] P(t) + \sum_i \lambda_i C_i(t) \quad (2)$$

$$\frac{dC_i(t)}{dt} = \frac{\beta_i(t)}{\Lambda(t)} P(t) - \lambda_i C_i(t) \quad (3)$$

The shape function equation is:

$$\frac{1}{v} \left[\frac{d\psi}{dt} + \frac{1}{P(t)} \frac{dP}{dt} \psi \right] + \Omega \cdot \nabla \psi + \Sigma_T \psi = S \quad (4)$$

where S, the source term in the ordinary transport equation, includes an inscatter integral and all fission sources (prompt and delayed).

The derivation of the preceding equations is subject to the following constraint for all times.

$$\left\langle \frac{\phi_o^* \psi}{v} \right\rangle = C, \text{ constant} \quad (5)$$

where ϕ_o^* is the steady-state adjoint flux. The parameters in the kinetics equations are defined by the following integrals:

$$\rho(t) = \frac{\left\langle \frac{\phi_o^* \Delta \Sigma \psi}{v} \right\rangle}{\left\langle \frac{\phi_o^* v \Sigma_f \psi}{v} \right\rangle} \quad (6)$$

$$\Lambda(t) = \frac{\left\langle \frac{\phi_o^* \psi}{v} \right\rangle}{\left\langle \frac{\phi_o^* v \Sigma_f \psi}{v} \right\rangle} \quad (7)$$

If the delayed neutron spectra χ_1 are different from the prompt spectrum, χ_p , there will be an additional integral, $\beta_1(t)$, as shown in reference 1. The $\Delta\Sigma$ in Eq. (6) represents the perturbation (cross section changes) from the initial state at time zero, t_0 , to the conditions at time t .

$$\Delta\Sigma = -[\Sigma_T(\bar{r}, \bar{E}, t) - \Sigma_T(\bar{r}, \bar{E}, t_0)] + \int d\bar{E}' [\Sigma_s(\bar{r}, \bar{E}' \rightarrow \bar{E}, t) - \Sigma_s(\bar{r}, \bar{E}' \rightarrow \bar{E}, t_0)] + \chi(E) \int d\bar{E}' [v \Sigma_f(\bar{r}, \bar{E}', t) - v \Sigma_f(\bar{r}, \bar{E}', t_0)] \quad (8)$$

If the system is not critical at t_0 , the second term in the fission integral must be divided by the unperturbed k_{eff} . In the adiabatic approximation of the quasi-static method, the bracketed term in Eq. (4) is ignored, and the prompt and delayed fission terms are combined. The shape equation now is identical to the static transport equation with ψ replacing the flux term. It is this equation that is solved by Monte Carlo at time t , similar to an ordinary k_{eff} calculation, each time an updated shape calculation is needed in the overall time sequence. The integral quantities in Eqs. (5) through (8) are determined simultaneously with the new shape, and the constraint in Eq. (5) is met by a simple normalization procedure after each shape calculation.

The ψ term in the bracket in Eq. (4) can be easily included in the shape calculation by combining it with Σ_T . The amplitude and its derivative at time t are determined from Eqs. (2) and (3). The Monte Carlo calculation then proceeds with a modified total cross section.

$$\Sigma_T' = \Sigma_T + \frac{1}{vP(t)} \frac{dP}{dt} \quad (9)$$

However, the effect of this extra term is usually so small as to be completely masked by the statistical uncertainty of the calculation. If the shape derivative term, $d\psi/dt$, were included, Eq. (4) would have the appearance of the time-dependent transport equation. This is, of course, the original equation for which it was determined that some approximation, such as the quasi-static method, was necessary. Analogous Monte Carlo techniques do exist for treating time-dependent multiplying systems, but to include the effects of delayed neutrons, if necessary, would be virtually impossible. For perturbations below prompt-critical,

delayed neutrons are so important in effect but so insignificant in number, as compared to prompt fission neutrons, that ordinary time-dependent Monte Carlo analysis would be totally unreliable. Time-dependent Monte Carlo calculations of multiplying systems near critical represent an order of magnitude increase in running time over static k_{eff} calculations, and there is no convenient way to interrupt the procedure, as with the quasi-static method, to include any feedback mechanisms.

A procedure sometimes used in deterministic codes is to represent the shape derivative as a difference term

$$\frac{d\psi}{dt} \approx \frac{\psi(t) - \psi(t - \Delta t)}{\Delta t} \quad (10)$$

where Δt is the time interval corresponding to a previous shape calculation. When Eq. (10) is substituted into Eq. (4), the resulting static transport-like equation has a further cross-section modification, the addition of $1/(v \Delta t)$ to Eq. (9), and a non-fission source term, $\psi(t - \Delta t)/(v \Delta t)$. This extra source term creates two such formidable difficulties that attempts to include Eq. (10) in the development of SPQR were discarded. First, the correct normalization of fixed and fission sources in a static Monte Carlo calculation of a multiplying system near critical is uncertain in concept, without consideration of the statistical uncertainty. Second, the constraint condition in Eq. (5) can no longer be met by a simple normalization procedure, and an iterative approach such as that used in deterministic codes is necessary.² The combination of increased calculation time and statistical uncertainty in an iterative procedure of this kind prohibits its use.

III. OUTLINE OF THE CODE

The SPQR code is basically the combination of a point kinetics code and a general Monte Carlo code. The MORSE³ multigroup code has been modified to include a fourth-order Runge-Kutta point kinetics module. Other special routines have been written to handle the adjoint information and to compute the integrals in Eqs. (5) through (7). Most of the special routines are problem-oriented and must be altered or rewritten for

different problems, which is a standard practice for general Monte Carlo codes. The procedure begins with a Monte Carlo calculation to determine the initial (usually critical) shape and integral parameters of the unperturbed system at time t_0 . The input data for this calculation is the same as that given in the MORSE manual. If the initial shape and integral parameters are known, the first shape calculation could be delayed for some time Δt into perturbation after a point kinetics solution over Δt .

A brief discription of the new or altered routines will now be presented.

SOURCE

This routine must describe all variables for the initialization of the first shape calculation. It is assumed that each succeeding shape calculation will use the preceeding distribution as a starting point.

BANKR

This is the standard MORSE routine which interfaces the random walk and analysis portions of the code. If the collision density estimator is utilized for the shape calculation, RELCOL is called from the standard location. For any other type estimator, RELCOL would be called as indicated in the comment cards. Subroutine FGAMF is called before the first batch of the first shape calculation and after the last batch of all shape calculations. Depending on the method of normalization for the constraint, Eq. (5), subroutine RESNT, is called either after every batch or only after the last batch of each shape calculation.

RELCOL

From this routine, all others needed in the calculation of the integral parameters are called.

READX

This routine reads in the steady-state adjoint fluxes and associated data and also the delayed neutron fractions, BET. For the adjoint data the following definitions are given corresponding to a DOT^4 calculation.

NG = number of energy groups
NA = number of angles
NR = number of radial intervals
NZ = number of axial intervals
PHE (NA, NR, NZ, NG) = adjoint flux
GAM (NA) = polar angle
BETA (NA) = azimuthal angle
DELSA (NA) = quadrature weight
RR (NR) = radial intervals
ZR (NZ) = axial intervals

GETRZ

This routine relates the random walk collision position to the adjoint flux spatial mesh.

DIFSP

This routine (problem-dependent) determines if the random walk collision occurs in a perturbed region of phase space. If not, the $\Delta\Sigma$ in Eq. (6) will be zero. However, the other integral parameters must still be calculated.

TRANF

This routine transfers the direction cosine of the particle history, both before (I=2) and after collision (I=1), to the coordinate system of the adjoint calculation. It is assumed that fission neutrons are produced with isotropic distributions.

GETUVW

The routine determines the adjoint flux direction, $-\Omega_1$, corresponding to the random walk direction, Ω_0 . The smallest dot product specifies the angle; $\mu = -\Omega_0 \cdot \Omega_i$ $i=1, \dots, NA$. This is done for pre-collision (I=2), post-collision (I=1), and for a fissionable material (I=3).

ESIM

This routine evaluates Eqs. (5) through (8). The adjoint fluxes are obtained from subroutine GETFLU. Although this is a problem-oriented routine depending on the perturbations involved, the following contributions to the integrals will be necessary.

$$C = \frac{WTBC \phi_0^*(\bar{r}, IGO, \bar{\Omega}_2)}{v(IGO) \Sigma_T(\bar{r}, IGO, t)} \quad (11)$$

$$\begin{aligned} \rho = & \frac{1}{D} \left\{ -WTBC \left[1 - \frac{\Sigma_T(\bar{r}, IGO, t_0)}{\Sigma_T(\bar{r}, IGO, t)} \right] \phi_0^*(\bar{r}, IGO, \bar{\Omega}_2) \right. \\ & + WATE \left[1 - \frac{\Sigma_s(\bar{r}, IG, t_0)}{\Sigma_s(\bar{r}, IG, t)} \frac{f(IGO \rightarrow IG, \mu, t_0)}{f(IGO \rightarrow IG, \mu, t)} \right] \phi_0^*(\bar{r}, IG, \bar{\Omega}_1) \\ & \left. + WTBC \left[\frac{v\Sigma_f(\bar{r}, IGO, t)}{\Sigma_T(\bar{r}, IGO, t)} - \frac{v\Sigma_f(\bar{r}, IGO, t_0)}{\Sigma_T(\bar{r}, IGO, t_0)} \right] \phi_0^*(\bar{r}, IGF, \bar{\Omega}_3) \right\} \quad (12) \end{aligned}$$

$$D = WTBC \frac{v\Sigma_f(\bar{r}, IGO, t)}{\Sigma_T(\bar{r}, IGO, t)} \phi_0^*(\bar{r}, IGF, \bar{\Omega}_3) \quad (13)$$

The contribution to $\Lambda(t)$ is C/D from Eqs. (11) and (13). Since the integral parameter in Eqs. (2) and (3) appears only as ratios, Eq. (13) is not needed. However, to relate $\rho(t)$ and $\Lambda(t)$ to the reactivity and generation time, the denominator in Eqs. (6) and (7) is necessary. In Eqs. (11) through (13) WTBC and WATE are the pre- and post-collision random walk statistical weights. The IGO and IG are the corresponding pre- and post-collision energy groups, and IGF is a group picked from the critical adjoint fission spectrum (see subroutines GETFG and GETFLU). The adjoint directions are those determined in GETUVW. In the cross sections $\bar{\sigma}$ corresponds to the medium of the collision site and in the adjoint fluxes $\bar{\phi}$ corresponds to the spatial intervals from GETRZ. The cosine of the random walk scattering angle is μ .

The cross section ratios in the above equations could be obtained using the standard MORSE routines NSIGTA and FISGEN. The scattering functions could be determined through the use of PTHETA, such as in the standard MORSE RELCOL routine for next-flight estimation.

GETFLU

This routine determines the value of the adjoint flux for use in ESTM according to the angle index from GETUVW, the spatial intervals from GETRZ, and the random walk energy group. The energy group structure is inverted in compliance with the forward-adjoint energy relation. The calling parameter is II=1 for post-collision energy flux, II=2 for pre-collision energy flux, and II=3 for post-fission energy flux.

GETFG

The energy for the fission flux term in GETFLU is determined in this routine.

FGAMF

This routine, called from BANKR, is the link between the Monte Carlo shape calculation and the point kinetics module. It is user written and its form depends on the calculation in question. FGAMF should be first called preceding the first batch of the first shape

function calculation to perform any necessary initialization tasks. It should then be called following the last batch of each shape calculation. Here the coupling to the kinetics module and the preparation for the next shape calculation is made. All perturbation and feedback effects which might alter the cross sections or geometry are included in this routine. Depending on the situation, the necessary problem-oriented programming could become extensive.

RESNT

This routine renormalizes the shape calculation to satisfy the constraint condition in Eq. (5). The normalization could be performed after each batch or only after each shape calculation is complete. All just-completed calculations must be adjusted, as well as the source and weight standards (Russian roulette data, etc.) for the next calculation.

MORSE

This routine has been modified to allow the fission distribution of the last batch of the last shape calculation to be used as the source of the first batch of the next shape calculation. This is done with ITSTR in subroutine MSOUR.

NRUN

This routine, together with its calling routine BANKR, has been written to calculate the statistical uncertainty on all calculated quantities resulting from unequally weighted batches.

PKT

This is the point kinetics routine called by FGAMF. All necessary parameters including the decay constants must be transferred to PKT. The amplitude function in Eq. (1) is calculated over a time interval selected to correspond to the integral parameters determined in the shape calculation. The initial amplitude is set to unity and the initial precursor densities are determined with the left side of Eq. (3) set to zero. Each succeeding calculation uses the final values of the preceding calculation as a starting point. This routine, with its

calling routine FGAMF, can be programmed to calculate the amplitude for a future time interval in addition to the current one. This would be done using integral parameters determined from the current shape based upon a projected perturbation (first-order perturbation). Some procedure such as this would be necessary in order to determine the extra term in Eq. (9). If it were shown that this term was of significance but incorrectly predicted, iteration might be necessary. In the call to POINT, L and BETA are the decay and group constants, TU and TL are the shape time interval limits, and DT is the interval used in POINT. The derivative in Eq. (9) is given by DER.

POINT

This routine solves Eqs. (2) and (3) based on a fourth-order Runge-Kutta approximation. There are several print options in this routine which must be controlled depending on the time intervals involved.

IV. SAMPLE PROBLEMS

The first tests of the SPQR code were based on some one-dimensional, two-group sample problems devised by Yasinsky and Henry.⁵ The system investigated is a 30-cm core with a 15-cm blanket region on each side. One delayed-neutron group with $\beta = 0.0064$ was used. All necessary data are given in reference 5. The first perturbation was a step increase of the fission cross sections in one blanket region of 20.6%, followed by a linear decrease of these cross sections to 78.5% of its original value at 10 msec. A second perturbation consisted of a linear increase of the same cross sections to 121.1% of their original value at 10 msec.

Some SPQR time dependent results for these perturbations are given in Figs. 1-4, and they are compared with TDA (time-dependent AINSN) calculations. The spatial dependent comparisons (SPQR and TDA) for the second perturbation are similar in shape, but they differ in magnitude by the amount indicated in the time-dependent fluxes. The SPQR calculations excluded the shape derivative term Eq. (4) but they included the addition amplitude term, Eq. (9). The disagreement in the time 0^+ flux

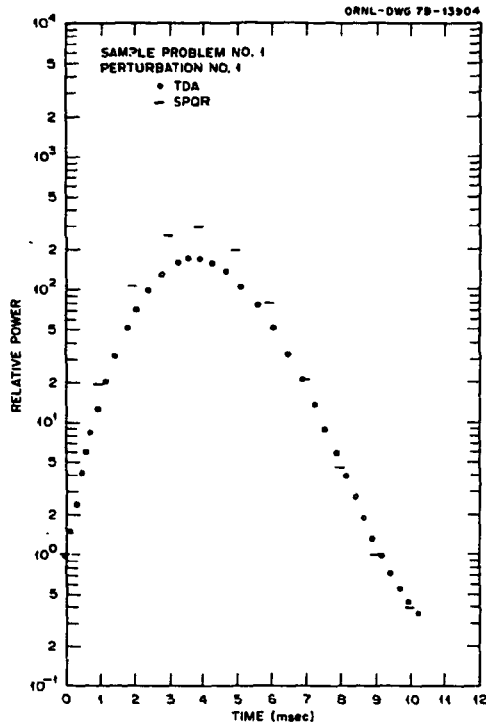


Fig. 1. Power Distribution for Sample Problem No. 1, Perturbation No. 1.

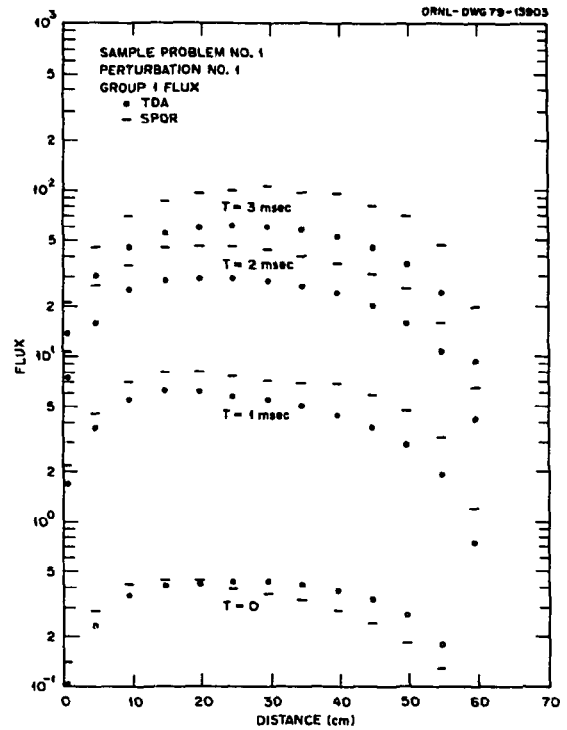


Fig. 2. Flux distributions for Sample Problem No. 1, Perturbation No. 1, Up to Three msec.

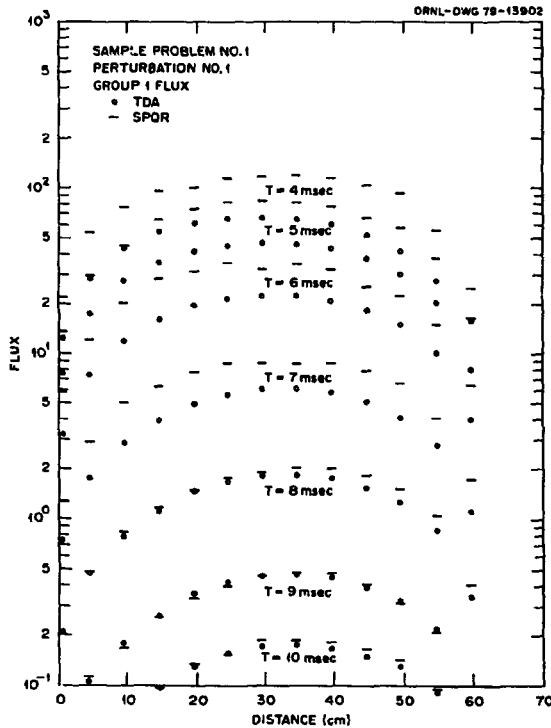


Fig. 3. Flux Distributions for Sample Problem No. 1, Perturbation No. 1, After Three msec.

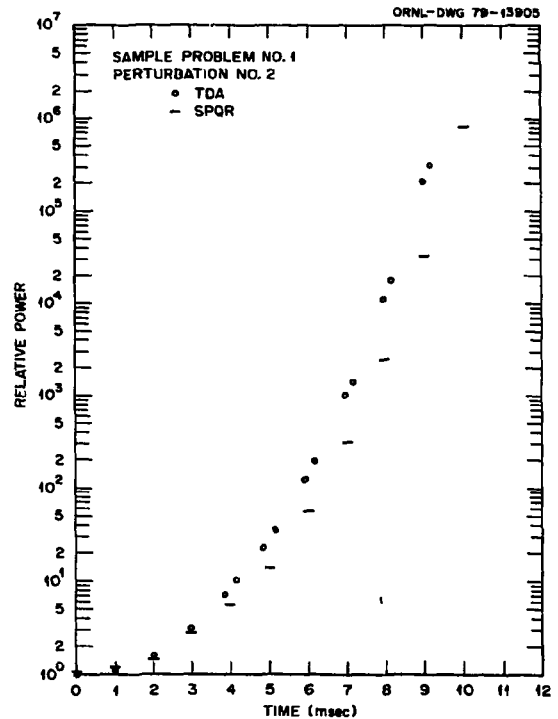


Fig. 4. Power Distribution for Sample Problem No. 1, Perturbation No. 2.

shape for the first perturbation contributes to the difference seen at later times. There are no error bars shown for the Monte Carlo results as there was no attempt to propagate the statistical error from one shape calculation to the next. The standard deviations for the individual calculations were about 10% for each data point in Figs. 1 and 4 and about 20% for Figs. 2 and 3.

A second sample problem was taken from the Argonne benchmark book.⁶ This problem, 6-A4, represents a large, uncoupled reactor with neutron velocities chosen to simulate a fast reactor. Time-dependent results from the perturbation are shown in Table 1. In the initial SPQR calculation no special spatial biasing was employed, but in the final results a strong bias based on TDA calculations was incorporated into the spatial distribution. It is clear that completely non-physical results can be obtained without a reasonable compilation of the shape function. This sample problem was included to show that for large systems, in terms of neutron mean free paths, the correct biasing factors would be needed prior to the calculation; however, these would not generally be available.

In order to further test the code, several sample problems were devised in order to simulate time-dependent behavior in a large LMFBR. The problems are presented in the Appendix in the standard benchmark problem format. The perturbations in these problems have been selected so as to represent simplistic accident conditions, such as density changes and material motion, rather than individual reaction type changes.

In Fig. 5 are presented SPQR and TDA results for problem 16-A2. Two independent SPQR calculations were made to illustrate the difficulties caused by the statistical uncertainty. The cause of this uncertainty can be traced to the form of the perturbation operator in Eq. (6). In Eq. (8) or Eq. (12) it is seen that there are three contributions to the perturbation: (1) a negative total cross-section term, (2) a positive scattering term, and (3) a positive fission term. For perturbations in which the change in one reaction type dominates, e.g. control rod movement, the algebraic sign of $\Delta\Sigma$ is always the same. However, for perturbations such as material density changes, all three terms are affected, leading to both positive and negative contributions to $\Delta\Sigma$

Table 1. Relative power comparisons for Benchmark Problem 6-A4

Time (msec)	Benchmark*	SPQR (Initial)	SPQR (Final)
0.0	1.000	1.000	1.000
1.0	1.178	1.162	1.291
2.0	1.558	1.425	1.701
3.0	2.797	2.024	2.925
3.5	5.284	2.934	5.989
4.0	20.72	4.546	22.93
4.5	472.0	13.45	640.2
5.0	153,700.0	215.9	490,800.0

*See reference 6.

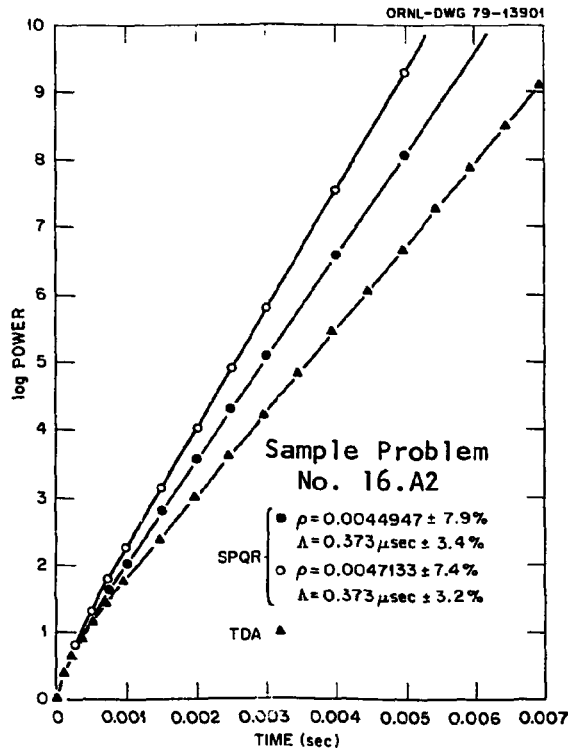


Fig. 5. Power Distribution for Sample Problem No. 16.A6.

and to large statistical errors. In general, it has been found that for perturbations causing changes in the scattering cross section of comparable magnitude to that in other reaction types, Monte Carlo perturbation techniques are sometimes not adequate.^{7,8}

Two final sample problems, 16-A6 and 16-A7, present combinations of control rod movement, material density changes, and material motion. These results are shown in Figs. 6 and 7. It is seen in the sample ramp perturbation results, Fig. 6, that although peak power rates differ by a factor of five, the comparisons are reasonable. But for step perturbations, the different methods diverge at early times and differ by several orders of magnitude at later times. These discrepancies can be attributed to various combinations of the problems associated with the preceding sample problems.

V. SUMMARY AND CONCLUSIONS

The Monte Carlo method has been utilized in the SPQR code to calculate the shape function portion of the adiabatic quasi-static model. The sample problem results in the preceding section illustrate some of the difficulties associated with Monte Carlo and its incorporation into a quasi-static code. The omission of the derivative terms in the shape equation (the adiabatic approximate) is usually overshadowed by the statistical uncertainty in the results. A potentially more serious limitation of the Monte Carlo method is the uncertainty in the reactivity calculation for perturbations which cause significant changes in the scattering cross sections. An uncertainty of a few percent in reactivity at early times in the perturbation can lead to order-of-magnitude differences in the power level at later times. It was also shown that the Monte Carlo method has difficulty following the spatial changes in the neutron distribution resulting from asymmetrical perturbations in large, uncoupled systems.

The calculation times involved in the sample problems were, of course, much longer than needed for deterministic methods. These times were dictated by the number of shape functions required, the average number of collisions in the lifetime of a neutron for a particular

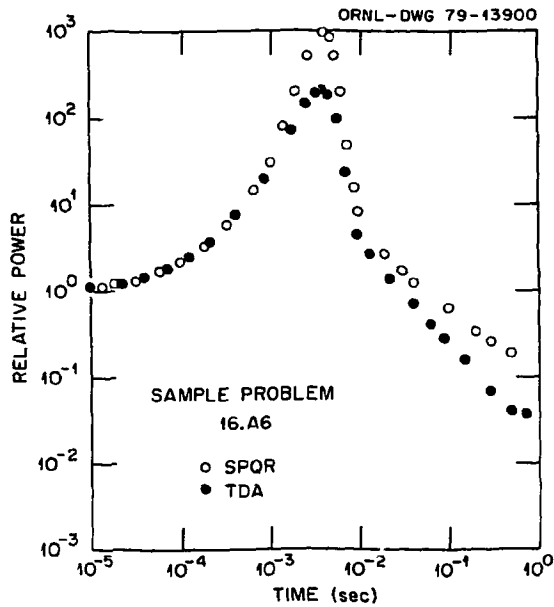


Fig. 6. Power Distribution for Sample Problem No. 16.A6.

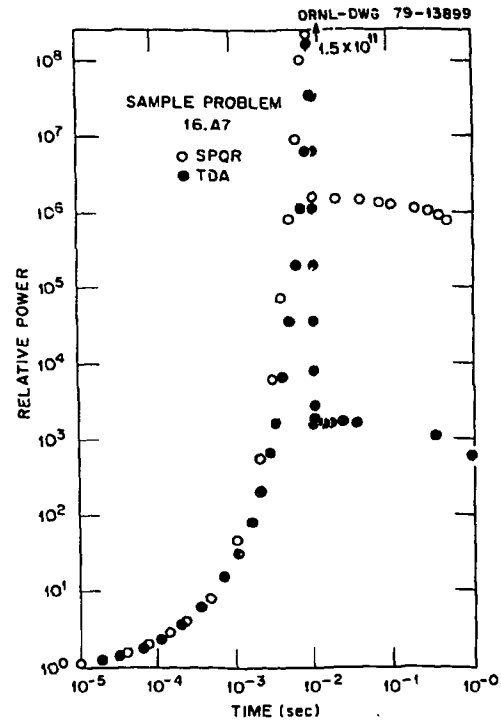


Fig. 7. Power Distribution for Sample Problem No. 16.A7.

reactor system, and the degree of statistical error desired. However, the SPQR calculation time would not increase substantially for three-dimensional problems of comparable design. The determination of the proper adjoint function for a three-dimensional problem could become a formidable task. These problems will need more study before realistic three-dimensional problems involving feedback and material motion can be addressed.

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Attached herewith is a proposed series of fast reactor kinetics benchmark problems. The problems are documented in the format required by the ANS M & C Division Benchmark Problems Committee. The problems (and solutions, when obtained) will eventually be submitted to the committee for publication in the benchmark book (ANL-7416).

There are nine problems, all in one-dimensional slab geometry, with cross sections and region sizes that are representative of a large LMFBR including core, blanket, and control rod (mixed with sodium) materials. The problems are directed toward testing transport theory methods (particularly, the discrete ordinates method) with two energy groups, and six precursor groups, but with isotropic scattering. All of the problems begin with the same steady state (critical) initial conditions.

Problems A1, A2, A3, A7, and A9 involve only step changes in reactivity while problems A4 and A5 require ramp perturbations. Problems A6 and A8 involve a step change followed by a ramp change. T. R. Hill (LASL) and W. Engle (ORNL) have agreed to provide solutions of the first three problems with TIMEX and TDA (Time-dependent ANISN), respectively.

The following suggestions are made regarding the times at which information is edited for the first seven problems.

1. Follow each transient out to $t = 0.5$ sec or until the power has increased by a factor of 10^9 , whichever occurs first.
2. Edit total reactor power and region-averaged power fractions at intervals of
 - (a) 0.001 sec for problems 16-A1 and 16-A4
 - (b) 0.0001 sec for problems 16-A2, 16-A3, 16-A5, 16-A6, and 16-A7.
3. Edit group scalar flux distributions at least three times during each transient (at $t = 0.0$ sec, near the middle of the transient, and at the end of the transient) or, more often, at intervals of
 - (a) 0.01 sec for problems 16-A1 and 16-A4.
 - (b) 0.001 sec for problems 16-A2, 16-A3, 16-A5, 16-A6, and 16-A7.

Needless to say, these problems have yet to be solved by any method and, therefore, are subject to changes. Any comments that you may have regarding improvements in the problem definitions and/or changes which will more easily facilitate obtaining solutions to the problems will be appreciated.



H. L. Dodds, Jr.
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HLD/co

Attachment

BENCHMARK SOURCE SITUATION

Identification: 16

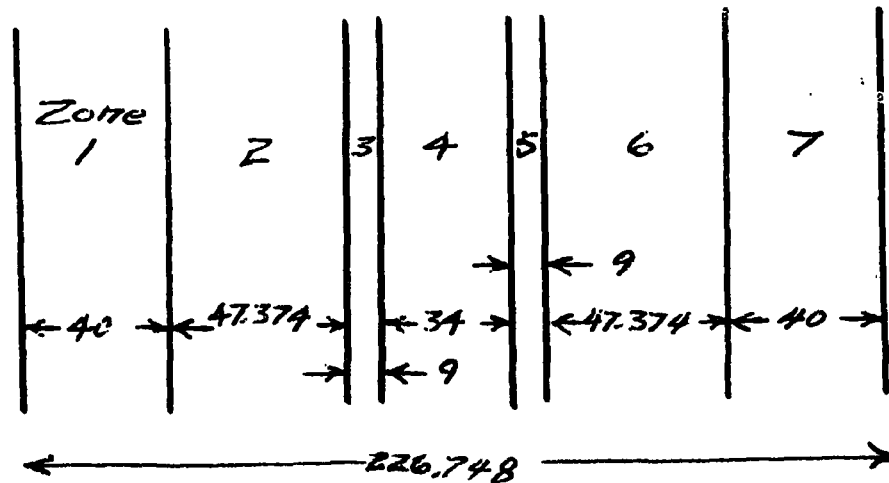
Date Submitted: November 1977 By: H. L. Dodds, Jr. (Univ. of Tenn.)

Dated Adopted: By:

Descriptive Title: *One-Dimensional Slab Reactor Model*

Suggested Function: Test one-dimensional neutron transport transient solutions

Reactor Configuration:



Note: All Dimensions
in Centimeters

BENCHMARK PROBLEM

Identification: 16-A1 Source Situation: ID.16
Date Submitted: November 1977 By: H. L. Dodds, Jr.
(University of Tennessee)
Date Accepted: By:

Descriptive Title: *Delayed Supercritical Transient; One-Dimensional,
Two-Group Neutron Transport Problem in a Fast Reactor*

Reduction of Source Situation:

1. One-dimensional (slab), two-group neutron transport theory
2. Isotropic scattering
3. Zero return current boundary conditions on external surfaces
4. Steady-state initial conditions
5. Six delayed neutron precursor groups

Data: Initial two-group constants shown in Table I. Delayed neutron parameters, prompt, and delayed spectra, and $1/v$ values shown in Table II.

The initial configuration is made critical by dividing the production cross sections by k -eff, and the initial precursor concentrations are in equilibrium with the initial critical flux distribution.

Initiating Perturbation:

At time $t = 0.0$ sec, the density of the material in Zone 2 is increased by 5% and the density of the material in Zone 6 is decreased by 5% (resulting in a step insertion of reactivity at time $t = 0.0$ sec).

Expected Primary Results:

1. Initial k -eff and initial scalar flux distribution for each group
2. Convergence requirements on flux (and eigenvalue) if an iterative solution is used

Table I. Initial Two-Group Constants^a (cm⁻¹)

<u>Zone</u>	<u>Group i</u>	<u>$v\Sigma_f^i$</u>	<u>Σ_t^i</u>	<u>$\Sigma_s^{i\rightarrow i}$</u>	<u>$\Sigma_s^{i\rightarrow j}$</u>
1,7 ^b	1	8.3441-4	2.411-1	2.33644-1	3.598-3
	2	3.2776-4	4.172-1	4.07004-1	0.0
2,4,6 ^c	1	7.4518-3	1.849-1	1.77711-1	2.085-3
	2	1.10612-2	3.668-1	3.53721-1	0.0
3,5 ^d	1	0.0	9.432-2	8.571-2	1.7168-3
	2	0.0	1.8762-1	1.7131-1	0.0

$${}^a\Sigma_a^i = \Sigma_t^i - \Sigma_s^i \text{ and } \Sigma_s^i = \Sigma_s^{i\rightarrow i} + \Sigma_s^{i\rightarrow j} .$$

^bBlanket material in Zones 1 and 7.

^cCore material in Zones 2, 4, and 6.

^dMixture of sodium and control rod material in Zones 3 and 5.

Table II. Delayed Neutron Parameters^a

<u>Type</u>	<u>β</u>	<u>λ (sec⁻¹)</u>
1	0.81-4	0.0129
2	6.87-4	0.0311
3	6.12-4	0.134
4	11.38-4	0.331
5	5.12-4	1.26
6	1.70-4	3.21

^aPrompt and delayed neutron spectra are identical with $\chi_1 = 1.0$ and $\chi_2 = 0.0$. Also, $1/v_1 = 1.851-9 \frac{\text{sec}}{\text{cm}}$ and $1/v_2 = 1.088-8 \frac{\text{sec}}{\text{cm}}$.

Table III
S₄ Angular Quadrature

<u>Cosine (μ)</u>	<u>Weight</u>
-1.0	0.0
-0.788675	0.25
-0.211325	0.25
+0.211325	0.25
+0.788675	0.25

Table IV
Spatial Mesh

<u>Zone</u>	<u>Number of Equal Intervals</u>
1	20
2	24
3	5
4	16
5	5
6	24
7	20

3. Total reactor power versus time (normalized such that the total power at $t = 0.0$ is 1.0 Mw)
4. Time-dependent group flux (i.e., scalar flux) distributions
5. Sensitivity of results to time step size
6. CPU time, wait (I/O) time, and core storage requirements

Possible Additional Results:

7. Zone-averaged power fractions versus time
8. Sensitivity of results to spatial mesh size
9. Sensitivity of results to angular quadrature (if solution is obtained by the discrete ordinates method)

Based on preliminary static k-eff calculations of the initial critical configuration using ANISN,¹ an S_4 quadrature with 114 spatial intervals (as defined in Tables III and IV) is a sufficiently accurate representation for the angular and spatial discretization. Specifically, by using a finer spatial mesh (i.e., 228 intervals), k-eff changed by 0.0001 and using an S_8 and S_{16} quadrature, k-eff changed by 0.0003 and 0.0003, respectively. Therefore, it is suggested that the "Expected Primary Results" requested above be obtained initially using the discretization indicated in Tables III and IV if the conventional discrete ordinates method is used to obtain solutions.

¹W. W. Engle, "A User's Manual for ANISN, A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering," K-1693, Computing Technology Center, Oak Ridge Gaseous Diffusion Plant (1967).

BENCHMARK PROBLEM

Identification: 16-A3 Source Situation: ID.16
 Date Submitted: November 1977 By: H. L. Dodds, Jr.
 (University of Tennessee)
 Date Accepted: By:

Descriptive Title: *Transient Initially Prompt Supercritical, then Subcritical; One-Dimensional, Two-Group Neutron Transport Problem in a Fast Reactor*

Reduction of source situation, initial data, expected primary results, and possible additional results are the same as in Problem 16-A1.

Initiating Perturbation:

At time $t = 0.0$ sec, the material in Zone 5 is changed from a mixture of sodium and control rod materials to 100% sodium (i.e., control rod bank ejection). Then, at $t = 0.0001$ sec, the material in Zone 3 is changed from a mixture of sodium and control rod materials to 100% control rod material (i.e., full insertion of the control rod bank). The cross section for sodium and for the control rod material are shown in the following table:

Two-Group Constants^a for Sodium and Control Rod Material (cm⁻¹)

Material	Group i	Σ_t^i	$\Sigma_s^{i \rightarrow i}$	$\Sigma_s^{i \rightarrow j}$
Sodium	1	6.83-2	6.3293-2	1.294-3
	2	1.257-1	1.21099-1	0.0
Control Rod Material	1	1.795-1	1.59078-1	3.101-3
	2	3.903-1	3.35661-1	0.0

$$^a \Sigma_a^i = \Sigma_t^i - \Sigma_s^i \text{ and } \Sigma_s^i = \Sigma_s^{i \rightarrow i} + \Sigma_s^{i \rightarrow j}$$

In addition, for the time interval between $t = 0.0$ sec and $t = 0.5$ sec, the densities of the materials in Zones 1, 2, 4, 6, and 7 are changed linearly resulting in final cross sections for each zone at $t = 0.5$ sec as shown below:

Two-Group Constants for Ramp Perturbations in
Zones 1, 2, 4, 6, and 7 (at $t = 0.5$ sec)

Zone No.	Group i	$u\Sigma_f^i$	Σ_t^i	$\Sigma_s^{i \rightarrow i}$	$\Sigma_s^{i \rightarrow j}$
1	1	1.71696-3	2.62999-1	2.54691-1	3.84493-3
	2	1.63779-3	4.60642-1	4.48897-1	0.0
2	1	6.70661-3	1.6641-1	1.5994-1	1.8765-3
	2	9.95507-3	3.3012-1	3.18349-1	0.0
4,6	1	2.98072-3	7.39599-2	7.10843-2	8.33999-4
	2	4.42448-3	1.4672-1	1.41488-1	0.0
7	1	9.93014-3	4.66791-1	4.50559-1	6.14297-3
	2	1.38292-2	8.64919-1	8.38759-1	0.0

The latter perturbations are representative of material motion; specifically, movement of core material from Zones 4 and 6 into the blanket in Zone 7 and movement of core material from Zone 2 into the blanket in Zone 1. The perturbed cross sections for each zone (i.e., Zones 1, 2, 4, 6, and 7) at each point in time between $t = 0.0$ and $t = 0.5$ sec are determined by linear interpolation of the cross sections given above at $t = 0.5$ sec, and the steady state cross sections given in Table I of Problem 16-A1. The cross sections in Zone 3, the control rod bank on the left, are not perturbed.

BENCHMARK PROBLEM

Identification: 16-A8

Source Situation: ID.16

Date Submitted: May 1979

By: H. L. Dodds, Jr.
(University of Tennessee)

Date Accepted:

By:

Descriptive Title: *Sodium Voiding-Fuel Movement Transient Initially Prompt Supercritical (Step Perturbation), then Subcritical (Ramp Perturbation); One-Dimensional, Two-Group Neutron Transport Problem in a Fast Reactor*

Reduction of the source situation, initial data, expected primary results, and possible additional results are the same as in Problem 16-A1, except for the termination of the transient which occurs at $t = 0.1$ sec.

Initiating Perturbation:

At time $t = 0.0$ sec, the sodium and stainless steel materials in core Zones 2, 4, and 6 are removed from the system resulting in the following cross sections for Zones 2, 4, and 6 at $t = 0.0$ sec:

Table I. Two-Group Constants for Step Perturbation
in Zones 2, 4, and 6 at $t = 0.0$ sec

Group i	$\nu\Sigma_f^i$	Σ_t^i	$\Sigma_s^{i \rightarrow i}$	$\Sigma_s^{i \rightarrow j}$
1	6.53879-3	1.26360-1	1.21890-1	2.60740-4
2	2.54410-2	1.59930-1	1.36410-1	0.0

In addition, for the time interval between $t = 0.0$ sec and $t = 0.0001$ sec, the densities of the materials in Zones 1, 2, 4, 6, and 7 are changed linearly resulting in final cross sections for each zone at $t = 0.0001$ sec as shown below:

Table II. Two-Group Constants for Ramp Perturbations in Zones 1, 2, 4, 6, and 7 (at $t = 0.0001$ sec)

Zone No.	Group i	$\nu\Sigma_f^i$	Σ_t^i	$\Sigma_s^{i \rightarrow i}$	$\Sigma_s^{i \rightarrow j}$
1	1	1.60883-3	2.56065-1	2.4808-1	3.62888-3
	2	3.3437-3	4.36141-1	4.23159-1	0.0
2	1	5.88491-3	1.13724-1	1.09701-1	2.34666-4
	2	2.29185-2	1.43937-1	1.22769-1	0.0
4,6	1	2.61552-3	5.05440-2	4.87560-2	1.04296-4
	2	1.01860-2	6.39719-2	5.4564-2	0.0
7	1	8.81573-3	3.95336-1	3.82424-1	3.91626-3
	2	3.14106-2	6.12412-1	5.73507-1	0.0

The latter perturbations are representative of fuel motion; specifically, movement of fuel material from Zones 4 and 6 into the blanket in Zone 7 and movement of fuel material from Zone 2 into the blanket in Zone 1. The perturbed cross sections for each blanket zone (i.e., Zones 1 and 7) at each point in time between $t = 0.0$ and $t = 0.0001$ sec are determined by linear interpolation of the cross sections given above at $t = 0.0001$ sec, and the steady state cross sections for Zones 1 and 7 given in Table I of Problem 16-A1. The cross sections in Zones 2, 4, and 6 are determined by linear interpolation of the cross sections given above at $t = 0.0001$ sec, and the perturbed cross sections given in Table I of this problem (i.e., 16-A8). The cross sections for the control rod banks in Zones 3 and 5 are unperturbed in this problem.

BENCHMARK PROBLEM

Identification: 16-A9

Source Situation: ID.16

Date Submitted: May 1979

By: H. L. Dodds, Jr.
(University of Tennessee)

Date Accepted:

By:

Descriptive Title: *Sodium Voiding-Fuel Movement Transient Initially Prompt Supercritical (Step Perturbation), then Subcritical (Step Perturbation); One-Dimensional, Two-Group Neutron Transport Problem in a Fast Reactor*

Reduction of the source situation, initial data, expected primary results, and possible additional results are the same as in Problem 16-A1, except for the termination of the transient which occurs at $t = 0.1$ sec.

Initiating Perturbation:

This perturbation is identical to the perturbation for Problem 16-A8 except for the ramp representing fuel motion. Specifically, the ramp between 0.0 sec and 0.0001 sec is replaced by a step which occurs at $t = 0.0001$ sec. The magnitude of this step change at $t = 0.0001$ is determined by the cross sections given in Table II of Problem 16-A8.