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A NUMERICAL COMPARISON OF DIFFUSION
AND TRANSPORT (S_n) CODES FOR SELECTED
FAST REACTOR CONFIGURATIONS

March 1969

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A NUMERICAL COMPARISON OF
DIFFUSION AND TRANSPORT (S_n) CODES
FOR SELECTED FAST REACTOR CONFIGURATIONS

By

L. D. O'Dell
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Reactor Physics and Operations Department
FFTF Project

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L. D. O'Dell, R. W. Hardie, and W. W. Little, Jr.

ABSTRACT

Numerical comparisons between the one-dimensional diffusion code, 1DX, and the one-dimensional transport code, DTF-IV, are described. The objective of the comparison is to determine under what circumstances diffusion codes are sufficiently accurate to be used in place of transport codes. For large breeder reactors, it is found that diffusion theory is adequate to compute virtually all preliminary design parameters -- including control rod worths and neutron fluxes far from the core.

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I. INTRODUCTION

This report describes the results of identical diffusion and transport (S_n) calculations for a wide range of fast reactor systems. The objective is to determine, by numerical experiment, under what conditions diffusion theory is adequate for computing fast reactor design parameters.

The well-known Los Alamos DTF-IV⁽¹⁾ and 2DF⁽²⁾ codes were used for all transport calculations. The Battelle 1DX⁽³⁾ and 2DB⁽⁴⁾ codes, which use the same input specifications as the Los Alamos codes, were used for all diffusion computations. Identical 5-group cross sections were used by each code in all calculations. The S_n quadrature parameters were taken from Lee's documentation⁽⁵⁾.

The diffusion and transport calculations are compared with respect to k_{eff} , reactivity coefficients, flux profiles, and flux magnitudes far from the source (core). In addition, the effects of mesh spacing, geometry, and core volume are described.

II. SPECIFICATIONS FOR BASE CASE

Various general rules are followed throughout the comparison calculations unless otherwise specified. A single 5-group cross section set is used for both the core and reflector. The mesh intervals are equally spaced in each region; 30 intervals are used in the core and 20 in the reflector. The convergence criterion on the total fission source rate is 10^{-6} .

The core, reflector, and control rod compositions are given in Tables 2.I and 2.II. The geometry and core radius will be specified for each calculation. A 30 cm Fe reflector is used in the base case, although uranium reflectors are also considered.

TABLE 2.I

Material Compositions (atoms/b-cm)

Material	Core	Fe Refl.	U. Refl.	Control Rod
^{239}Pu	*	0.000	0.000	0.000
^{238}U	0.005	0.000	0.010	0.000
O	0.010	0.000	0.020	0.000
Na	0.010	0.005	0.005	0.020
Fe	0.020	0.050	0.010	0.020
^{10}B	0.000	0.000	0.000	0.000→0.025

* See Table 2.II

TABLE 2.II

²³⁹Pu Atom Densities (atoms/b-cm)

Geometry	C o r e R a d i u s		
	25 cm	50 cm	100 cm
PLANE	0.00104	0.000726	0.000604
SPHERE	0.00394	0.00151	0.000816
CYLINDER	0.00211	0.00104	0.000695

The critical ²³⁹Pu densities listed in Table 2.II were calculated using the 1DX code and the specifications given in Table 2.I.

III. EFFECT OF QUADRATURE ORDER ON k_{eff} COMPARISON

Using the base case specifications and core radii of 25, 50 and 100 cm, DTF-IV calculations were performed for quadratures from S_2 to S_{12} . The calculated k_{eff} values are tabulated in Tables 3.I and 3.II for cylindrical and spherical geometry, respectively. 1DX results and the corresponding computation times for the 50 cm cases are also shown.

TABLE 3.I

*k_{eff} Ratio as a Function of Quadrature Order
for Cylindrical Reactors*

Calculation	Computation Time (min) a.	$k_{eff}/k_{eff} (S_{12})$		
		25 cm	50 cm	100 cm
DTF-IV, S_2	0.45	1.00465	1.00168	1.00043
S_4	0.98	1.00414	1.00140	1.00036
S_6	1.70	1.00104	1.00030	1.00008
S_8	2.65	1.00043	1.00014	1.00006
S_{12}	5.08	1.00000	1.00000	1.00000
1DX	0.02	0.98443	0.99633	0.99944

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TABLE 3.II

k_{eff} Ratio as a Function of Quadrature Order
for Spherical Reactors

Calculation	Computation Time (min)	$k_{eff}/k_{eff} (S_{12})$		
		25 cm	50 cm	100 cm
DTF-IV, S_2	0.46	1.03298	1.01350	1.00347
S_4	0.69	1.00383	1.00115	1.00020
S_6	0.92	1.00160	1.00046	1.00008
S_8	1.14	1.00084	1.00024	1.00004
S_{12}	1.59	1.00000	1.00000	1.00000
1DX	0.02	0.96518	0.99126	0.99860

The difference between the diffusion and transport calculations decreases with increasing core volume and increasing quadrature order. Note that the transport k_{eff} 's are always greater than the diffusion k_{eff} 's. Plots of k_{eff} versus quadrature order are shown in Figs. 3.1 and 3.2.

FIGURE 3.1.

*Effect of Quadrature Order on k_{eff}
Calculation for Cylindrical Reactors*

FIGURE 3.2.

Effect of Quadrature Order on k_{eff}
Calculation for Spherical Reactors

IV. EFFECT OF NUMBER OF MESH INTERVALS ON k_{eff} COMPARISON

1DX and DTF-IV k_{eff} calculations were performed using 13, 25, 50, 75, and 100 equally spaced (in each region) mesh intervals. The ratio of core intervals to reflector intervals was 3:2 (except for the 13 interval case, where the ratio was 8:5). All calculations were based on a 50 cm core in cylindrical geometry with an Fe reflector. The results are shown in Figure 4.1.

Two significant observations can be made from Figure 4.1: (1) both codes show only slight variation above 30 intervals, and practically no variation above 50 intervals and (2) the diffusion code is significantly more sensitive to mesh spacing than the transport code.

FIGURE 4.1.

*Effect of Number of Mesh
Intervals in k_{eff} Calculation*

V. EFFECT OF REFLECTOR MATERIAL ON k_{eff} COMPARISON

The influence of reflector material on the comparison between 1DX and DTF-IV was investigated by performing identical calculations for both natural uranium and Fe reflectors. See Table 2.I for the specific reflector compositions. All calculations were performed in cylindrical geometry with core radii of 25, 50, and 100 cm.

The results, in the form of k_{eff} ratios as a function of core radius, are given in Figure 5.1. As one would expect, the 1DX and DTF-IV eigenvalues merge at large radii. Note, however, that the merger rate is virtually the same for both U and Fe reflectors.

FIGURE 5.1.

k_{eff} Comparison Between Codes
1DX and DTF-IV (S_4)

VI. EFFECT OF GEOMETRY ON k_{eff} COMPARISON

To discover the effect of geometry on the comparison between 1DX and DTF-IV (S_4), plane, cylindrical, and spherical, k_{eff} calculations were performed on 25, 50, and 100 cm configurations.

Figure 6.1 gives the results in the form of eigenvalue ratios as a function of core radius. The difference between diffusion and transport theory obviously increases as one goes from plane to cylindrical to spherical geometry. For all three geometries, the difference between diffusion and transport theory decreases as the volume increases.

FIGURE 6.1.

Effect of Geometry on k_{eff} Comparison
Between Codes 1DX and DTF-IV (S_4)

VII. EFFECT OF NUMBER OF MESH INTERVALS ON
REACTIVITY COEFFICIENT CALCULATIONS

In Section IV it was shown that rather crude mesh spacings are adequate for computing k_{eff} in systems that do not contain control rods. This section will show the sensitivity of the worth of a central ^{10}B rod to the number of mesh intervals.

A 5 cm (radius) test loop was placed in the center of a 50 cm cylindrical reactor surrounded by an Fe reflector. The worth of ^{10}B ($\delta N = 0.005$ atoms/b-cm) in the test loop was then computed by 1DX and DTF-IV (S_4) using 30, 60, and 120 mesh intervals. The results are shown in Table 7.I.

TABLE 7.I

δk_{eff} as a Function of the Number of Mesh Intervals

Number of Intervals (loop, core, reflector)	δk 1DX	δk DTF-IV (S_4)	1DX DTF-IV
30 (5, 15, 10)	-0.02199	-0.02166	1.015
60 (10, 30, 20)	-0.02211	-0.02161	1.023
120 (20, 60, 40)	-0.02216	-0.02160	1.025

As before, observe that the DTF-IV results are less sensitive to mesh spacing than the 1DX results. Both codes, however, show no significant variation above about 30 intervals.

VIII. EFFECT OF ^{10}B DENSITY ON δk_{eff} COMPARISON
FOR A CENTRAL CONTROL ROD

The effect of successively larger increases in the ^{10}B density of a central control rod on the 1DX - DTF-IV comparison was examined. The geometry used here was the same as that employed in Section VII, and the total number of mesh intervals was set at 60. The ^{10}B density in the 5 cm central control rod was varied from 0 to 0.025 atoms/b-cm.

Figure 8.1 shows the rod worth as a function of ^{10}B concentration. As anticipated, the difference between the diffusion and transport predictions increase as the rod worth increases. The diffusion results are virtually indistinguishable from the transport results for rod worths less than about 0.02 -- which is the range of interest in practically all designs.

Figures 8.2 and 8.3 show the diffusion and transport flux profiles for ^{10}B concentrations of 0.001 and 0.025 atoms/b-cm. Significant differences are apparent in the flux profiles in the control rod region.

FIGURE 8.1.

δk_{eff} Comparison Between Codes 1DX and DTF-IV (S₄)
for a Central Control Rod

FIGURE 8.2.

Flux Profile for a Central Rod, $N(B^{10}) = 0.001$

FIGURE 8.3.

Flux Profile for a Central Rod, $N(B^{10}) = 0.025$

IX. EFFECT OF ^{10}B DENSITY ON δk_{eff} COMPARISON
FOR A PERIPHERAL CONTROL ROD

As a test to see whether the close agreement between 1DX and DTF-IV for central rods was just a fluke, worth calculations were run for a peripheral ^{10}B annulus with a thickness of 5 cm. Thirty mesh intervals were used in the core, 10 in the poison annulus, and 20 in the reflector.

Figure 9.1 gives the diffusion and transport worths as a function of ^{10}B density. Again, the two models display surprisingly good agreement over a rather wide range of ^{10}B concentrations. A comparison of selected flux profiles is shown in Figures 9.2 and 9.3.

FIGURE 9.1.

δk_{eff} Comparison Between Codes 1DX and DTF-IV (S_4)
 for a Peripheral Control Rod

FIGURE 9.2.
Flux Profile for a Peripheral Rod, $N(B^{10}) = 0.001$

FIGURE 9.3.
Flux Profile for a Peripheral Rod, $N(B^{10}) = 0.025$

X. COMPARISON OF CENTRAL REACTIVITY COEFFICIENTS

1DX and DTF-IV were used to compute the reactivity change caused by perturbations in the ^{239}Pu , ^{10}B , and sodium densities. The perturbations were made in a 5 cm (radius) central zone of a 50 cm cylindrical reactor. See Tables 2.I and 2.II for the specific compositions. The computed reactivity worths, together with the density variations, are given in Table 10.I.

Clearly, the diffusion and transport reactivity coefficients agree remarkably well. The close agreement for the small but important sodium coefficient is particularly gratifying since it indicates that the oft-repeated Na void calculation can be performed using diffusion theory.

TABLE 10.I

Central Reactivity Coefficients for ^{239}Pu , ^{10}B , and Sodium

Material	$\delta N(\text{atoms/b-cm})$	δk 1DX	δk DTF-IV (S_4)	$\frac{\delta k (1DX)}{\delta k (DTF)}$
^{239}Pu	+0.002	+0.02118	+0.02150	0.985
^{10}B	+0.001	-0.00580	-0.00581	0.998
Sodium	-0.020	+0.00085	+0.00083	1.030

XI. COMPARISON OF FLUXES FAR FROM SOURCE

In order to compare the flux calculated by 1DX and DTF-IV at large distances from the core, the reflector thickness was increased from 30 cm to 450 cm, and the total number of mesh intervals was expanded to 130 (30 intervals in the core and 100 in the reflector). All calculations were based on a 50 cm spherical core with Fe and U reflectors. A plot of the total radial flux profile for Fe and U reflectors is given in Figures 11.1 and 11.2, respectively. The flux greater than 0.8 MeV is shown in Figures 11.3 and 11.4.

Figures 11.1 and 11.2 show very good agreement between 1DX and DTF-IV (S_4 and S_8) for the total flux in both reflectors. For the Fe reflector, the deviation between the two codes starts at less than 1% near the core center and steadily increases to about 10% at 4.5 meters from the core center. The fluxes above 0.8 MeV do not display the same good agreement as the total fluxes. The deviation between the values calculated by 1DX and those calculated by DTF-IV (S_4 and S_8) for the high energy flux is less than 1% near the core center, but increases to approximately 50% at 2.5 meters from the core center. It is interesting to observe that the diffusion flux profiles are more accurate (i.e., agree better with S_4 and S_8 calculations) than the S_2 profiles.

FIGURE 11.1.

*Radial Flux Profile at Large Distances
from Source Through an Fe Reflector*

FIGURE 11.2.

*Radial Flux Profile at Large Distances
from Source Through a U Reflector*

FIGURE 11.3.

Flux Profile Above 0.8 MeV for Fe Reflector

FIGURE 11.4.

Flux Profile Above 0.8 MeV for U Reflector

XII. COMPARISON OF 1DX AND DTF-IV CELL CALCULATIONS

For this comparison between the two codes, a plane geometry cell problem with seven plates was considered. The heterogeneous cell arrangement is shown in Figure 12.1, and the plate compositions are given in Table 12.I.

Figure 12.1. Plate Arrangement for Heterogeneous Cell

TABLE 12.I

Material Densities for Plates (atoms/b-cm)

Material	U ₃ O ₈	Na ₂ CO ₃	Fuel	Na	SS
²³⁹ Pu	0.0	0.0	0.007432	0.0	0.0
²³⁸ U	0.013416	0.0	0.021223	0.0	0.0
C	0.0	0.009595	0.0	0.0	0.0
Fe	0.002837	0.010291	0.002837	0.010976	0.032655
Cr	0.000892	0.002785	0.000892	0.003018	0.010306
Ni	0.000496	0.001263	0.000496	0.001333	0.005740
Na	0.0	0.019191	0.0	0.018538	0.0
O	0.035869	0.028786	0.0	0.0	0.0

Using this geometric arrangement, diffusion and transport calculations were performed using periodic boundary conditions. The resulting eigenvalues are given in Table 12.II and a plot of the low energy and total flux profiles are shown in Figure 12.2. Even though the eigenvalues show little variation, it is clear that transport theory is required if accurate local flux profiles are desired.

TABLE 12.II

k_{eff} For Diffusion and Transport Cell Calculations

Calculation	k_{eff}
1DX	1.2139
DTF-IV, S_2	1.2141
S_4	1.2142
S_8	1.2149
S_{16}	1.2161

FIGURE 12.2.

Flux Comparison for a Heterogeneous Cell

XIII. COMPARISON OF TWO-DIMENSIONAL MODELS

To conserve computer time, all comparisons described in the foregoing sections have been based on one-dimensional models. In order to see if the general trends displayed by the one-dimensional models are valid for two-dimensional models, identical two-dimensional diffusion and transport k_{eff} calculations were performed using the 2DB⁽³⁾ and 2DF⁽⁴⁾ codes. The computations were based on a cylindrical reactor with a radius of 50 cm and a height of 100 cm. The core composition was that of the 50 cm spherical reactor described in Tables 2.I and 2.II. A 30 cm Fe reflector was used in both the axial and radial dimensions.

To save computer time, the convergence criterion on the total fission source was relaxed to 10^{-5} and the total number of mesh intervals used in each direction was reduced to 30, with 20 intervals in the core and 10 intervals in the reflector. The 2DB and 2DF results are shown in Table 13.I.

TABLE 13.I

Comparison of 2DB and 2DF

Parameter	2DB	2DF (S_2)	2DF (S_4)
k_{eff}	1.0810	1.0955	1.0888
Computation Time (Minutes)	2.1	12.7	30.0

Observe that the S_4 calculation yields about 1% greater reactivity than the diffusion calculation. This difference agrees on sign and magnitude with the one-dimensional results. The S_2 calculation gives no significant improvement over diffusion theory--and requires about six times more computer time.

XIV. CONCLUSIONS

From the results described herein, it is clear that diffusion theory is adequate for computing preliminary design parameters in moderate ($R \sim 50$ cm) to large fast reactor configurations. Indeed, diffusion calculations are often more accurate than S_2 calculations.

Diffusion calculations of reactivity coefficients (fuel, poison, and sodium) and global flux profiles agree quite well with transport calculations. However, if precise estimates of k_{eff} are required, transport corrections should be made for radii less than about 100 cm. Also, if precise local flux profiles (e.g., flux in a cell or control rod) or precise flux magnitudes far from the source are desired, transport theory must be employed.

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P. L. Hofmann	Legal (2)
E. M. Johnston	