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Flux Extrapolation Models used in the DOT IV Discrete Ordinates Neutron Transport Code

E. T. Tomlinson
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Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
NTIS price codes—Printed Copy: A04; Microfiche A01

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Contract No. W-7405 eng 26

Engineering Physics Division

FLUX EXTRAPOLATION MODELS USED IN THE DOT IV DISCRETE ORDINATES NEUTRON TRANSPORT CODE

E. T. Tomlinson*
W. A. Rhoades
W. W. Engle, Jr.

Date Published - May 1980

Sponsor: D. E. Bartine

NOTE

Work Sponsored by
DEFENSE NUCLEAR AGENCY
Under Subtask Code V99QAXNA010

*Computer Sciences Division.

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ACKNOWLEDGMENTS

The authors would like to express their appreciation to M. B. Emmett for her help in obtaining the numerical results presented in this report. The efforts of B. O. Neeley and B. R. Ferguson in the preparation of the final report are also appreciated. The funds in support of this work were provided by the Defense Nuclear Agency.

ABSTRACT

The DOT IV[1] code solves the Boltzmann transport equation in two dimensions using the method of discrete ordinates. Special techniques have been incorporated in this code to mitigate the effects of flux extrapolation error in space meshes of practical size. This report presents the flux extrapolation models as they appear in DOT IV. A sample problem is also presented to illustrate the effects of the various models on the resultant flux. Convergence of the various models to a single result as the mesh is refined is also examined. A detailed comparison with the widely used TWOTRAN II[2] code is reported. The features which cause DOT and TWOTRAN to differ in the converged results are completely observed and explained.

I. INTRODUCTION

The solution to the Boltzmann transport equation in two dimensions can be readily obtained using the method of discrete ordinates.[3] The diamond difference technique, which is usually employed to solve the difference form of the discrete ordinates equation, produces spurious oscillations in regions where the flux gradients are steep and the spatial and directional meshes are coarse. This oscillation often results in the calculation of negative angular fluxes. Various alternate flux extrapolation techniques have been developed to enhance the solution stability and to remove the negative angular fluxes. Each of these techniques is, in effect, an assumption relating mean flux within an interval to the boundary valves, i.e., a flux-shape model.

The use of alternate flux extrapolation models leads to concerns about the convergence of the various models to a single solution. That is, when the spatial and directional meshes are refined, do all the models produce the same solution?

This report presents the flux extrapolation models as they appear in the DOT IV discrete ordinates transport code. A discussion, with a sample case, of the convergence of the models to a single solution is also presented. Comparisons with the widely used TWOTRAN II code are also reported. The features that make DOT and TWOTRAN differ in the converged results are discussed. A discussion of the relative merits of the use of zero-weight directions in angular quadrature set is presented.

II. THE DIFFERENCE FORM OF THE DISCRETE ORDINATES EQUATION

The finite difference representation of the discrete ordinates equations can be written as Eq. (1):[2]

$$
\begin{aligned}
& W_m|\mu_m|\left(A_{i+c,j}N_{i+c,j,m} - A_{i-c,j}N_{i-c,j,m}\right) \\
& +W_m|\eta_m|\left(B_{i,j+d,}N_{i,j+d,m} - B_{i,j-d,}N_{i,j-d,m}\right) \\
& + \left(A_{i+c,j} - A_{i-c,j}\right)\left(\alpha_{m+\frac{1}{2}}N_{i,j,m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{i,j,m-\frac{1}{2}}\right) \\
& + \sigma_t W_m V_{i,j}N_{i,j,m} = W_m V_{i,j}S_{i,j,m} \quad , \qquad (1)
\end{aligned}
$$

where we define

$$V_{i,j} = \int_i\int_j dV = \int_i\int_j dAdB \quad , \qquad (2)$$

i - direction surface area

$$A_{i+c,j} = \int_j dA_{i+c} \quad , \qquad (3)$$

j - direction surface area

$$B_{i,j+c} = \int_i dB_{j+c} \quad , \qquad (4)$$

quadrature weight

$$W_m = \iint_m d\Omega \quad , \qquad (5)$$

$$c = \tfrac{1}{2}Sg(\mu);\ d = \tfrac{1}{2}Sg(\eta),\ \text{and}$$

$$\alpha_{m+\frac{1}{2}} = \alpha_{m-\frac{1}{2}} - W_m \mu_m \quad . \tag{6}$$

The recursion for the α's is initialized by setting the first α in each η level equal to zero. For sets of (μ,η) which are symmetric in μ, this insures that the sum of the α's in each η level is zero. Thus, if Eq. (1) is summed over all directions, the terms in α will sum to zero, and there is no net particle loss or gain due to angular redistribution in an area of uniform flux, a property of the analytic equation.

The direction set implied by the pairs of (μ,η) is organized into contiguous subsets (η levels) having a common η. The terms containing α couple adjacent directions in each η level, thus accounting for the effects of curved geometry. This is called "angular flow." Since sums over the direction set are used to approximate intergrals over solid angle, the collection of μ, η, and W are often referred to as a "quadrature set."

Following Reference 2, obvious subscripts, such as those describing the spatial dependence of σ_t, are omitted. Fractional subscripts refer to values associated with the boundary between adjacent intervals; e.g., $N_{i+\frac{1}{2},j,m}$ is the boundary value between intervals i and i+1.

III. FLUX EXTRAPOLATION MODEL USED IN DOT IV

In order to solve Eq. (1), a flux extrapolation model relating the incoming, outgoing, and cell average fluxes must be assumed. In DOT IV, the analyst can choose among a number of models. The following flux extrapolation models are available in DOT IV and will be described in this section.

linear (diamond difference)

step

zero fix-up

weighted

theta-weighted

Linear can be used as the primary model, with either zero or theta-weighted used as an alternative when the linear model results in a negative flux. All models except the zero fix-up model can be used alone.

Equation (1) has been recast in the following form for implementation in the code:

$$|\mu|\left(A_{i+c}N_{i+c} - A_{i-c}N_{i-c}\right) + |\eta|B\left(N_{j+d} - N_{j-d}\right)$$

$$+ \frac{1}{2}\Delta A\left[\left(\beta_m - \mu_m\right)N_{m+\frac{1}{2}} - \left(\beta_m + \mu_m\right)N_{m-\frac{1}{2}}\right] + V\sigma_T N = VS \quad . \tag{7}$$

Equation (7) is obtained by applying the following relationship to Eq. (1):

$$\beta_m = \frac{1}{W_m}\left(\alpha_{m+\frac{1}{2}} + \alpha_{m-\frac{1}{2}}\right) \quad . \tag{8}$$

The recursion relationship for the β_m can be obtained from Eq. (6) and (8):

$$W_m\beta_m = \alpha_{m+\frac{1}{2}} + \alpha_{m-\frac{1}{2}}$$

$$W_{m+1}\beta_{m+1} = \alpha_{m+3/2} + \alpha_{m+\frac{1}{2}} \tag{9}$$

$$\alpha_{m+\frac{1}{2}} = \alpha_{m-\frac{1}{2}} - W_m\mu_m$$

$$\alpha_{m+3/2} = \alpha_{m+\frac{1}{2}} - W_{m+1}\mu_{m+1} \tag{10}$$

Therefore

$$W_{m+1}\beta_{m+1} = W_m\beta_m - (W_{m+1}\mu_{m+1} + W_m\mu_m) \quad . \tag{11}$$

A. Zero-Weight Directions

DOT IV, requires an initial "zero-weight" direction at the beginning of each η level. TWOTRAN uses a "step formulation" in angle for the first direction in each η level, together with a nonzero weight. The zero-weight directions are located such that, physically, the angular flow into, but not out of, the initial μ interval must be zero. This implies that

$$\alpha_{1/2} = 0 \tag{12a}$$

$$\alpha_{3/2} = -W_1\mu_1 \tag{12b}$$

$$\beta_1 = -\mu_1 \quad . \tag{12c}$$

As the width of the angular interval approaches zero, and thus the weight approaches zero, it can be seen that the angular interval boundary flux, $N_{m+\frac{1}{2}}$, approaches the average interval flux, N; i.e.,

$$N_{3/2} = N_1 \quad . \tag{13}$$

Equations (12) and (13) define the conditions used in the derivation of the zero-weight direction equations. If the initial weight is not zero, these same conditions are then arbitrarily assumed; the so-called "step-initialization." The use of zero-weight directions means that, in general, more fluxes must be calculated. The relative merits of zero-weight directions are discussed in Section VI of this report.

The aforementioned extrapolation models will now be derived from Eqs. (7), (8), and (11). In each case, the assumptions concerning the variation of the flux across the interval will be presented, as well as the results. Obvious intermediate steps are not shown. The zero-weight direction equations are also presented.

In each of the models presented, it is assumed that N_{i-c}, N_{j-d}, and $N_{m-\frac{1}{2}}$ are known fluxes either from a boundary condition or the calculation in an adjoining interval.

1. <u>The Linear Model</u>

The linear model (diamond difference model) is an arithmetic mean model.

Assume

$$N_{i+c} = 2N - N_{i-c} \tag{14a}$$

$$N_{j+d} = 2N - N_{j-d} \tag{14b}$$

$$N_{m+\frac{1}{2}} = 2N - N_{m-\frac{1}{2}} \tag{14c}$$

$$\bar{A} = \frac{1}{2}\left(A_{i+\frac{1}{2}} + A_{i-\frac{1}{2}}\right) \tag{14d}$$

$$\Delta A = A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}} \tag{14e}$$

$$2|\mu|A_{i+c} + \Delta A\left(\beta-\mu\right) = 2|\mu|\bar{A} + \Delta A\beta \tag{14f}$$

$$N = \frac{VS + 2|\mu|\bar{A}N_{i-c} + 2|\eta|BN_{j-d} + \Delta A\beta N_{m-\frac{1}{2}}}{V\sigma_T + 2|\mu|\bar{A} + 2\ |\eta|B + \Delta A\beta} \tag{15}$$

Zero-Weight Direction

$$N = \frac{VS + 2|\mu|\bar{A}N_{i-c} + 2|\eta|BN_{j-d}}{V\sigma_T + 2|\mu|\bar{A} + 2|\eta|B} \tag{16}$$

Eqs. (14) can result in negative values for N_{i+c}, N_{j+d}, and $N_{m+\frac{1}{2}}$ due to over-extrapolation in a region with steep flux gradients. In a region where the source is negative due to truncation in the Legendre expansion of the cross sections, negative fluxes may also be calculated. The latter can cause the cell average flux to be negative, also, and in these cases no attempt to "fix-up" the negative fluxes is attempted. In the former case, one of the negative flux fix-up models can be invoked to provide a result closer to the true positive flux. These fix-up models include zero fix-up and weighted difference, both of which guarantee non-negative fluxes if a positive source is present.

2. <u>The Step Model</u>

The step fix-up model assumes that the extrapolated fluxes are equal to the cell average flux.

Assume

$$N_{i+c} = N \tag{17a}$$

$$N_{j+d} = N \tag{17b}$$

$$N_{m+\frac{1}{2}} = N \tag{17c}$$

$$N = \frac{VS + |\mu|A_{i-c}N_{i-c} + |\eta|BN_{j-d} + \frac{1}{2}\Delta A(\beta+\mu)N_{m-\frac{1}{2}}}{V\sigma_T + |\mu|A_{i-c} + |\eta|B + \frac{1}{2}\Delta A(\beta+\mu)} \tag{18}$$

Zero-Weight Direction

$$N = \frac{VS + |\mu|A_{i-c}N_{i-c} + |\eta|BN_{j-d}}{V\sigma_T + |\mu|A_{i-c} + |\eta|B} \tag{19}$$

This model, when invoked assumes a step representation of the flux in all three dimensions. The step model results in very slow attenuation of a source with intervals of practical size, and tends to always overestimate fluxes. In older versions of DOT, it was used as a negative fix-up.

3. <u>The Zero Fix-up</u>

Unlike the step model, the zero fix-up model cannot be used as a stand-alone model. This fix-up model is also more selective in the way it removes the negative fluxes. That is, the linear model is assumed in the dimensions that give positive fluxes, and only the negative fluxes are set to zero. This leads to seven sets of fix-up equations, rather than a single set as for step.

If any flux is negative, it is set to zero, and the cell average flux is recalculated assuming that that particular flux is zero. If the new cell average flux is negative, the fix-up attempt is terminated. This usually implies a negative source or boundary flux. If the cell average

flux is non-negative, the remaining two fluxes are extrapolated using the linear models. If either of these fluxes is negative, the cell average flux is recalculated assuming two fluxes are zero. If the cell average flux is positive, the remaining flux is extrapolated. If it is negative, then all three boundary fluxes are set to zero, and the cell averaged flux recomputed (assuming the total cross section is not zero).

A set of seven equations results from the zero fix-up strategy:

(1) Assume

$$N_{i+c} = 0.0 \tag{20a}$$

$$N_{j+d} = 2N - N_{j-d} \tag{20b}$$

$$N_{m+\frac{1}{2}} = 2N - N_{m-\frac{1}{2}} \tag{20c}$$

$$N = \frac{VS + |\mu|A_{i-c}N_{i-c} + 2|\eta|BN_{j-d} + \Delta A\beta N_{m-\frac{1}{2}}}{V\sigma_T + 2|\eta|B + \Delta A(\beta-\mu)} \tag{21}$$

Zero-Weight Direction

$$N = \frac{VS + |\mu|A_{i-c}N_{i-c} + 2|\eta|BN_{j-d}}{V\sigma_T + 2|\eta|B - \Delta A\mu} \tag{22}$$

(2) Assume

$$N_{i+c} = 2N - N_{i-c} \tag{23a}$$

$$N_{j+d} = 0.0 \tag{23b}$$

$$N_{m+\frac{1}{2}} = 2N - N_{m-\frac{1}{2}} \tag{23c}$$

$$N = \frac{VS + 2|\mu|\bar{A}N_{i-c} + |\eta|BN_{j-d} + \Delta A\beta N_{m-\frac{1}{2}}}{V\sigma_T + 2|\mu|\bar{A} + \Delta A\beta} \tag{24}$$

Zero-Weight Directions

$$N = \frac{VS + 2|\mu|\bar{A}N_{i-c} + |\eta|BN_{j-d}}{V\sigma_T + 2|\mu|\bar{A}} \tag{25}$$

(3) Assume

$$N_{i+c} = 2N - N_{i-c} \tag{26a}$$

$$N_{j+d} = 2N - N_{j-d} \tag{26b}$$

$$N_{m+\frac{1}{2}} = 0.0 \tag{26c}$$

$$N = \frac{VS + 2|\mu|\ \bar{A}N_{i-c} + 2|\eta|BN_{j-d} + \frac{1}{2}\Delta A(\beta+\mu)N_{m-\frac{1}{2}}}{V\sigma_T + 2|\mu|\bar{A} + 2|\eta|B + \Delta A\mu} \tag{27}$$

Zero-Weight Direction

$$N = \frac{VS + 2|\mu|\bar{A}N_{i-c} + 2|\eta|BN_{j-d}}{V\sigma_T + 2|\mu|\bar{A} + 2|\eta|B} \tag{28}$$

(4) Assume

$$N_{i+c} = 0.0 \tag{29a}$$

$$N_{j+d} = 0.0 \tag{29b}$$

$$N_{m+\frac{1}{2}} = 2N - N_{m-\frac{1}{2}} \tag{29c}$$

$$N = \frac{VS + |\mu|A_{i-c}N_{i-c} + |\eta|BN_{j-d} + \Delta A\beta N_{m-\frac{1}{2}}}{V\sigma_T + \Delta A(\beta-\mu)} \tag{30}$$

Zero-Weight Direction

$$N = \frac{VS + |\mu|A_{i-c}N_{i-c} + |\eta|BN_{j-d}}{V\sigma_T - \Delta A\mu} \tag{31}$$

(5) Assume

$$N_{i+c} = 0.0 \tag{32a}$$

$$N_{j+d} = 2N - N_{j-d} \tag{32b}$$

$$N_{m+\frac{1}{2}} = 0.0 \tag{32c}$$

$$N = \frac{VS + |\mu|A_{i-c}N_{i-c} + 2|\eta|BN_{j-d} + \frac{1}{2}\Delta A(\beta+\mu)N_{m-\frac{1}{2}}}{V\sigma_T + 2|\eta|B} \tag{33}$$

Zero-Weight Directions

Same as Eq. (22)

(6) Assume

$$N_{i+c} = 2N - N_{i-c} \tag{34a}$$

$$N_{j+d} = 0.0 \tag{34b}$$

$$N_{m+\frac{1}{2}} = 0.0 \tag{34c}$$

$$N = \frac{VS + 2|\mu|\bar{A}N_{i-c} + |\eta|BN_{j-d} + \frac{1}{2}\Delta A(\beta+\mu)N_{m-\frac{1}{2}}}{V\sigma_T + 2|\mu|\bar{A} + \Delta A\mu} \tag{35}$$

Zero-Weight Direction

Same as Eq. (25)

(7) Assume

$$N_{i+c} = 0.0 \tag{36a}$$

$$N_{j+d} = 0.0 \tag{36b}$$

$$N_{m+\frac{1}{2}} = 0.0 \tag{36c}$$

$$N = \frac{VS + |\mu| A_{i-c} N_{i-c} + |\eta| B N_{j-d} + \frac{1}{2}\Delta A(\beta+\mu) N_{m-\frac{1}{2}}}{V\sigma_T} \tag{37}$$

Zero-Weight Direction

Same as Eq. (31)

4. The Weighted Model

The weighted-difference model provides a smooth transition between the linear model in the case of small mesh spacing and the step model in the large. This smooth transition promotes rapid convergence of the iteration process and guarantees a non-negative emergent flux value if the source term is positive. The weighted-difference model uses three new parameters to interpolate between the linear and step models.

Assume

$$a = \frac{N - N_{i-c}}{N_{i+c} - N_{i-c}} \tag{38a}$$

$$b = \frac{N - N_{j-d}}{N_{j+d} - N_{j-d}} \tag{38b}$$

$$c = \frac{N - N_{m-\frac{1}{2}}}{N_{m+\frac{1}{2}} - N_{m-\frac{1}{2}}} \tag{38c}$$

so that

$$N_{i+c} = \frac{1}{a} N - \left(\frac{1 - a}{a}\right) N_{i-c} \tag{39a}$$

$$N_{j+d} = \frac{1}{b} N - \left(\frac{1 - b}{b}\right) N_{j-d} \tag{39b}$$

$$N_{m+\frac{1}{2}} = \frac{1}{c} N - \left(\frac{1 - c}{c}\right) N_{m-\frac{1}{2}} \tag{39c}$$

Then defining

$$X = |\mu| \left[(1/a - 1)\ A_{i+c} + A_{i-c}\right] \tag{40a}$$

$$Y = |\eta| \left[(1/b - 1)\ B_{j+d} + B_{j-d}\right] \tag{40b}$$

$$Z = \tfrac{1}{2}\Delta A \left[(1/c - 1)(\beta - \mu) + (\beta + \mu)\right] \tag{40c}$$

yields

$$N = \frac{VS + XN_{i-c} + YN_{j-d} + ZN_{m-\frac{1}{2}}}{V\sigma_T + X + Y + Z} \tag{41}$$

The values of a, b, and c are determined by first solving for the outgoing boundary fluxes and then, by examination, choosing these coefficients to ensure positivity of the boundary flux. Non-negativity of the flux can be assured by bounding a, b, and c between 1/2 (linear) and 1 (step) and using Eqs. (42) between these limits.

$$1 - a = \frac{SV\theta_s + \left[|\eta|BN_{j-d} + \tfrac{1}{2}\Delta A(\beta + \mu)\ N_{m-\frac{1}{2}}\right]\theta_n + |\mu|A_{i-c}\ N_{i-c}}{2\left[\tfrac{1}{2}\ V\sigma_T + |\eta|B + \tfrac{1}{2}\Delta A(\beta - \mu)\right]\ N_{i-c}} \tag{42a}$$

$$1 - b = \frac{SV\theta_s + \left[|\mu|A_{i-c}N_{i-c} + \tfrac{1}{2}\Delta A(\beta + \mu)\ N_{m-\frac{1}{2}}\right]\theta_n + |\eta|BN_{j-d}}{2\left[\tfrac{1}{2}V\sigma_T + |\mu|A_{i+c} + \tfrac{1}{2}\Delta A(\beta - \mu)\right]N_{j-d}} \tag{42b}$$

$$1 - c = \frac{SV\theta_s + \left[|\mu|A_{i-c}N_{i-c} + |\eta|BN_{j-d}\right]\theta_n + \tfrac{1}{2}\Delta A(\beta + \mu)N_{m-\frac{1}{2}}}{2\left[\tfrac{1}{2}V\sigma_T + |\mu|A_{i+c} + |\eta|B\right]N_{m-\frac{1}{2}}} \tag{42c}$$

The parameters θ_s and θ_n in Eq. (42) are arbitrary and can be related to previous formulations. In the 1968 version of TWOTRAN (x,y)[4] the formulation is equivalent to:

$$\theta_s = \theta_n = 0$$

This method never generates non-positive results, but will produce inaccurate results for large intervals with a source or for long, narrow intervals.

In 1969 a Lathrop paper[5] had $\theta_s = \theta_n = 1$, but in-house testing has shown this method to lead to many degenerate results near zero, which thwart convergence. In the 1973 version of DOT III[6], a compromise; $\theta_s = 1$, $\theta_n = 0$ was used. This worked well in source-dominated regions, but gave inaccurate results for source-free intervals of long, narrow shape. The present version of DOT IV differs from its predecessor in that the m-flow terms (i.e., terms involving $N_{m-\frac{1}{2}}$) are grouped with the source term with a multiplier of θ_s.

Zero-Weight Direction

$$N = \frac{VS + XN_{i-c} + YN_{j-d}}{V\sigma_T + X + Y} \tag{43}$$

The weighting coefficients a and b are defined by Eqs. (44). There is no c weighting coefficient for the zero-weight direction. The coefficients a and b are derived in a similar manner as for Eqs. (42).

$$1 - a = \frac{SV\theta_s + |\eta|BN_{j-d}\theta_n + |\mu|A_{i-c}N_{i-c}}{\left[V\sigma_T + 2|\eta|B - \Delta A\mu\right] N_{i-c}} \tag{44a}$$

$$1 - b = \frac{SV\theta_s + |\mu|A_{i-c}N_{i-c}\theta_n + |\eta|BN_{j-d}}{\left[V\sigma_T + 2|\mu|A_{i+c} - \Delta A\mu\right]N_{j-d}} \tag{44b}$$

5. <u>The Theta-Weighted Model</u>

The theta-weighted model[7] is essentially a specific case of the weighted difference model. An arbitrary multiplier is used to avoid degeneracy yet to use the accurate linear model when the source or flow from adjacent boundaries actually controls N;

$$\theta_s = \theta_n = \theta$$

Values of θ ranging from 0.5 to 0.9 have been tested with satisfactory results. Apparently any value near 1, but not near enough to produce numerical degeneracy, is acceptable. At present a value of 0.9 is used in DOT IV. This gives results which are often very similar to those of the linear model with zero fix-up and often converges faster, and is therefore less expensive.

IV. SOLUTION TO THE DOT-TWOTRAN DISCREPANCY

The DOT and TWOTRAN series of discrete ordinates codes were developed by different teams of researchers, each with their own ideas concerning approximations that would be incorporated in their code. The DOT codes were developed primarily for use in the area of deep penetration shielding analysis, which is characterized by problems with fixed sources, highly anisotropic fluxes, and large flux attenuations. The TWOTRAN codes have found their largest use in reactor core problems, i.e., eigenvalue problems, which are usually characterized by more isotropic fluxes. Owing to this difference in objectives, two very different philosophies were adopted.

The recent TWOTRAN codes offer only the linear-zero difference model (other versions had other models), while the DOT code provides the user with a number of difference models to choose among, depending on the problem at hand. TWOTRAN's treatment of the initial direction is also different from that used in DOT. TWOTRAN uses the step-initiation model in angle in the first direction of each η level, while the DOT codes traditionally use the zero-weight approach. Due to these differences, DOT and TWOTRAN gave different results to many problems,[8] and the explanation in a given case could only be incomplete. In an attempt to find any discrepancies between DOT and TWOTRAN, TWOTRAN's zero fix-up and step-initiation features were incorporated into a temporary version of DOT. A number of X-Y geometry problems were run in both codes without the use of flux rebalance. X-Y geometry was chosen first because the angular flow terms are not present in this geometry, and thus the zero-weight

directions have no effect. The rebalance acceleration was omitted since DOT and TWOTRAN rebalance in a different manner. In all cases DOT and TWOTRAN agreed exactly.

The second set of test problems was run in R-Z geometry. When DOT and TWOTRAN were run using the linear "diamond difference" model they once again agreed exactly with each other. However, when a negative flux was calculated and it became necessary to invoke the zero fix-up model the codes were in gross disagreement. After extensive investigation it was found that there was a basic flaw in TWOTRAN.

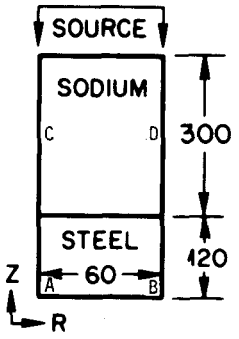
In the initial direction, TWOTRAN uses the step model in angular space, which guarantees a positive flux in the angular dimension, but not necessarily in the spatial dimensions. When one of the extrapolated spatial fluxes is negative, the fix-up equations are invoked. TWOTRAN does not have a special set of fix-up equations for the initial directions, where the step model in angle is employed. The effects of this approximation are discussed later in this report. The fix-up equations are derived assuming a linear variation of the flux for the direction that is not being fixed up. For the initial direction, this is inconsistent with the step model that was used originally and leads to a term coupling the mean flux to a previous flux that does not exist [see Eq. (19) or (22)]. The value that was used by TWOTRAN was the value that was left in the computer's memory by previous calculations. This is obviously in error. The equations do not indicate what should be used. A correction was made to TWOTRAN to set the undefined flux to zero if the fix-up equations were invoked, corresponding to the DOT treatment. This brought DOT and TWOTRAN

back into agreement. TWOTRAN was run to convergence with and without the correction, to assess the effects of the error (reported later).

A different formulation of the zero fix-up model is being made available in DOT IV. Zero-weight directions are used rather than the step model in the first angle in each η level. The corresponding equations were listed previously. Running this DOT option allowed isolation of the effects of zero-weight directions. The problem chosen was the 20 X 50 R-Z sodium-steel problem described later in this report. The results are presented in Table 1. The correction to TWOTRAN decreased the emergent flux along the bottom of the mesh by a factor of 3.56 at the center line and 1.65 at the edge. The larger error at the center line is due to the more frequent use of the fix-up model in this region of the problem. The use of zero-weight directions increased the emergent flux at the center line by a factor of 1.10 and decreased it by a factor of 1.13 at the edge. However, the leakage from the right and bottom boundaries of the problem agree within 1 percent.

The fluxes closer to the source behave in a manner consistent with the flux model being employed. That is: linear-zero gives the smallest flux values, as would be expected by the nature of the fix-up model; weighted gives the largest flux values, as expected, since we know it is approximately the same as the step model for coarsely meshed problems; and theta-weighted flux values lie between these models. However, this is not true of the fluxes further away from the source, indicating that knowledge of the behavior of the flux model locally does not necessarily imply knowledge of the behavior of the flux model over the entire problem.

Table 1. TWOTRAN Versus DOT Flux Comparison for the First Group of the R-Z Sodium-Steel Problem



Code	Flux at A	Flux at B	Flux at C	Flux at D
TWOTRAN II	3.07152-18	3.25054-19	3.16834-7	1.00751-7
TWOTRAN II (corrected)*	8.63367-19	1.97081-19	2.25276-7	1.13672-7
DOT IV (linear-zero)	9.53677-19	1.73965-19	2.00958-7	9.09857-8
DOT IV (weighted)	8.68320-19	1.41253-19	5.01178-7	1.99149-7
DOT IV (θ-weighted)	6.42672-19	1.20006-19	2.63975-7	1.12762-7

*DOT IV gives identical results for this case when the step-initiation model is used together with the corrected zero fix-up equations.

Therefore, it is impossible to *a priori* determine a "conservative" flux model.

The linear-zero model tended to yield higher bottom leakage than either the weighted or theta-weighted models. This could be a result of the selectiveness of the zero fix-up; that is, only the fluxes that need to be fixed-up are fixed, while the linear model is used in the remaining dimensions. In principle, weighted tends to yield a higher flux than linear zero, since it uses the linear model for small intervals, making a smooth transition to non-negative values for large intervals. Examining the flux at the midplane of the problem, we see that weighted has caused more neutrons to migrate to the side of the problem and to leak. The higher leakage flux ultimately lead to lower flux at the problem boundary.

It should be noted that the corrected linear-zero model described herein is not truly consistent when used without zero-weight direction. In fact, a careful derivation of the zero fix-up equations to be used for the step-initialization directions shows that they are identical to the zero-weight equations. This is not equivalent to setting $N_{\frac{1}{2}} = 0$, as was done in this study. In a later section, it will be seen that this inconsistency, not the type of initialization, is responsible for much of the remaining difference between the linear-zero and corrected step-initialization results noted in this section.

V. EXTRAPOLATION MODEL EVALUATION

The convergence of the various flux extrapolation models to a unique solution with refinement of the spatial mesh has always been a matter of concern to users of transport codes. It has been tacitly assumed that if the mesh is refined until the maximum interval is less than two mean free paths, $\left[\frac{\sigma\Delta r}{\mu}\right]$, in any direction, negative fluxes will not be generated if the source and incoming boundary fluxes are positive.

In order to assess the validity of this assumption, three small sample problems that have characteristics similar to those encountered in shielding analysis and one cell eigenvalue problem were solved on a number of spatial grids. Each successive mesh was halved until all intervals in the problems were less than two mean free paths. Isotropic scattering was assumed in all cases and an S_8 fully symmetric quadrature was used. The linear-zero model with zero-weight directions, the linear zero model with step-initialization, the theta-weighted model and the weighted model were all used in this study. The mesh spacing was extrapolated to zero using a three parameter fit of the following form:

$$L^{\infty} = C_1 + C_2(\sigma\Delta x)^{C_3} \tag{45}$$

The results for the first group leakage opposite the source versus mesh size and a description of each of the shielding problems are shown in Figs. 1 through 3.

In all cases, the weighted model yielded extrapolated leakage fluxes that were higher than those calculated with the other models. This is

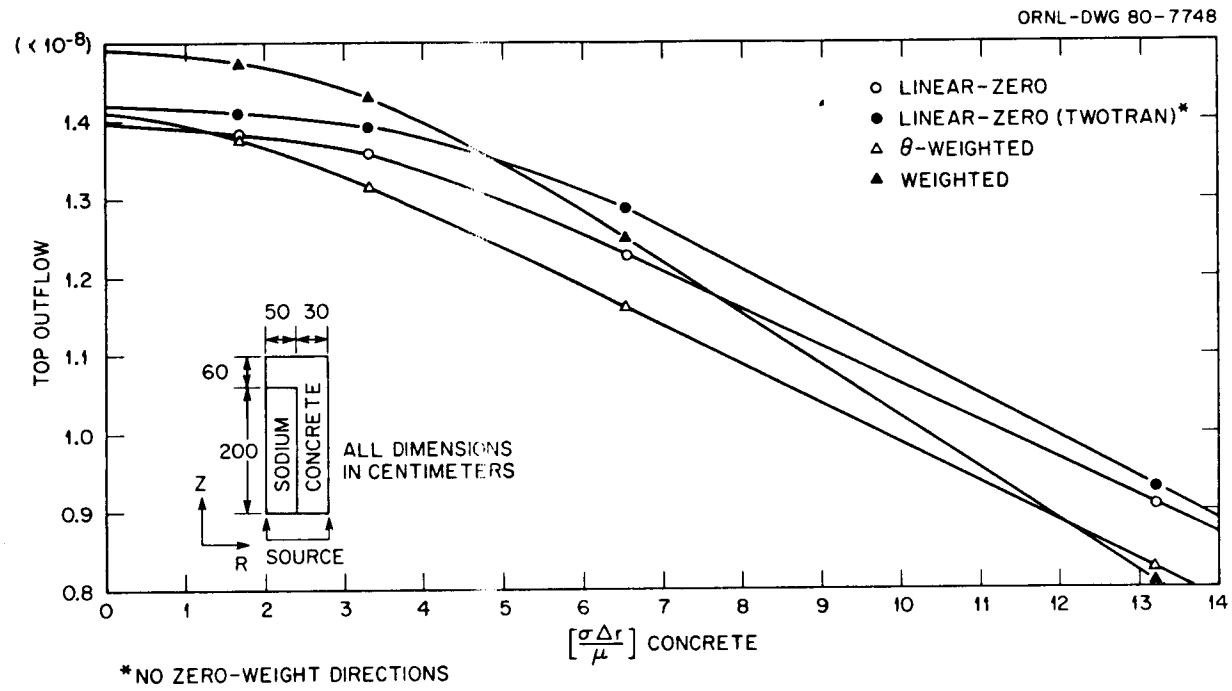


Fig. 1. Top leakage versus mesh size for a sodium-concrete system.

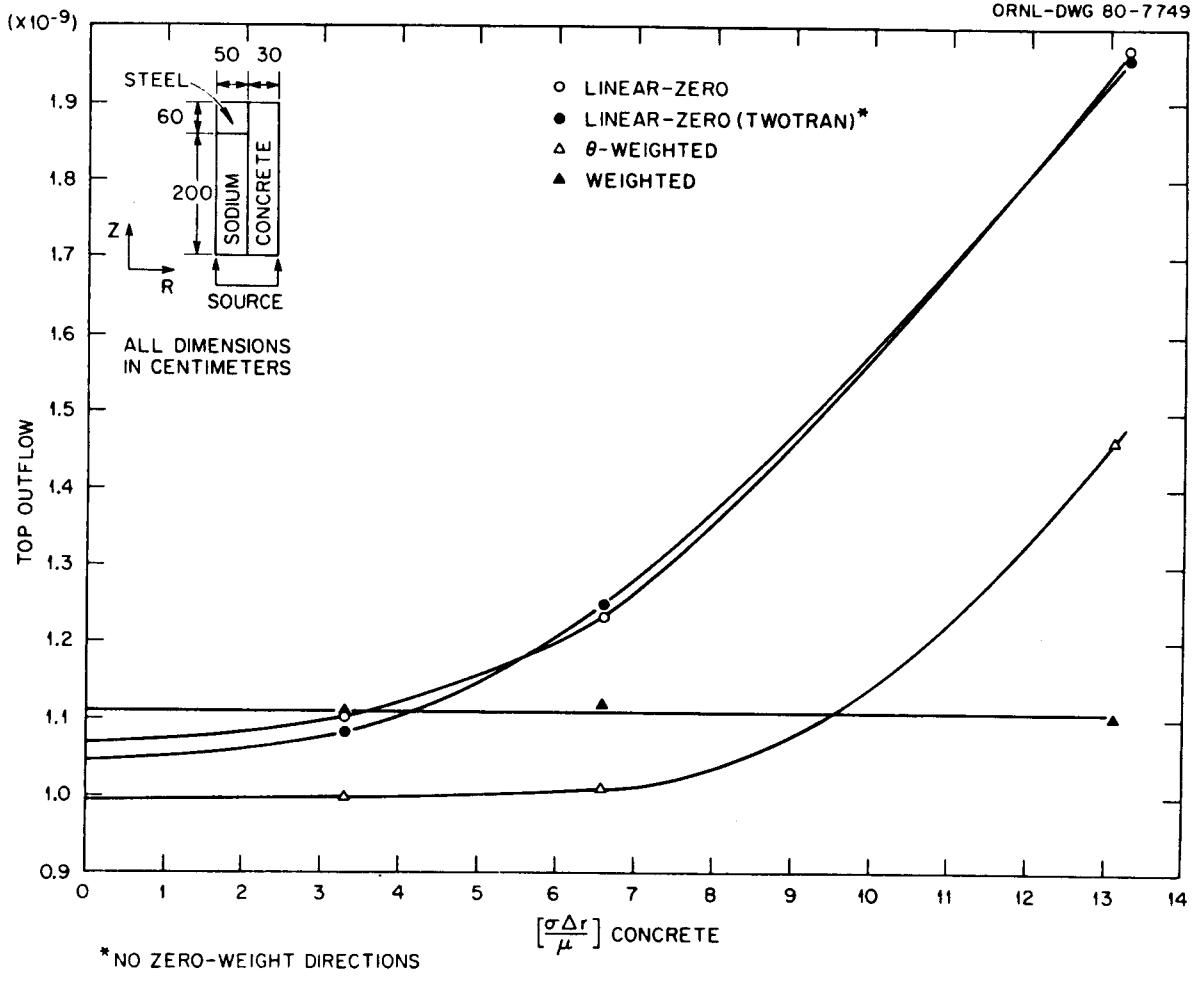


Fig. 2. Top leakage versus mesh size for a sodium-concrete-steel system.

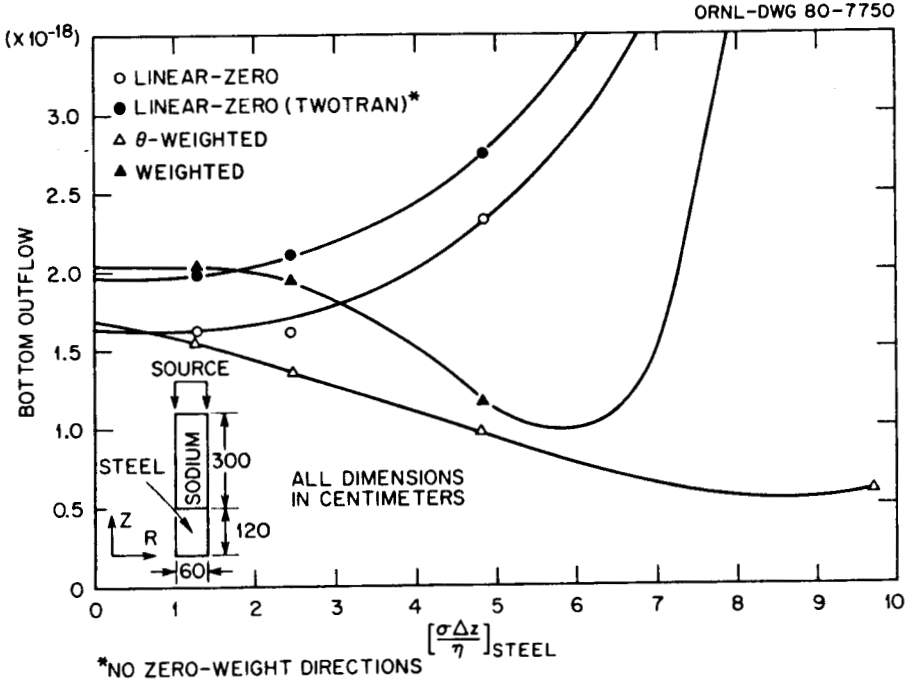


Fig. 3. Bottom leakage versus mesh size for a sodium-steel system.

in agreement with general experience. The remaining models give approximately the same result, although the theta-weighted model sometimes converges faster than either of the linear-zero models. Since shielding problems are often performed using mesh spacings corresponding to abscissas of 5-7 on these plots the error introduced by finite mesh spacing can be larger than the difference between models. Other mesh-spacing considerations such as the "factor-of-two-flux-variation-between-intervals" rule are now suspected of producing poor results.

As the mesh was refined, all models except the weighted model became more difficult to converge. Calculations with meshes below the two mean free path limit, where all models should be solving the linear (diamond difference) equations with no negative flux fix-up, could not be made to converge. The material densities were reduced until almost void conditions existed and this phenomenon persisted. Further understanding of this phenomenon can be gained by examining the linear equation for the cell averaged flux:

$$N = \frac{VS + 2|\mu|\bar{A}N_{i-c} + 2|\eta|BN_{j-d} + \Delta A\beta N_{m-\frac{1}{2}}}{V\sigma_T + 2|\mu|\bar{A} + 2\ |\eta|B + \Delta A\beta} \tag{15}$$

The source term in Eq. (15) is usually small for the first groups in typical shielding problems because the majority of the source in these groups is the self-scatter source, and also, V is small as the mesh is refined. The N_{i-c} term in the first groups is small especially near the right boundary for problems with top or bottom boundary sources. The $N_{m-\frac{1}{2}}$ term is usually small in these groups because of the forward peaked scattering. These conditions lead to Eq. (46).

$$\bar{N} \simeq \frac{|\eta| B \, N_{j-d}}{|\mu| \bar{A} + |\eta| B + \frac{1}{2}\Delta A \beta} \tag{46}$$

Since A and B are usually of comparable magnitude, $\bar{N}$ for some directions will be less than $\frac{1}{2}N_{j-d}$, resulting in a negative value of N_{j+d}. This effect is not seen in the 1-D geometries. It results in the use of negative fix-up procedures in typical 2-D shielding calculations no matter how fine the mesh becomes. In such cases, the converged result depends upon the extrapolation model, and convergence of the iterative process becomes more difficult.

The emergent scalar flux from the bottom of the sodium-steel problem is presented in Fig. 4. The spatial oscillations in the flux resulting from the use of the models based on the linear formulation are evident. The weighted model however calculates a flux shape that is smooth and more representative of the physical situation, but results in a higher total leakage from the bottom of the system. The theta-weighted model calculates results that are somewhat smoother than the linear formulations with fix-up, but gives a lower leakage. However, inspection of Figs. 1 through 3 indicates that the theta-weighted model gave results that were closer to the extrapolated zero mesh spacing results.

The cell eigenvalue problem is shown in Fig. 5. This problem is characterized by long narrow intervals, which tend to cause difficulty with the weighted-difference model. The scattering was assumed to be linearly anisotropic, and an S_4 fully symmetric quadrature set was used for these calculations. The results are shown in Table 2.

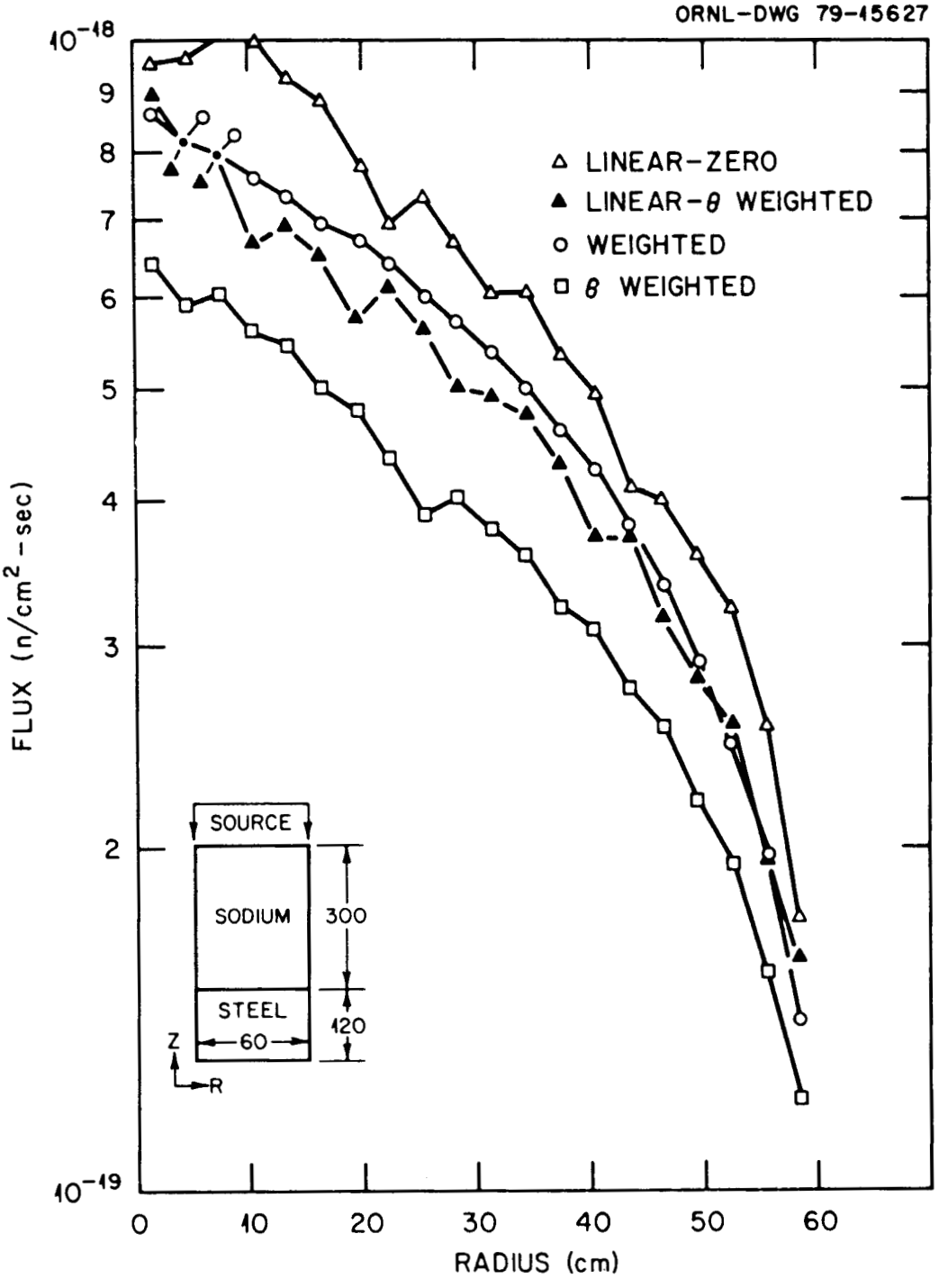


Fig. 4. Emergent flux from the 20 x 50 sodium-steel problem.

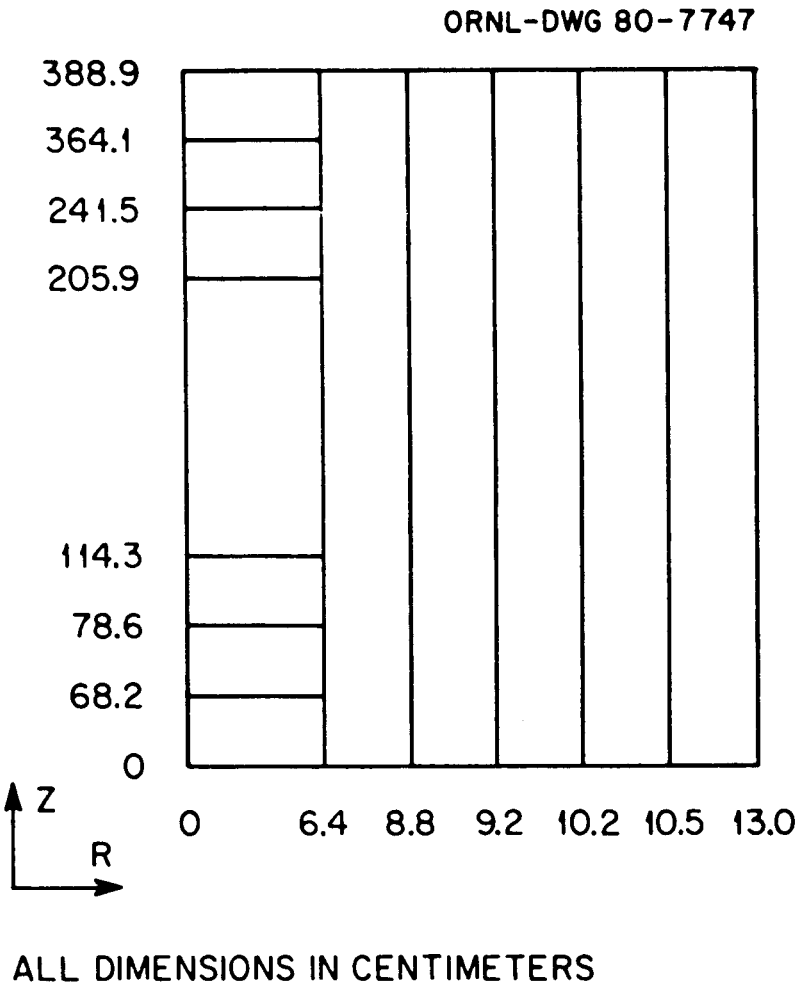


Fig. 5. Cell eigenvalue problem geometry.

Table 2. The Calculted k-eff for the Cell Eigenvalue Problem Various Flux Models

Model	k-eff
Linear-zero	0.9926
Linear-zero (TWOTRAN)	0.9927
-weighted	0.9897
Weighted	0.9519
Monte Carlo	0.986 ± 0.015
Point fission source convergence of <0.025 for DOT cases.	

As was seen previously, the weighted model gave the higher leakage, which resulted in a lower k_{eff} eigenvalue. The other models gave essentially the same results, and are in agreement with the MORSE Monte Carlo calculation.

As to which model is preferable, the study has shown that the weighted model converges to a higher leakage, which is in agreement with general experience. It is preferred for shielding calculations where the maximum leakage is sought, but is unsuitable for eigenvalue problems for the same reason. The remaining models give approximately the same results. The theta-weighted model sometimes converges faster than the linear-zero models, and may be preferred where convergence difficulty is expected. The linear-zero model is inexpensive, and is applicable to most eigenvalue problems which are not expected to present flux convergence difficulty.

VI. ZERO-WEIGHT DIRECTION EVALUATION

As stated earlier in this report, one of the basic differences between DOT and TWOTRAN is that DOT traditionally requires zero-weight directions in its angular quadrature set, while TWOTRAN uses step-initialization. TWOTRAN also uses a zero fix-up model that is based on the linear extrapolation model, and implies an undefined flux, as discussed previously. When the zero fix-up equations are derived approximately, the resultant equations are identical to the equations for the zero-weight directions.

In order to assess the effectiveness of zero-weight directions, a simple two zone, 21 energy group, R-Z problems were constructed. An isotropic boundary source was applied at the top boundary. Nonreturn boundary conditions were applied at the right and bottom of the problem. An S_8 direction quadrature set from the TWOTRAN code, with zero-weight directions added, was used in all problems. The problem was 60.0 cm in radius and 420.0 cm in height. The top boundary source is incident on 300.0 cm of sodium followed by 120.0 cm of steel. In this case there were 20 equally spaced mesh intervals in the radial direction, 20 equally spaced mesh intervals axially in the sodium, and 30 equally spaced mesh intervals in the steel. The scattering was assumed to be linearly anisotropic. The following calculations were performed:

1. Standard DOT IV linear-zero model with zero-weight directions
2. Standard TWOTRAN linear-zero with the corrected initial angle fix-up based on the linear extrapolation model
3. DOT IV linear-zero with the step-initialization consistently derived

4. Standard TWOTRAN linear-zero model without the initial angle correction. The results of these calculations are presented in Figs. 6 and 7. Only the group one fluxes are presented.

Figure 6 presents the scalar flux along the top mesh row in the sodium. The zero-weight direction calculation and the step in angle with the consistent fix-up equations are in excellent agreement. The standard TWOTRAN models, both with and without the correction, give results that indicate a depression in the flux along the center of the cylinder; obviously not physically correct.

Figure 7 presents the scalar fluxes in the last interval in the steel. The uncorrected TWOTRAN yields results that are in greatest disagreement with the other calculations. All four models give poor results, marred by spatial oscillation.

In summary, both the zero-weight direction model and the step initial-direction model with a consistent fix-up model give results that are physically acceptable near the source. None of the fix-up models give particularly good results at the bottom of the cylinder.

These results seem to indicate that the step initiation model with a consistent fix-up is computationally more cost efficient, since fewer directions need be calculated using this method, and the results are no worse. However, examination of the quadrature sets supplied with the TWOTRAN code reveals that the initial (and final, due to symmetry) directions have large η values (near 1) compared to a set of equivalent order that would be used in DOT. It appears that these directions may behave like zero-weight directions which also have η values near unity. This raises the question of the adequacy of a given quadrature set.

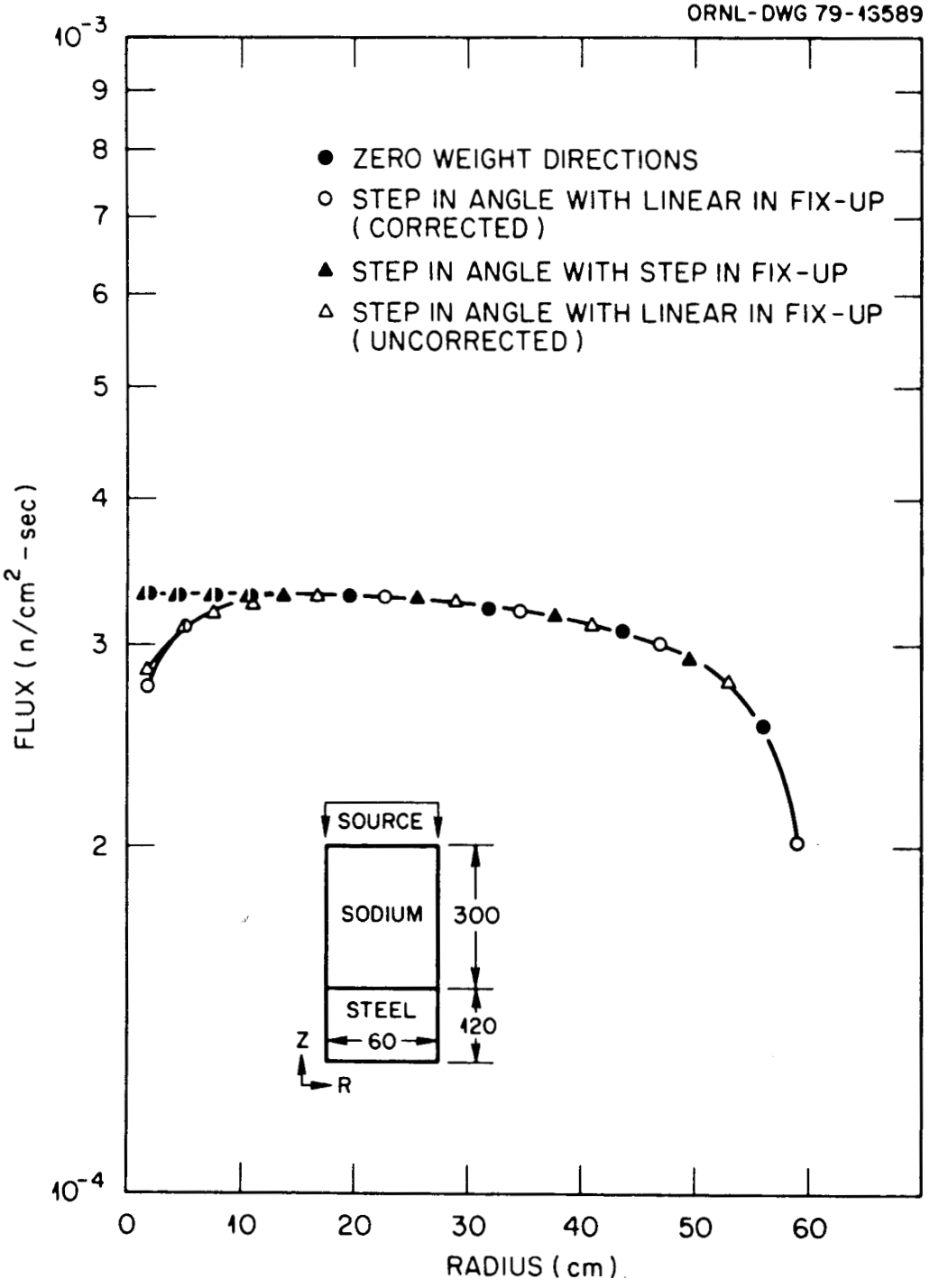


Fig. 6. Scalar flux at the top boundary of sodium-steel system.

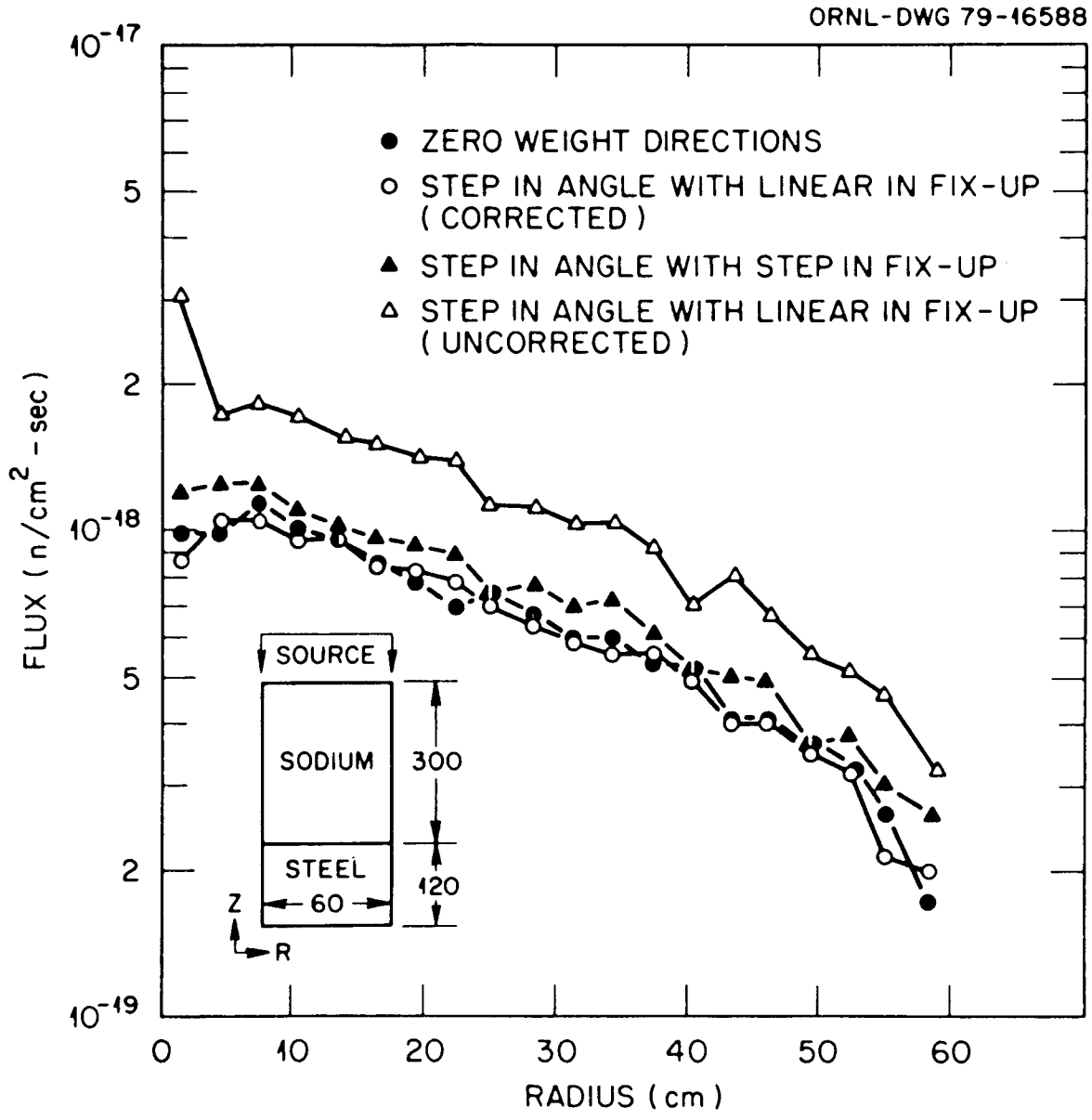


Fig. 7. Emergent scalar flux from the sodium-steel system.

An R-Z model of a SNAP reactor was chosen to evaluate the effect of zero-weight directions on eigenvalue calculations. This system is characterized by relatively high radial leakage. Four three group, S_4P_3 problems were run. The linear-zero model, with and without zero-weight directions, was used with the standard DOT and TWOTRAN quadratures. The results of these calculations are shown below. Again, the difference in k_{eff} results from the inclusion of zero-weight directions was insignificant.

	DOT Quadrature	TWOTRAN Quadrature
With zero-weight directions	0.923213	0.924330
Without zero-weight directions	0.923685	0.924770

VII. CONCLUSIONS

The DOT IV discrete ordinates transport code allows the user to choose among various flux extrapolation models to mitigate the effects of over-extrapolation error in shielding problems. The assumptions for each of these models and the resultant equations have been present in this report to enhance the user's understanding of the code.

A detailed comparison between DOT and TWOTRAN uncovered a model deficiency in the TWOTRAN code. With this deficiency in modeling treated identically in both codes, it was shown that DOT and TWOTRAN produced identical results for all the problems studied. Thus, the decade-old discrepancy was resolved.

The study has shown that for the problems studied, the flux models do not converge to a single solution as the spatial mesh is refined. It was also discovered that, regardless of the degree to which the mesh is refined, the negative flux fix-up models will always be needed during a calculation. This sometimes thwarts the convergence of fine-mesh problems. The error in the converged results due to finite mesh spacing may be greater than the difference between flux extrapolation models. This is particularly true in the range of mesh sizes commonly used in shielding analysis.

The inclusion of zero-weight boundary directions in the quadrature set was shown to have no significant effect on the converged results for the problems studied.

Since no exact solutions are available for judging the accuracy of the various models it may be appropriate to seek a model which most consistently avoids erratic behavior as the mesh spacing is increased. In this and other studies, the theta-weighted model appears to be the best choice to achieve this end. It converges in fewer iterations than the linear-zero model. The use of contemporary coding techniques makes the execution speed of the theta-weighted model approximately the same as that of the linear-zero model. The differences in the zero-mesh results are probably insignificant compared to the mesh size effects. Thus, theta-weighted is the appropriate choice in the absence of indications to the contrary.

Weighted was seen to give smoother flux shapes, and gives higher (and thus conservative) leakage currents for some problems. This study has shown that weighted leakage is not higher for all problems. However, it sometimes converges better than all other models.

The use of linear-zero should probably be restricted to eigenvalue calculations which are to be compared to other linear-zero results. The older linear-step model (not included in this study) should not be used at all.

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