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TITLE: AN ADAPTIVE WEIGHTED DIAMOND DIFFERENCING METHOD FOR THREE-DIMENSIONAL, XYZ GEOMETRY

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AN ADAPTIVE WEIGHTED DIAMOND DIFFERENCING METHOD FOR THREE-DIMENSIONAL, XYZ GEOMETRY

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I. INTRODUCTION

About sixteen years ago, Bengt Carlson[1] introduced a method for discretizing the neutral particle transport equation to achieve a positive solution while at the same time retaining much of the accuracy of the diamond differencing method. About six years later Russian researchers[2] applied this work to their problems and extended it somewhat to enhance the flexibility of the method to incorporate monotonic properties of the solution. This latter work came to the attention of U.S. researchers in late 1991 where it verified much of Carlson's conclusions in theory and in test problems. This method, called the adaptive weighted diamond (AWDD) method, is based upon a weighted diamond discretization of the transport equation with the weights chosen from a diamond difference prediction of the solution so as to correct it for positively and monotonicity. This work reexamines the method and extends it to three-dimensional XYZ geometry and demonstrates its potential for solving such problems accurately while achieving a much smoother solution than diamond with set-to-zero fixup and is as effective as the theta-weighted fixup method[3] while theoretically and operationally more satisfying.

II. SKETCH OF THE ADAPTIVE WEIGHTED DIAMOND METHOD AND ITS PROPERTIES

We begin with the discretized, three-dimensional XYZ transport balance equation written in the form

$$\mu h_y h_z(\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}) + \eta h_x h_z(\psi_{j+\frac{1}{2}} - \psi_{j-\frac{1}{2}}) + \xi h_x h_y(\psi_{k+\frac{1}{2}} - \psi_{k-\frac{1}{2}}) + \sigma_t V \psi = SV \tag{1}$$

where h is the mesh size in the x, y, or z directions; μ, η, and ξ are the direction cosines in each direction, and the other symbols have their usual meaning.

To obtain a weighted diamond equation, we assume the following relationship between the cell center and cell edge fluxes:

$$(1+P_x)\psi = \begin{cases} P_x\psi_{i+\frac{1}{2}} + \psi_{i-\frac{1}{2}} & \text{for } \mu < 0 \\ \psi_{i+\frac{1}{2}} + P_x\psi_{i-\frac{1}{2}} & \text{for } \mu > 0 \end{cases}$$

$$(1+P_y)\psi = \begin{cases} P_y\psi_{j+\frac{1}{2}} + \psi_{j-\frac{1}{2}} & \text{for } \eta < 0 \\ \psi_{j+\frac{1}{2}} + P_y\psi_{j-\frac{1}{2}} & \text{for } \eta > 0 \end{cases} \tag{2}$$

$$(1+P_z)\psi = \begin{cases} P_z\psi_{k+\frac{1}{2}} + \psi_{k-\frac{1}{2}} & \text{for } \xi < 0 \\ \psi_{k+\frac{1}{2}} + P_z\psi_{k-\frac{1}{2}} & \text{for } \xi > 0 \end{cases}$$

where the weight,

$$O \le P_x \le 1, O \le P_y \le 1, O \le P_z \le 1 .$$

Combining Eqs. (1) and (2), we find that the cell averaged flux in the octant $\mu < 0, \eta < 0, \xi < 0$ is

$$\psi = \frac{SV + |\mu|h_yh_z(1+P_x)\psi_{i+\frac{1}{2}} + |\eta|h_xh_z(1+P_y)\psi_{j+\frac{1}{2}} + |\xi|h_xh_y(1+P_z)\psi_{k+\frac{1}{2}}}{\sigma_t V + |\mu|h_yh_z(1+P_x) + |\eta|h_xh_z(1+P_y) + |\xi|h_xh_y(1+P_z)} \tag{3}$$

We now determine the weights such that a positive solution is obtained and desired properties of monotonicity of solution are attained. To do this we consider each coordinate direction independently, and using the x direction as representative, we rewrite Eq. (1) with assumptions of Eq. (2) as

$$\mu(\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}) + \sigma_x h_x \psi = S_x h_x \tag{4}$$

where

$$\sigma_x h_x = \sigma_t h_x + |\eta|\frac{h_x}{h_y}(1+P_y) + |\xi|\frac{h_x}{h_z}(1+P_z)$$

$$S_x h_x = Sh_x + |\eta|\frac{h_x}{h_y}(1+P_y)\psi_{j+\frac{1}{2}} + |\xi|\frac{h_x}{h_z}(1+P_z)\psi_{k+\frac{1}{2}}$$

As a first step, we solve Eq. (4) using diamond differencing ($P_x = 1$, $\mu < 0$) with the results

$$2\left(\frac{\psi - \psi_{i+\frac{1}{2}}}{\psi}\right) + \epsilon_x\left(1 - \frac{S_x}{\sigma_x\psi}\right) = 0 \tag{5}$$

where

$$\epsilon_x = \frac{\sigma_x h_x}{|\mu|}$$

or rewriting

$$2U_x = \epsilon'_x \tag{6}$$

where

$$U_x = \frac{\psi_{i+\frac{1}{2}} - \psi}{\psi}, \quad \epsilon'_x = \epsilon_x\left(1 - \frac{S_x}{\sigma_x \psi}\right)$$

Thus U_x is the diamond difference estimate of the logarithm derivative of the flux while ϵ'_x is a measure of the effective optical size of the cell which may be much smaller than the physical optical depth ϵ_x and is a more appropriate measure of the domain of applicability of the diamond method which infact we shall make use of subsequently.

We now return to solving Eq. (4) using weighted diamond form and, after some manipulation, we can write the cell exiting flux in the form

$$\psi_{i-\frac{1}{2}} = \frac{\left[1 - (2U_x - 1)P_x\right]\psi_{i+\frac{1}{2}} + (1 - P_x U_x)\epsilon_x \frac{S_x}{\sigma_x}}{1 + P_x + \epsilon_x} \tag{7}$$

From Eq. (7) it is seen that

$$\text{if} \quad U_x \le 1 \quad \text{and} \quad P_x = 1, \quad \text{then} \quad \psi_{i-\frac{1}{2}} \ge 0$$

$$\text{if} \quad U_x \ge 1 \quad \text{and} \quad P_x = \frac{1}{2U_x - 1}, \quad \text{then} \quad \psi_{i-\frac{1}{2}} \ge 0 \quad . \tag{8}$$

Thus Eq. (8) gives the sufficient condition for a non-negative exiting flux; we see that the weights depend upon the value of the logarithm derivative estimate Ux. We wish now to inject the issue of monotonically of solution. We can show that the solution to the analytic equation upon which Eq. (4) is based, has the property:*

$$\frac{\psi_{i-\frac{1}{2}} - \frac{S_x}{\sigma_x}}{\psi_{i+\frac{1}{2}} - \frac{S_x}{\sigma_x}} = e^{-\epsilon_x} > 0 \tag{9}$$

From Eq. (7), we can derive

$$\psi_{i-\frac{1}{2}} - \frac{S_x}{\sigma_x} = \frac{(1 - P_x)(\psi_{i+\frac{1}{2}} - \frac{S_x}{\sigma_x}) - P_x U_x(2\psi_{i+1/2} + \epsilon_x \frac{S_x}{\sigma_x})}{1 + P_x + \epsilon_x} \tag{10}$$

* A generalization of this appears in Ref. 2, p. 72

Thus for $\psi_{i+\frac{1}{2}} - \frac{S_x}{\sigma_x} > 0$, we require $\psi_{i-\frac{1}{2}} - \frac{S_x}{\sigma_x} < 0$ for monotonicity, which means that $P_x U_x$ may need to be adjusted from that implied by Eq. (8). To do this, we define two parameters U_{ox} and b_x to extend Eq. (8).

Using these parameters, we prescribe

$$\begin{aligned} &\text{for} \quad b_x U_x \le U_{ox} \quad \text{set} \quad P_x = 1 \\ &\text{for} \quad b_x U_x \ge U_{ox} \quad \text{set} \quad P_x = \frac{U_{ox}}{b_x U_x} \end{aligned} \qquad (11)$$

The prescription of Eq. (11) gives a smooth transition from the diamond to weighted diamond and also allows flexibility in obtaining a monotonic solution by adjusting PxUx more favorably as is motivated by Eq. (10). This is explored in the example given in the next section.

III. EXAMPLE PROBLEM AND CONCLUSIONS

The example used for this paper is a simple iron water shielding problem based upon that of Ref. 4. The problem is cubic, 50 cm x 50 cm x 50 cm, with symmetry boundary condition on the left bottom and front faces. This is a three group problem solved in S-8 quadrature with a 10 x 10 x 10 cm source region in the bottom-left front corner, surrounded with 10 cm of iron in turn surrounded by 30 cm of water. A 1 cm spatial mesh was used in all dimensions. Flux profiles are presented on selected x-y planes for the outside j levels in Fig. 1 and on the front face in Fig. 2. These calculations are compared with diamond set-to-zero, theta weighted diamond and the present AWDD with Uo = 1/2, and b = 2 for group 1 and b = 1 for group 3. A further comparison curve in group 3 is for b = 2 which shows some adverse effect of being too vigorous with monotonicity. Briefly, it is seen that the AWDD method is successful in achieving a much smoother solution while retaining accuracy. It achieves accuracy comparable with the theta-weighted method in this case. In a typical 3D eigenvalue problem whose k is 0.96236, theta weighted gives 0.96193 whereas AWDD gives 0.96226. These and many other results also point up to the fact that one must be careful in the choice of the value of the parameters Uo and b. In the near future we intend to make their choice less empirical and more based upon the needs of the solution itself.

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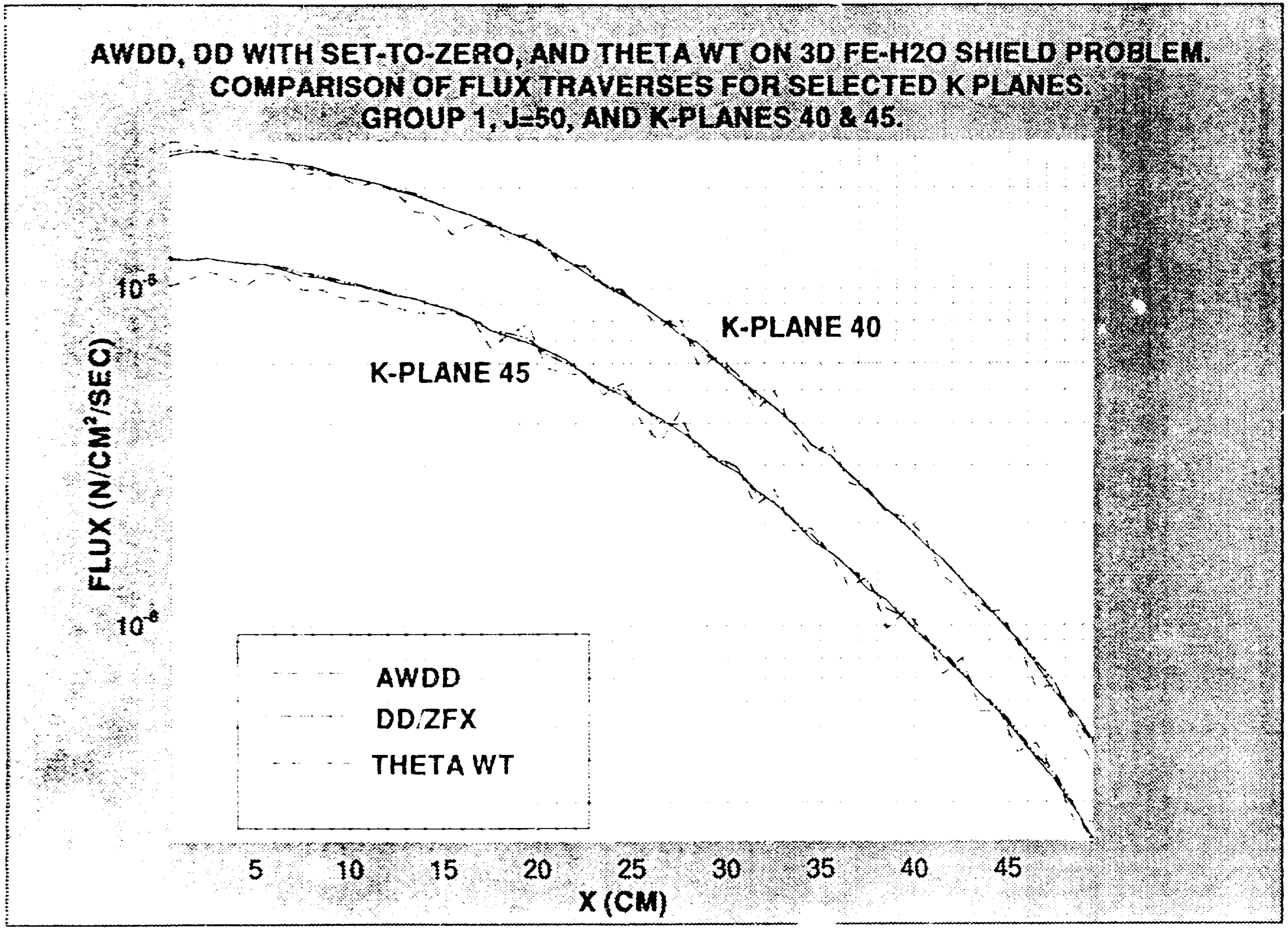
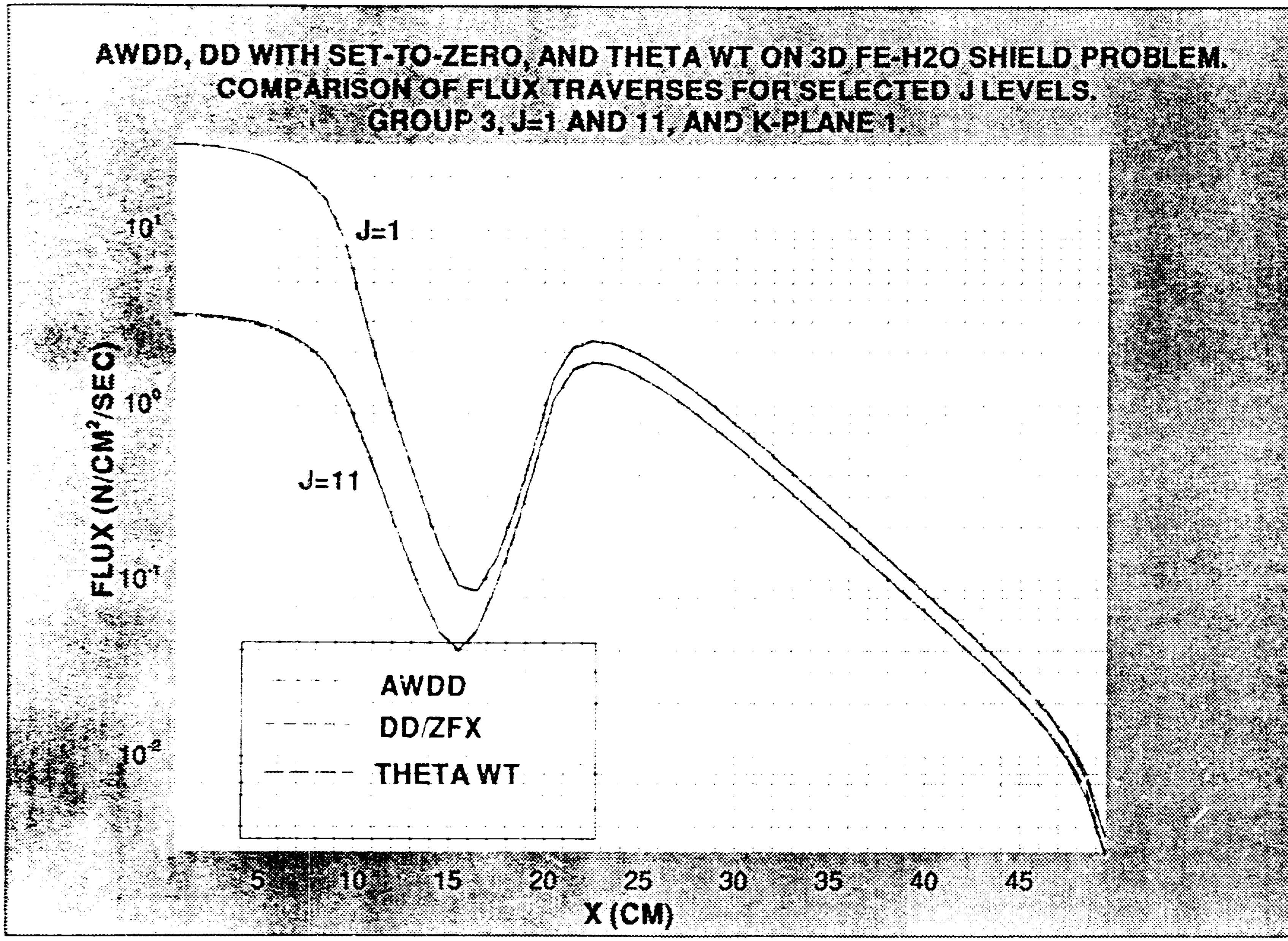
Figure


AWDD, DD WITH SET-TO-ZERO, AND THETA WT ON 3D FE-H2O SHIELD PROBLEM.
COMPARISON OF FLUX TRAVERSES FOR SELECTED K PLANES.
GROUP 1, J=50, AND K-PLANES 40 & 45.
FLUX (N/CM²/SEC)
10⁻⁵
10⁻⁶
K-PLANE 40
K-PLANE 45
AWDD
DD/ZFX
THETA WT
5
10
15
20
25
30
35
40
45
X (CM)


AWDD, DD WITH SET-TO-ZERO, AND THETA WT ON 3D FE-H2O SHIELD PROBLEM.
COMPARISON OF FLUX TRAVERSES FOR SELECTED J LEVELS.
GROUP 3, J=1 AND 11, AND K-PLANE 1.
J=1
J=11
FLUX (N/CM²/SEC)
10¹
10⁰
10⁻¹
10⁻²
AWDD
DD/ZFX
THETA WT
5
10
15
20
25
30
35
40
45
X (CM)