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COMPARISON OF REBALANCE STABILIZATION METHODS FOR TWO-DIMENSIONAL TRANSPORT CALCULATIONS*

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INTRODUCTION

The introduction of the space-dependent rebalance method in 1968[1] resulted in dramatic improvement in the convergence of deep-penetration transport problems. The value of the method was limited, however, by its tendency to overcorrect. In the DOT III code,[2] rebalance was applied to only every third iteration. That method was so successful that the code is still in use today.

In 1971, however, Reed showed a better way.[3] He showed that stability could be insured, at least in 1-D geometry with uniform mesh and cross sections, by adding fictitious boundary flows at each boundary. Since then, the extension of this work to general multidimensional problems has led to several interpretations. This paper will compare three of these interpretations and show a sound basis for the generalization.

DEVELOPMENT

With the 1-D discrete-ordinates iteration process for some group:

$$\mu_m \left(A_{i+\frac{1}{2}}\psi^k_{i+\frac{1}{2}} - A_{i-\frac{1}{2}}\psi^k_{i-\frac{1}{2}} \right) + \left(\gamma_{m+\frac{1}{2}}\psi^k_{m+\frac{1}{2}} - \gamma_{m-\frac{1}{2}}\psi^k_{m-\frac{1}{2}} \right) + V_i \left(\sigma^R_i + \sigma^S_i \right) \psi^k_{m,i}$$

$$= V_i Q_{m,i} + V_i \sum_{m'} W_{m'} \psi^{k-1}_{m',i}\, \sigma_{m'\to m,i} \qquad 1$$

$$\psi^{k-1}_{m,i} = \tfrac{1}{2} \left(\psi^{k-1}_{m,i+\frac{1}{2}} + \psi^{k-1}_{m,i-\frac{1}{2}} \right) \qquad 2$$

$$\sigma^S_i = \sum_m W_m \sigma_{m'\to m,i} \qquad 3$$

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where:

m = direction index
i = space interval index
k = iteration index
μ = direction cosine with x axis
x = space dimension
Q = fixed source + inscatter
W = direction weight
σ^s = cross section for self scatter
σ^R = cross section for capture + outscatter
$\sigma_{m'\to m,i}$ = cross section for scattering from direction m' to direction m
γ = curvature coupling coefficient
ψ = directional flux
v = mesh cell volume

and the $\pm\frac{1}{2}$ subscripts refer to mesh cell boundaries, it is evident that the failure of ψ to be perfectly converged is equivalent to a fictitious source of magnitude:

$$\sigma_i^s \psi_{m,i}^k - \sum_{m'} W_{m'} \psi_{m',i}^{k-1} \sigma_{m'\to m} \qquad 4$$

This source has a different magnitude and shape at each iteration, can be positive or negative, and can thwart convergence indefinitely. Defining leftward partial boundary flows at boundary $i-\frac{1}{2}$ as:

$$F_{i-\frac{1}{2}}^L = A_{i-\frac{1}{2}} \sum_m W_m |\mu_m| \psi_{m,i-\frac{1}{2}}^k ; \ \mu_m < 0 \qquad 5$$

and similarly for rightward flow and flows at boundary $i+\frac{1}{2}$, we have, by integrating Equation 1 over direction:

$$F_{i+\frac{1}{2}}^R - F_{i+\frac{1}{2}}^L - F_{i-\frac{1}{2}}^R + F_{i-\frac{1}{2}}^L + V_i\left(\sigma_i^R + \sigma_i^s\right)\phi_i^k + \sum_m \left(\gamma_{m+\frac{1}{2}}\psi_{m+\frac{1}{2}} - \gamma_{m-\frac{1}{2}}\psi_{m-\frac{1}{2}}^k\right) W_m$$

$$= V_i S_i + V_i \sum_m W_m \sum_{m'} W_{m'} \psi_{m',i}^{k-1} \sigma_{m'\to m,i} \qquad 6$$

$$\phi_i^k = \sum_m W_m \psi_{m,i}^k \qquad 7$$

$$S_i = \sum_m W_m Q_{m,i}^k \qquad 8$$

The γ's are defined such that the last term on the left side of Equation 6 is 0. The order of the summation on the right can be reversed, giving:

$$-\left[F_{i+\frac{1}{2}}^L + F_{i-\frac{1}{2}}^R - F_{i+\frac{1}{2}}^R - F_{i-\frac{1}{2}}^L\right] + V_i\left(\sigma_i^R + \sigma_i^s\right)\phi_i^K = V_iS_i + V_i\sigma_i^s\phi_i^{k-1} \qquad 9$$

In this equation, we define correction factors for the flux in, and the flow emerging from, each interval such that balance is reached without the fictitious non-convergence source:

$$-\left[F_{i+\frac{1}{2}}^L f_{i+\frac{1}{2}} + F_{i-\frac{1}{2}}^R f_{i-\frac{1}{2}}\right] + \left[F_{i+\frac{1}{2}}^R + F_{i-\frac{1}{2}}^L + V_i\left(\sigma_i^R + \sigma_i^s\right)\phi_i^k\right] f_i$$

$$= V_iS_i + V_i\sigma_i^s\phi_i^k f_i \qquad 10$$

This can be simplified by eliminating either S_i or σ_i^R from Equations 9 and 10. From a numerical point of view, elimination of σ_i^R is preferable:

$$-\left[F_{i+\frac{1}{2}}^L f_{i+\frac{1}{2}} + F_{i-\frac{1}{2}}^R f_{i-\frac{1}{2}}\right] + \left[F_{i+\frac{1}{2}}^L + F_{i-\frac{1}{2}}^R + V_iS_i - V_i\sigma_i^s\left(\phi_i^k - \phi_i^{k-1}\right)\right] f_i$$

$$= V_iS_i \qquad 11$$

For large V_i the solution approaches:

$$f_i = \frac{S_i}{S_i - \sigma_i^s\left(\phi_i^k - \phi_i^{k-1}\right)} \qquad 12$$

which can obviously produce negative values of f_i, resulting in oscillitory non-convergence.

END TYPING

Reed showed that stability can be ensured in the case of uniform space mesh and constant cross section by adding, to each boundary flow, a fictitious flow:

$$G_{i+\frac{1}{2}} = A_{i+\frac{1}{2}} \frac{Y}{4} \sigma^s \Delta x \max \left(\phi_i^k, \phi_{i+1}^k \right) \quad ; Y \geq 1 \qquad 13$$

The augmented flows satisfy Equation 9, as did the original flows, but as G becomes large, Equation 11 is satisfied by f_i near unity. This damping effect is space-dependent, having its strongest effect in regions of large Δx and σ^s, where the instability is likely to occur.

Returning to Equation 11, we can observe that the f_i are positive if $\phi_i^{k-1} \geq 0$ and if each boundary flow is augmented by:

$$G_{i+\frac{1}{2}} = \frac{1}{2} \max \left(V_i \sigma_i^s \phi_i^k, V_{i+1} \sigma_{i+1}^s \phi_{i+1}^k \right) \qquad 14$$

In the case of uniform mesh and σ^s, this is equivalent to Reed's criterion with Y = 2. In other words, Y = 1 guarantees stability, while Y = 2 guarantees non-negativity. In later examples, we will see that even larger values of Y may promote rapid convergence.

An equation equivalent to 14 can be written directly for 2-D geometries. In this case, the flow terms of Equation 11 are joined by an upward and a downward term, so that four fictitious flows affect each cell:

$$G_{i+\frac{1}{2}} = \frac{Z}{4} \max \left(V_i \sigma_i^s \phi_i^k, V_{i+1} \sigma_{i+1}^s \phi_{i+1}^k \right) \qquad 15$$

$$G_{j+\frac{1}{2}} = \frac{Z}{4} \max \left(V_j \sigma_j^s \phi_j^k, V_{j+1} \sigma_{j+1}^s \phi_{j+1}^k \right) \qquad 16$$

$$Z \geq 1 \qquad 17$$

This method is an option in the DOT IV code, called the "ϕ method." The value of Z can be adjusted by the user and can increase with each iteration. This last feature has brought convergence to very difficult problems which would otherwise oscillate hopelessly.

A somewhat similar approach is described in reports of the cylindrical-geometry SIMMER code,[4,5] although they use a form emphasizing the common area between cells:

$$G_{i+\frac{1}{2}} = \frac{\Delta r}{4}\sigma^{s}_{i+\frac{1}{2}} A_{i+\frac{1}{2}} \max\left(\phi^{k}_{i},\phi^{k}_{i+1}\right) \qquad 18$$

$$G_{j+} = \frac{\Delta z}{4}\pi\left(r^{2}_{i+\frac{1}{2}} - r^{2}_{i-\frac{1}{2}}\right) \max\left(\phi^{k}_{j},\phi^{k}_{j+1}\right) \qquad 19$$

It may not be clear which Δz or Δr is to be used in this formulation.

Yet another interpretation was made by the developers of DOT 3.5. Observing that Reed's criterion had its basis in a diffusion-theory analogue, they chose to interpret the $\phi/4$ term which recurs in these equations as the one-sided diffusion-theory current, resulting in the "J method:"

$$G_{i+\frac{1}{2}} = Z \max\left(F^{L}_{i+\frac{1}{2}},F^{R}_{i+\frac{1}{2}}\right) \qquad 20$$

$$G_{j+\frac{1}{2}} = Z \max\left(F^{D}_{j+\frac{1}{2}},F^{U}_{j-\frac{1}{2}}\right) \qquad 21$$

This method is used in DOT 3.5 and as an option into DOT IV. The lack of dependence on interval width seems to be an omission in the context of this discussion, but the proof of a convergence method is in the testing!

RESULTS

The first illustration (P1 of Table 1 and Figure 1) is a study of neutron transmission along an annular gap surrounding a sodium-filled pipe which penetrates a thick concrete wall. A 30-direction biased quadrature is used to detail streaming. The table shows that any value of Z between 0.25 and 4 gives satisfactory convergence to this difficult problem, with the optimum being 0.5. The ϕ and J methods give nearly

Table 1. Results of Comparing the J-Method with the ϕ-Method On Two Realistic Problems

Problem description	Method	Z	Number of flux iterations	Flux convergence	Fission convergence
(P1) Pipe duct streaming with boundary source. Variable space and direction mesh. 28 X 35 maximum space mesh. 1 energy group of a 14-group P_3 cross section set is solved. Flux convergence of 1E-2 is sought.	J	4	9	7E-3	
	↓	2	8	8E-3	
	↓	1	8	3E-3	
	↓	.5	7	7E-3**	
	↓	.25	7	9E-3	
	ϕ or J	0	15*	2E-2	
	ϕ	.25	7	9E-3	
	↓	.5	7	7E-3**	
	↓	1	7	9E-3	
	↓	2	8	6E-3	
	↓	4	8	8E-3	
(P2) Fast critical assembly, 4-group P_0 cross sections. A K calculation with 20 source iterations and 4 flux iterations per source iteration is solved. The space mesh is 35 X 30. A low value of fission convergence is sought.	J	4	80		5E-5
	↓	2	↓		2E-5
	↓	1	↓		8E-6**
	↓	.5	↓		1E-4
	↓	.25	↓		2E-2
	ϕ or J	0	↓		1E-2
	ϕ	.25	↓		8E-3
	↓	.5	↓		1E-4
	↓	1	↓		2E-5**
	↓	2	↓		3E-5
	↓	4	↓		4E-5

*Iteration limit reached.
**Optimum value of Z

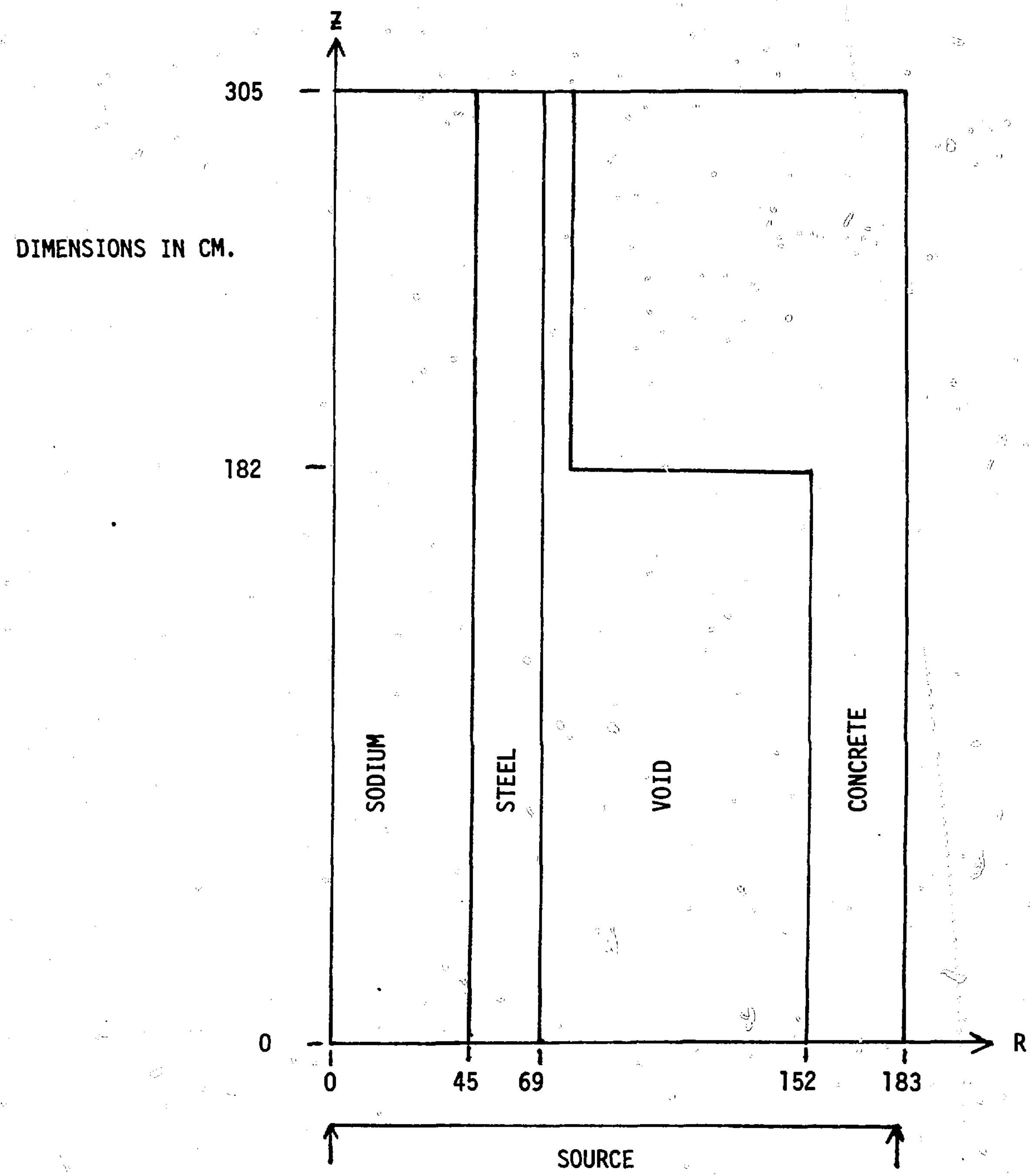

Figure 1. Pipe duct streaming problem.

comparable results. The solution with Z = 0, i.e., no stabilization, failed to converge within the iteration limit.

Problem P2 (Figure 2) is a conventional 4-group, P_0 calculation of k-effective. The directional quadrature has six directions. The best result was obtained from the J method, although results for Z near 0 are inferior to ϕ method results. The optimum Z was 1 for this problem.

Problem P3 (Table 2 and Figure 3) is a classical problem having a uniform source in one quadrant of an X-Y geometry. The source material has anisotropic scattering with:

$$\bar{\mu} = 1/3 \qquad 22$$

and a dominance ratio of 0.5. The volume outside the source region is filled with an isotropic material of dominance 0.5 or 0.99 as noted.

The table shows that the low-dominance problems could be solved very well with any value of Z less than or equal to 2. The first high dominance problem is greatly benefitted by either J or ϕ method smoothing, while the second is not. Overall, any Z between 0.5 and 2 gives satisfactory results, with the J method superior to the method in the more difficult problems.

A fourth problem, representing a reactor head compartment, is shown in Figure 4. Seven groups of a 14-group cross section set are solved. The principal interest is in the convergence of the difficult groups 6 and 7 (Table 3), which are given a maximum of 24 iterations each. Groups 1-5 are given only five interations each in order to stay within execution-time constraints. The value of Z is adjusted according to:

$$Z = C + (I-1)D \qquad 23$$

where I is the iteration count, and C and D are as noted. Various combinations of ϕ and J method damping are used as noted. Relatively large values of Z were required to converge groups 6 and 7. Although

Table 2. Number of Iterations to Converge a Hypothetical Test Problem

(P3) Classical source-in-a-box problem, 8 X 8 space mesh, uniform source in one quadrant with dominance = 0.5 in source region. Flux convergence criterion = 1E-4. Total cross section = 1.

Dominance ratio outside source region	Δx (mfp)	Δy (mfp)	Method	0	.125	.25	.5	1	2	4
.5	1	1	J	10	10	9	8	8	9	10
.5	1	1	ϕ	10	10	9	9	8	8	8
.5	.25	4	J	8	8	7	7	8	10	12
.5	.25	4	ϕ	8	8	8	8	8	10	12
.99	1	1	J	39	23	18	13	10	13	16
.99	1	1	ϕ	39	25	19	15	11	12	16
.99	.25	4	J	12	12	12	10	12	17	24
.99	.25	4	ϕ	12	12	13	13	19	27	35

CLASSIFICATION

Table 3. Groupwise Convergence of a Multigroup Head Compartment Problem

Case	A	B	C	D	E	F
C	0.5	0.5	2	1	1	1
D	0	0	0	0.25	1	1
Method	φ	J	J	J	J	φ
Convergence If Group						
1	[a]1.9^{-1}	9.2^{-2}	8.5^{-2}	6.8^{-2}	9.2^{-2}	2.7^{-2}
2	7.2^{-2}	5.4^{-2}	2.2^{-2}	4.0^{-2}	2.2^{-2}	8.4^{-2}
3	7.8^{-2}	2.4^{-2}	1.8^{-2}	9.0^{-3}	1.8^{-2}	3.4^{-2}
4	1.9^{-1}	7.0^{-2}	2.2^{-2}	2.0^{-2}	2.7^{-2}	8.0^{-2}
5	2.7^{-1}	1.2^{-2}	1.2^{-2}	2.9^{-2}	1.7^{-2}	1.4^{-1}
6	3.5^{-1}	3.4^{-1}	1.9^{-1}	5.4^{-3}	[b]$12/7.2^{-4}$	4.9^{-3}
7	[c]$(21/1.5^{-1})$	$(21/3.2^{-1})$	$(22/2.0^{-1})$	1.4^{-3}	$21/9.6^{-4}$	$17/9.6^{-4}$

[a] Interpreted as 1.9×10^{-1}

[b] Indicates convergence of <0.001 was reached in 12 iterations. Where only the convergence is shown, the iteration limit of 5 iterations (groups 1-5) or 24 iterations (groups 6 and 7) was reached.

[c] Results in parentheses are incomplete due to the standard time limit, 4 minutes on a CDC CYBER 76.

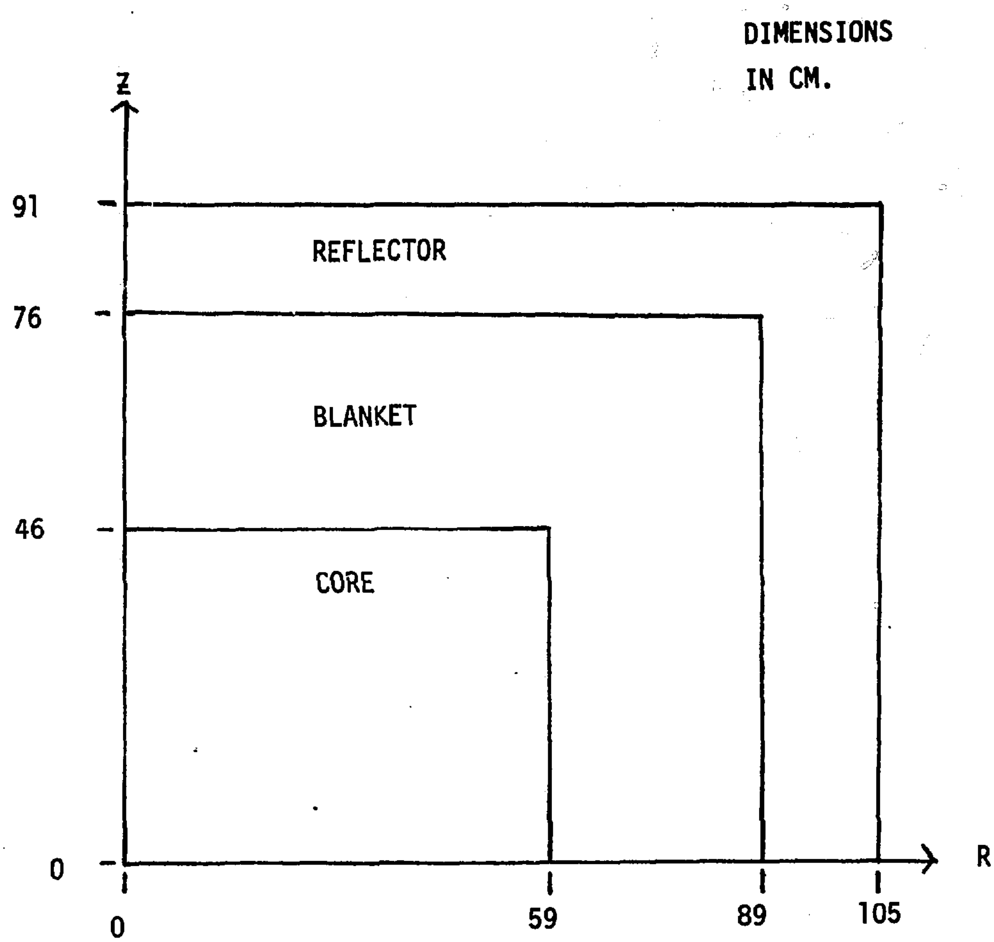

Figure 2. Fast critical assembly problem.

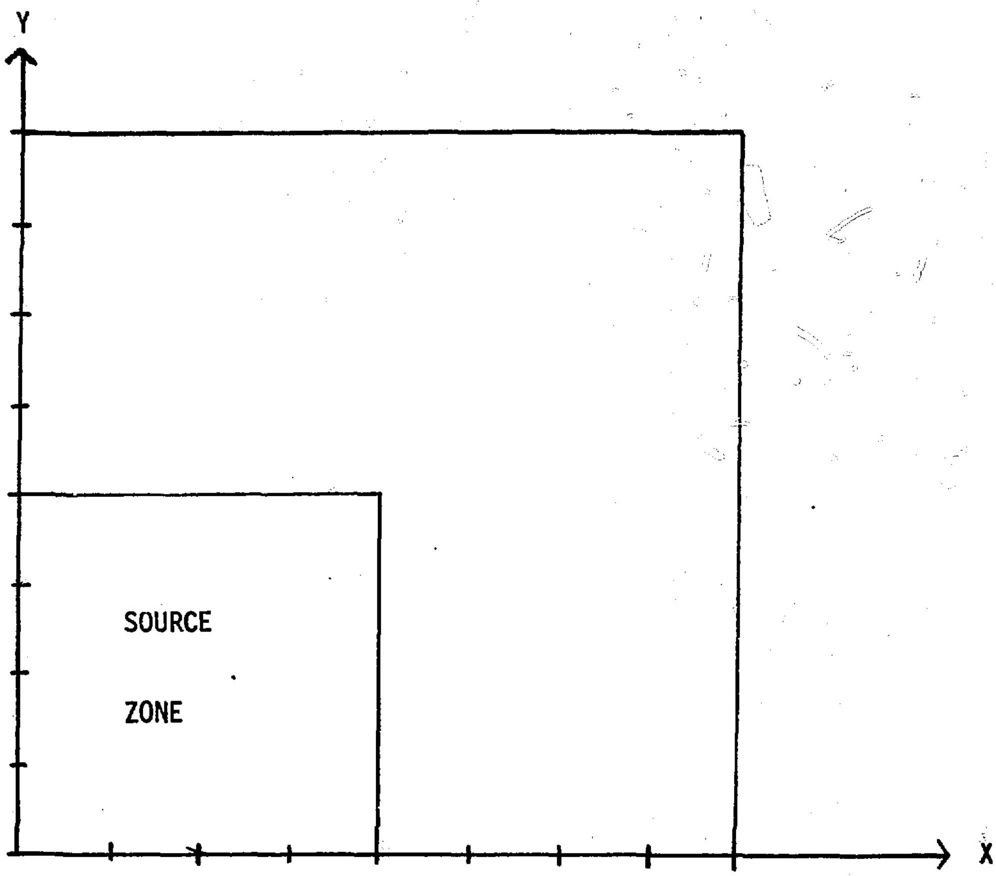

Figure 3. Box-in-a-corner problem.