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Evaluation of Spatial Differencing Practices for the Discrete-Ordinates Method

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Three popular spatial differencing practices for the discrete ordinates method are examined in detail for a basic two-dimensional Cartesian coordinates problem. These differencing schemes are 1) positive, 2) step, and 3) diamond schemes. The diamond scheme is shown to produce negative intensities under certain conditions *irrespective* of the number of control volumes employed, requiring some form of negative intensity fix-up. In absorbing-emitting or absorbing-emitting-scattering media, *grid refinement* can result in negative intensities when the diamond scheme is used. The diamond scheme and a positive scheme, which sets the negative intensities encountered in the diamond scheme to zero or very small number for purely absorbing media, can also produce physically unrealistic overshoots. The step scheme, although not considered as accurate as the diamond scheme, gives physically realistic results for the basic problem considered. Further evaluation of Fiveland's positive conditions, and variable weight and exponential-type schemes indicate a need for alternate spatial differencing schemes that describe the physics of radiative heat transfer more accurately.

Nomenclature

f = spatial differencing weights, Eq. (4)
I = actual intensity
L = total number of ordinates
S_m^l = modified source function, Eq. (2b)
w = angular weights
x, y = coordinate directions
β = extinction coefficient, $\kappa + \sigma$
β_m^l = modified extinction coefficient, Eq. (2a)
$\Delta x, \Delta y$ = x and y direction control volume widths
θ = polar angle
κ = absorption coefficient
μ = direction cosine in the x direction, $\cos\theta$
ξ = direction cosine in the y direction, $\sin\theta\cos\phi$
σ = scattering coefficient
τ = optical thicknesses
Φ = scattering phase function
ϕ = azimuthal angle

Subscripts
b = blackbody
E = neighbor in the positive x direction
e = control volume face between P and E
m = modified
N = neighbor in the positive y direction
n = control volume face between P and N
P = control volume
S = neighbor in the negative y direction
s = control volume face between P and S
W = neighbor in the negative x direction
x, y = in the x or y direction
w = control volume face between P and W

Superscripts
l, l' = angular directions

Introduction

OVER the past decade, the discrete ordinates method[1-3] has been used in computations of radiative heat transfer. One of the four popular spatial differencing practices is used in most published works. These are 1) positive,[4] 2) step,[5] 3) diamond,[5] and 4) variable-weight[6] schemes. Researchers in this area have attempted to prevent negative intensities from occurring, mostly with experience gained from one-dimensional analyses and computations. Recently, Fiveland[7] reported that it is not possible to ensure positive intensities for all directions when the diamond scheme is used in multidimensional computations.

Intensity is a positive quantity by definition. Negative intensities are physically unrealistic and can cause computational instabilities. Various ways of ensuring positive intensities have therefore been proposed. These include the negative intensity fix-up procedure,[2] a positive scheme,[4] a variable-weight scheme,[6] and positive intensities criteria.[7] All these procedures use zero intensity as the reference intensity. When a negative intensity is encountered, it is set to zero in the negative intensity fix-up procedure. Other procedures attempt to ensure zero intensity as the minimum.

Zero intensity is a physically realistic result only in a few limiting cases, e.g., an optically thick purely absorbing medium, or an unilluminated region of a nonscattering, nonemitting enclosure. Usually, zero intensity is physically unrealistic in an emitting and/or scattering medium. For a scattering medium, zero intensities are only useful as intermediate solutions in the iteration procedure.

Figure 1 illustrates the concept of physically realistic solutions. The curve marked "Exact" represents a normalized intensity solution in a purely absorbing medium. Curve B is a physically realistic solution to the problem, although it is

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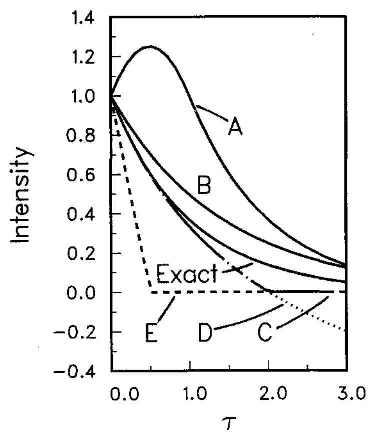

Fig. 1 Physically realistic and unrealistic solutions.

an approximation. Solution D with negative intensities (undershoots) and curve A with overshoots (intensities higher than the incident intensity) are physically unrealistic. Curve E, which contains zero intensity for $\tau << 2$, is also physically unrealistic. Trend C with zero intensity for $\tau > 2$ is a possible solution when the diamond scheme is used with the set-to-zero negative intensity treatment. Due to a lack of a better criterion, curve C is usually accepted as the lower limit to physically realistic solution. In this illustration, physically realistic solution contains intensities between the maximum intensity and the intensity produced by the diamond scheme with the negative intensity fix-up procedure.

The purpose of this article is to present a detailed analysis of the step, diamond, and positive spatial discretization methods as applied to a basic test problem. Fiveland's positive intensity conditions,[7] variable weight schemes,[6] and the modified exponential schemes[8] are also considered. A brief discussion on a better differencing practice is given at the end of this article, along with some concluding remarks.

Governing Equation

The linearized radiative heat transfer equation[8] for a two-dimensional square enclosure (Fig. 2a) is written for each ordinate direction l as

$$\mu^l \frac{\mathrm{d}I^l}{\mathrm{d}x} + \xi^l \frac{\mathrm{d}I^l}{\mathrm{d}y} = -\beta_m^l I^l + S_m^l \tag{1}$$

The modified extinction coefficient and the modified source term are

$$\beta_m^l = \beta - \frac{\sigma}{4\pi}\Phi^{ll}w^l \tag{2a}$$

$$S_m^l = \kappa I_b + \frac{\sigma}{4\pi}\sum_{l'=1,l'\neq l}^{L} \Phi^{l'l}w^{l'}I^{l'} \tag{2b}$$

Integrating Eq. (1) over a typical control volume shown in Fig. 2b gives

$$\mu^l(I_e^l - I_w^l)\Delta y + \xi^l(I_n^l - I_s^l)\Delta x = (-\beta_{mP}^l I_P^l + S_{mP}^l)\Delta x\Delta y \tag{3}$$

Spatial differencing relations are used to derive the final discretization equation for the nodal intensity. For the $\mu^l > 0$ and $\xi^l > 0$ directions, these relations are usually written as

$$I_P^l = f_y^l I_n^l + (1 - f_y^l)I_s^l = f_x^l I_e^l + (1 - f_x^l)I_w^l \tag{4}$$

where f_x^l, and f_y^l are appropriate weighting factors. The diamond and step schemes are obtained by setting $f = f_x^l = f_y^l$ to 0.5 and 1, respectively. When a positive scheme of Lathrop[4] is used, the corresponding weights are

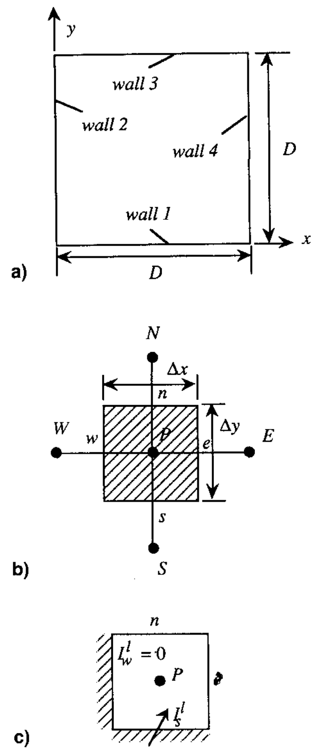

Fig. 2 Two-dimensional enclosure: a) schematic, b) typical internal control volume, and c) test problem (first internal control volume).

$$f_x^l = \max[1 - \gamma_y^l/\gamma_x^l(\gamma_y^l + 2), 0.5] \tag{5a}$$

$$f_y^l = \max[1 - \gamma_x^l/\gamma_y^l(\gamma_x^l + 2), 0.5] \tag{5b}$$

where

$$\gamma_x^l \equiv \frac{\beta\Delta x}{|\mu^l|}, \qquad \gamma_y^l \equiv \frac{\beta\Delta y}{|\xi^l|} \tag{6}$$

The final discretization equation for the nodal intensity then becomes

$$I_P^l = \frac{\mu^l f_y^l \Delta y I_w^l + \xi^l f_x^l \Delta x I_s^l + S_{mP}^l f_x^l f_y^l \Delta x \Delta y}{\mu^l f_y^l \Delta y + \xi^l f_x^l \Delta x + \beta_{mP}^l f_x^l f_y^l \Delta x \Delta y} \tag{7}$$

Equation (4) is used to solve for the downstream boundary intensities, with the nodal intensity obtained from Eq. (7). Since the step and positive schemes always produce positive downstream boundary intensities, no special treatment is needed. The diamond scheme sometimes produces negative downstream boundary intensities. When a negative boundary intensity is encountered, the negative intensity fix-up procedure proposed by Carlson and Lathrop[2] sets the negative intensity to zero. A new discretization equation is then formulated using Eqs. (3) and (4), and this equation is used to solve for a new nodal intensity. The set-to-zero boundary intensity remains zero in the current iteration to ensure energy conservation within the control volume.

Analysis

The physical situation considered is a square enclosure with one hot and three cold black walls (Fig. 2a). The hot wall is the south boundary (wall 1). The medium can emit, absorb, and scatter energy. The test problem considers the first in-

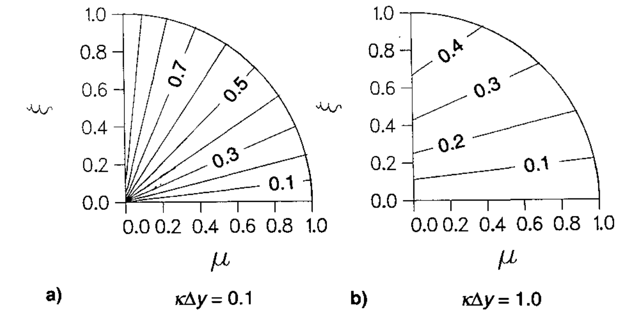

Fig. 3 Step scheme $I'_n/I'_s = I'_e/I'_s = I'_P/I'_s$ for a) $\kappa\Delta y = 0.1$ and b) $\kappa\Delta y = 1$.

ternal control volume at the lower left corner as shown in Fig. 2c. For the $\mu' > 0$ and $\xi' > 0$ directions, with $I'_w = 0$ (cold west wall) and $\Delta x = \Delta y$ for ease of presentation, Eq. (7) reduces to

$$I'_P = \frac{\xi' f'_x I'_s + S'_{mP} f'_x f'_y \Delta y}{\mu' f'_y + \xi' f'_x + \beta'_{mP} f'_x f'_y \Delta y} \tag{8}$$

This basic problem is important, because this is the most upstream control volume for all $\mu' > 0$ and $\xi' > 0$ directions; any error in the boundary intensities will propagate to the entire solution domain. Also, the left boundary intensity of an internal control volume can become zero due to a negative intensity fix-up, even if the left physical boundary is not cold.

Step Scheme

For the control volume shown in Fig. 2c, the east and north boundary intensities are obtained using

$$I'_e = I'_n = I'_P = \frac{\xi' I'_s + S'_{mP}\Delta y}{\mu' + \xi' + \beta'_{mP}\Delta y} \tag{9}$$

Figure 3 shows contours of constant intensities in the quadrant $\mu' > 0$ and $\xi' > 0$ obtained from Eq. (9) for the purely absorbing limit ($S'_{mP} = 0$ and $\beta'_{mP} = \kappa$). Comparing the results for $\kappa\Delta y$ of 0.1 and 1.0 shows the intensity in any given direction decreasing with increasing optical thickness. Consistent with published literature, no negative intensities are predicted by the step scheme. Since no attenuation is experienced between P and its downstream boundaries, the step scheme produces physically realistic solutions for fine grids.

Diamond Scheme

Using $f = f'_x = f'_y = 0.5$, the nodal intensities are

$$I'_P = \frac{\xi' I'_s + S'_{mP}\Delta y/2}{\mu' + \xi' + \beta'_{mP}\Delta y/2} \tag{10}$$

The corresponding north boundary intensities then become

$$I'_n = 2I'_P - I'_s = \frac{(\xi' - \mu' - \beta'_{mP}\Delta y/2)I'_s + S'_{mP}\Delta y}{\mu' + \xi' + \beta'_{mP}\Delta y/2} \tag{11}$$

Figure 4 shows I'_n/I'_s isopleths computed from Eq. (11) in the purely absorbing limit ($S'_{mP} = 0$ and $\beta'_{mP} = \kappa$). Negative north boundary intensities are encountered and must be set to zero by a fix-up procedure for the $\xi' \le \mu'$ directions. When $\xi' > \mu'$, negative intensities are more prominent in the optically thicker situation ($\kappa\Delta y = 1$).

The conditions for positive I'_n are derived from Eq. (11) for absorbing-emitting-scattering media

$$2I'_s(\xi' - \mu') \ge \beta'_{mP}\Delta y(I'_s - 2S'_{mP}/\beta'_{mP}) \tag{12}$$

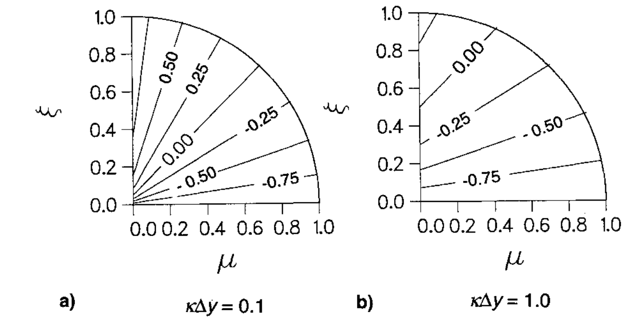

Fig. 4 Diamond scheme I'_n/I'_s for a) $\kappa\Delta y = 0.1$ and b) $\kappa\Delta y = 1$.

or

$$\frac{\beta'_{mP}\Delta y}{\xi'} \le \left(\frac{2I'_s}{I'_s - 2S'_{mP}/\beta'_{mP}}\right)\left(1 - \frac{\mu'}{\xi'}\right) \quad \text{for} \quad I'_s > \frac{2S'_{mP}}{\beta'_{mP}} \tag{13a}$$

$$\frac{\beta'_{mP}\Delta y}{\xi'} \ge \left(\frac{2I'_s}{I'_s - 2S'_{mP}/\beta'_{mP}}\right)\left(1 - \frac{\mu'}{\xi'}\right) \quad \text{for} \quad I'_s < \frac{2S'_{mP}}{\beta'_{mP}} \tag{13b}$$

In the purely absorbing limit, Eq. (13a) and (13b) reduces to $\kappa\Delta y/\xi' \le 2(1 - \mu'/\xi')$. Because both direction cosines are needed, this two-dimensional criterion is more complex than $\kappa\Delta y/\xi' \le 2$, the positive intensity criterion for one-dimensional planar geometry. When $\xi' \le \mu'$ for this two-dimensional problem, the diamond scheme will produce negative I'_n, irrespective of the number of control volumes used. When $\xi' > \mu'$, positive I'_n can be ensured for a sufficiently fine grid, although this is not always practical in high optical thickness computations.

For the two-dimensional absorbing-emitting-scattering problem, Eqs. (12) and (13a) show that negative intensities are encountered and must be set to zero regardless of the control volume size in two situations: 1) $\xi' < \mu'$ and $I'_s = 2S'_{mP}/\beta'_{mP}$, and 2) $\xi' \le \mu'$ and $I'_s > 2S'_{mP}/\beta'_{mP}$. A fine grid resolution and a restricted ordinate set including only the $\xi' > \mu'$ directions would be needed to ensure positive intensities for the test problem when $I'_s > 2S'_{mP}/\beta'_{mP}$. In media with strong modified source function or weak modified extinction coefficient (i.e., $I'_s < 2S'_{mP}/\beta'_{mP}$), Eq. (13b) implies that grid refinement can result in negative intensities. These results are contrary to the common belief that a sufficiently fine spatial discretization will ensure positive intensities when the diamond scheme is used.[2,3,9]

The diamond scheme east boundary intensities for the test problem can be written using Eqs. (4) and (8) as

$$I'_e = 2I'_P = \frac{2\xi' I'_s + S'_{mP}\Delta y}{\mu' + \xi' + \beta'_{mP}\Delta y/2} \tag{14}$$

Figure 5 shows the I'_e/I'_s contours for the μ' and $\xi' > 0$ directions in the purely absorbing limit ($S'_{mP} = 0$ and $\beta'_{mP} = \kappa$). Some east boundary intensities are seen to be greater than the upstream intensity I'_s, which is impossible for this nonemitting and nonscattering example. Furthermore, I'_e cannot exceed I'_P for this case, since the distance between the hot south wall and point P is identical to the distance between the hot wall and point e (Fig. 2c). The east boundary intensity predicted by Eq. (14) is twice I'_P, and can contain overshoots that are physically unrealistic.

Positive Scheme

Although it is possible to present an analysis for absorbing-emitting-scattering media, some interesting features are observed in purely absorbing media ($S'_{mP} = 0$ and $\beta'_{mP} = \kappa$).

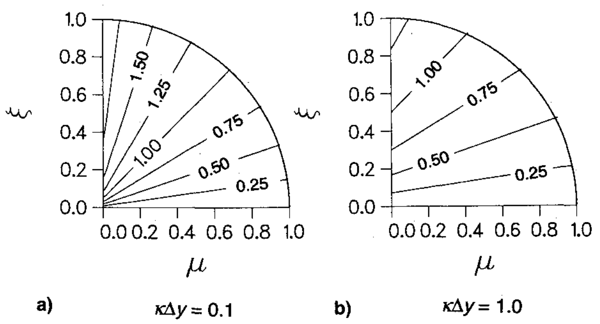

Fig. 5 Diamond scheme I_e^l/I_s^l for a) $\kappa\Delta y = 0.1$ and b) $\kappa\Delta y = 1$.

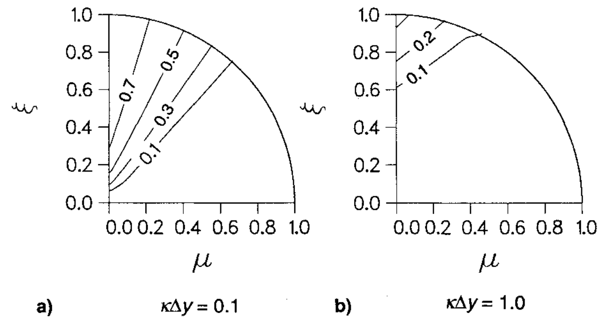

Fig. 6 Positive scheme I_n^l/I_s^l for a) $\kappa\Delta y = 0.1$ and b) $\kappa\Delta y = 1$.

The north boundary intensity obtained by the positive scheme is

$$I_n^l = \frac{1}{f_y^l}\left[\frac{\xi^l f_x^l}{\mu^l f_y^l + \xi^l f_x^l + \kappa f_x^l f_y^l \Delta y} - (1 - f_y^l)\right] I_s^l \quad (15)$$

where f_x^l and f_y^l are defined in Eq. (5). Plots of I_n^l/I_s^l for varying μ^l and ξ^l are shown in Fig. 6. Comparing Figs. 6 and 4 shows that the positive scheme sets the negative intensities encountered in the diamond scheme to zero or very small intensities. The east boundary intensity in the purely absorbing limit is

$$I_e^l = \frac{I_P^l}{f_x^l} = \frac{1}{f_x^l}\left(\frac{\xi^l f_x^l}{\mu^l f_y^l + \xi^l f_x^l + \kappa f_x^l f_y^l \Delta y}\right) I_s^l \quad (16)$$

Since f_x^l can be less than unity, I_e^l can be larger than I_P^l, which is physically unrealistic for this problem as explained for the diamond scheme.

Fiveland's Positive Intensity Conditions

Fiveland[7] suggests guidelines for maintaining positive intensity and avoiding unwanted oscillations throughout the computational domain. These conditions are written for purely absorbing media as

$$\Delta x < \frac{|\mu|}{\kappa(1 - f)}\chi, \quad \Delta y < \frac{|\xi|}{\kappa(1 - f)}\chi, \quad \Delta z < \frac{|\eta|}{\kappa(1 - f)}\chi \quad (17)$$

where χ is defined as

$$\chi = \frac{f^3 + (1 - f)^2(2 - 5f)}{f} \quad (18)$$

The ratio $\chi/(1 - f)$ is equal to $\kappa\Delta y/\xi$, and is shown in Table 1 for various values of spatial differencing weights. When $f = 0.5$ (diamond scheme), negative intensities will occur irrespective of the size of the control volumes employed. When $f = 1.0$ is used (step scheme), there is no limitation on the grid spacing. The values of $\chi/(1 - f)$ in Table 1 also indicate that if conditions in Eq. (17) are satisfied, positive intensities are ensured for $0.5 < f \leq 1.0$.

Table 1 Ratio of $\chi/(1 - f)$ for various f

f	$\chi/(1 - f) = \kappa\Delta y/\xi$
0.5	0.000
0.6	0.233
0.7	0.990
0.8	2.700
0.9	7.822
1.0	∞

Table 2 Level symmetric S_8 quadrature set for the first quadrant

Direction number	Ordinates μ^l	ξ^l
1	0.1422555	0.1422555
2	0.5773503	0.1422555
3	0.8040087	0.1422555
4	0.9795543	0.1422555
5	0.1422555	0.5773503
6	0.5773503	0.5773503
7	0.8040087	0.5773503
8	0.1422555	0.8040087
9	0.5773503	0.8040087
10	0.1422555	0.9795543

The north boundary intensities are given below for the two-dimensional test problem (Fig. 2c) in the purely absorbing limit

$$I_n^l = \frac{1}{f}\left[\frac{\xi^l}{\mu^l + \xi^l + \kappa f \Delta y} - (1 - f)\right] I_s^l \quad (19)$$

The criterion for positive north boundary intensities for this problem can be written as

$$\frac{\kappa\Delta y}{\xi^l} \leq \frac{1}{1 - f} - \frac{\mu^l}{\xi^l f} \quad (20)$$

This positive criterion is fundamentally different from Fiveland's conditions, where the ratio is only a function of f. For the right side of Eq. (20) to be greater than or equal to zero, the weighting factor must satisfy the following condition:

$$f \geq \frac{\mu^l}{\mu^l + \xi^l} \quad (21)$$

The positive intensity condition in Eq. (21) can be applied to a specific ordinate set for better comparison with Fiveland's condition.[7] If the S_8 quadrature set in Table 2 is used, negative intensities will occur for $f \leq 0.8$ in the direction number 2, irrespective of the number of control volumes employed. Fiveland's condition only required $f > 0.5$ for positive intensities. This simple test problem shows that while Fiveland's conditions are useful guidelines, they do not necessarily ensure positive intensities for all situations. Even if conditions in Eq. (17) are satisfied, a user should still check for negative intensities and apply necessary fix-up procedures.

Other Differencing Schemes

The analysis for the test problem considered in this article has shown that the diamond scheme can produce overshoots and undershoots. The positive scheme is also not free from overshoots. It seems, in general, any spatial differencing scheme defined by Eq. (4) with weighting factors less than unity can produce physically unrealistic overshoots when used in multidimensional Cartesian coordinates computations. This sec-

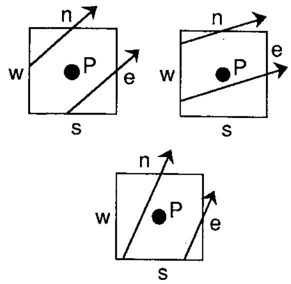

Fig. 7 Three possible radiation directions.

tion briefly discusses the variable weight[6] and exponential-type schemes.[2,8,10]

A variable-weight[6] scheme assigns a uniform spatial differencing weight for all directions by increasing f from 0.5 up to 1.0 until no negative intensities are encountered in any direction. Above consideration of Fiveland's positive conditions[7] indicates that some directions will require $f > 0.8$. Although not presented in this article, a similar three-dimensional analysis showed that $f > 0.9$ are required for some directions. A variable weight scheme[6] may well require additional computational effort merely to assign a differencing weight very close to the step scheme.

The exponential scheme[2] is generally regarded as a more accurate differencing scheme in one-dimensional computations. The modified-exponential scheme of Chai et al.[8] and a higher-order scheme of Raithby and Chui[10] are improvements on the exponential scheme. The modified-exponential weighting factor f_y^l is given as

$$f_y^l = \frac{1}{1 - \exp(-\tau_m^l)} - \frac{1}{\tau_m^l} \tag{22}$$

where $\tau_m^l = \beta_m^l \Delta y / |\xi^l|$. It can be seen from Eq. (22) that this weighting factor can also be less than unity. Since this can sometimes lead to physically unrealistic solutions when used with Eq. (4), exponential-type schemes may not ensure accuracy in multidimensional computations.

Possible Differencing Practices

One reason for the occurrence of physically unrealistic solutions lies in the failure of Eq. (4) to properly account for the directional effect of radiation. Figure 7 shows three possible radiation directions. Equation (4) does not describe these situations correctly, since for most of the rays $I_e^l \neq f(I_w^l)$ and $I_n^l \neq f(I_s^l)$.

A possible, although more complex alternative, is to trace the downstream intensity appearing in Eq. (3) to an upstream location where the intensity is known.[10] The north boundary intensity can then be evaluated using an exponential-type spatial differencing scheme.[2,8,10] Using the modified-exponential scheme of Chai et al.[8] would give

$$I_n^l = I_u^l e^{-\beta_m^l d^l} + (S_m^l/\beta_m^l)(1 - e^{-\beta_m^l d^l}) \tag{23}$$

where I_u^l is an upstream location appropriate for I_n^l, and d^l is the distance between u and n. The advantage of Eq. (23) is that the nodal intensities are evaluated from good boundary intensities. The upstream location u must be chosen carefully to avoid negative neighbor coefficients that can produce unwanted wiggles and negative nodal intensities.

Conclusions

A systematic evaluation of spatial differencing practices has been presented for a basic test problem in two-dimensional Cartesian coordinates. The following conclusions are drawn from this study:

1) When the diamond scheme is used, there are situations where negative intensities will occur *irrespective* of the number of control volumes employed, and some form of negative intensity fix-up procedure is needed.

2) Negative intensities can occur *with* grid refinement in certain absorbing-emitting and absorbing-emitting-scattering media, requiring, again, a negative intensity fix-up procedure.

3) For the purely absorbing problem tested, the positive scheme sets the negative intensities encountered in the diamond scheme to zero or small intensities.

4) As shown by the analysis with diamond and positive schemes, there are situations where a downstream boundary intensity can be *artificially* augmented when the weighting factor is less than unity.

5) A user should check for negative intensities even when the Fiveland positive conditions are satisfied.

6) Variable and exponential-type differencing schemes may still not be sufficient for multidimensional calculations when used with Eq. (4).

7) Spatial differencing schemes which describe the physics of radiative heat transfer more accurately are needed.

If a simple spatial differencing scheme is needed for Cartesian coordinates computations, the step scheme is recommended based on this study. A general recommendation would require further evaluations, especially in geometries with curvature effects. For those who continue to use either the diamond or positive scheme, care must be taken to minimize negative intensities and overshoots. In certain situations, the user must also be willing to accept zero intensity, overshoots, and undershoots as physically realistic solutions.

Acknowledgments

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