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Transport–Diffusion Interfaces in Radiative Transfer

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For radiative transfer problems involving both optically thick and thin regions, it is suggested that a coupled diffusion-transport treatment has certain advantages in numerical treatments. The well known Marshak (Milne) boundary treatment is extended in a straightforward way to give the connecting conditions at the diffusion-transport interface. It is found that these conditions give a diffusion radiative flux from a blackbody in excess of the physical blackbody limit. The Marshak conditions are modified to correct this discrepancy and the resulting diffusion description is found to be quite accurate for grey, as well as black, bodies. A previously suggested diffusion-transport interface treatment, due to Brockway, is discussed and shown to be a certain finite difference analogue of the unmodified Marshak treatment. The modification needed to give the correct black-body limit is applied to the Brockway formulation. The previously suggested interpretation of the Brockway equations in terms of probabilities leads to conceptual difficulties, and it is shown that such an interpretation is not needed to successfully apply these interface conditions.

1. INTRODUCTION

In the vast majority of radiative transfer problems, the well known equation of radiative transfer, together with the assumption of local thermodynamic equilibrium, is considered to be an accurate description of the interaction of radiation with matter. Unfortunately, this equation is sufficiently complex to prohibit analytic solutions for all but very simple problems. The numerical solution of this equation is also difficult. If photon scattering is an important interaction, then the equation of radiative transfer is an integro-differential equation. Even in the absence of scattering, the coupling of the radiation field to the material (temperature) field, as well as geometric considerations, give rise to difficulties in a numerical solution.

Because of this complexity, it is common to employ approximations to the equation of transfer. One of the more widely used approximations is the diffusion, or $P-1$, description. This follows from the equation of transfer by describing the angular dependence of the radiative intensity through its spherical harmonic components,

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and truncating the corresponding spherical harmonic expansion after a few terms. For optically thick, near thermodynamic equilibrium, problems the diffusion description is particularly appropriate. In this type of problem, the radiative intensity is known apriori to be nearly isotropic, and hence is accurately represented by a low order spherical harmonic expansion. Further, for this class of problems a numerical solution of the equation of transfer is difficult. In a deterministic (finite difference) solution of the equation of transfer, this difficulty is manifested in the need for many zones, or mesh points. This need arises because accuracy considerations dictate that the zone size be near that of a photon mean free path, and in an optically thick situation the size of the problem is, by definition, many mean free paths. In a stochastic (Monte Carlo) solution, the difficulty arises in the time required to track the photons. One has many absorptions and re-emissions, the effects of which tend to cancel. To gain adequate statistics, one needs track an inordinately large number of photons.

In this paper we will be concerned with problems which involve both an optically thin (transport) region and an optically thick (diffusion) region. A conceptually attractive method of solution for a problem of this type would be to use the equation of transfer as the description in the thin region, and the diffusion equation as the description in the thick region. The question then arises as to how to connect these descriptions at the transport-diffusion interface. It is this interface problem that we shall specifically address. It should be noted that the placement of a diffusion-transport interface is somewhat arbitrary. In a general problem there is no sharp position beyond which diffusion theory is obviously an adequate description. Even if one identifies a diffusive region, the interface placement still requires discussion. Ideally, one would like to place this interface several mean free paths into the diffusive region to assure a smooth transition across it. For multigroup problems, this is impractical because of the strong group dependence of the mean free path. That is, one would have to introduce an interface position which is group dependent. For problems involving hydrodynamic motion, it would be extremely difficult to maintain the transport-diffusion interface a few mean free paths into the diffusive region, even if one allowed a group dependence. This is because the hydrodynamics is continually changing the mean free path, as well as the location of the diffusive region. Thus, as a practical matter, the transport-diffusion interface must generally be placed at a material boundary, separating a highly absorbing (thick) region from a weakly absorbing (thin) region.

In the next section we briefly review the equation of transfer and the diffusion approximation, for the purpose of establishing notation and giving a starting point for the analysis to follow. Section 3 develops the interface condition from a straightforward extension of the Marshak, or Milne, boundary condition commonly used at a vacuum boundary in the diffusion description. The analytic solution of a model problem points out a basic discrepancy in the Marshak condition. This discrepancy is just a manifestation of the inaccuracy of the diffusion description in the vicinity of a vacuum boundary, and leads to a radiative flux in excess of the black body limit. A modification to the Marshak condition is suggested in the following section to remedy this problem. Section 5 discusses a previously suggested treatment of the transport-diffusion interface condition, and points out a conceptual difficulty with this earlier approach as presented. However, it is shown that this difficulty is more apparent than real, and an alternate interpretation of this earlier approach brings it into close conformity with the present (unmodified) method. The paper concludes with a summary section.

The development presented here is restricted, for simplicity, to the grey (mono-energetic, or one group) time independent radiative transfer problem in slab geometry. The underlying ideas apply to time and frequency dependent (multigroup) problems in any geometry. The extension required is only algebraic and offers no conceptual difficulties.

2. The Transport and Diffusion Descriptions

We assume a grey equation of transfer with an isotropic phase function describing the scattering. At steady state in slab geometry we have [1]

$$\mu \frac{\partial I(\tau, \mu)}{\partial \tau} + I(\tau, \mu) = \frac{[1 - \tilde{\omega}(\tau)]}{\pi} \sigma T^4(\tau) + \frac{\tilde{\omega}(\tau)}{2} \int_{-1}^{1} d\mu' \, I(\tau, \mu'), \tag{1}$$

where $I(\tau, \mu)$ is the specific intensity of radiation, $T(\tau)$ is the material temperature, $\tilde{\omega}(\tau)$ is the single scatter albedo, and the distance τ is measured in mean free paths. We assume there is a left hand boundary at $\tau = 0$. The boundary condition on Eq. (1) at $\tau = 0$ is that the incoming angular intensity is known, i.e.,

$$I(0, \mu) = \Gamma_+(\mu), \qquad \mu > 0, \tag{2}$$

where $\Gamma_+(\mu)$ is a known, specified, function. A similar boundary condition applies at the right hand boundary, say $\tau = b$. Equation (1), together with the boundary conditions at $\tau = 0$ and $\tau = b$, constitute the transport description of radiative transfer.

To obtain the diffusion approximation, we expand the specific intensity in Legendre polynomials in μ, and carry only the first two terms, i.e.,

$$I(\tau, \mu) = \frac{\sigma}{\pi} \theta^4(\tau) + \frac{3}{4\pi} \mu F(\tau) + \cdots \tag{3}$$

where $\theta(\tau)$ is the radiation temperature and $F(\tau)$ is the radiative flux. Computing the 2π solid angle (hemispherical) right and left going fluxes, we have, from Eq. (3),

$$F^+(\tau) \equiv 2\pi \int_0^1 d\mu \, \mu I(\tau, \mu) = \sigma\theta^4(\tau) + \tfrac{1}{2}F(\tau), \tag{4}$$

$$F^-(\tau) \equiv 2\pi \int_{-1}^0 d\mu \, |\mu| \, I(\tau, \mu) = \sigma\theta^4(\tau) - \tfrac{1}{2}F(\tau). \tag{5}$$

The total, or net, flux is given by the difference of these two quantities, namely

$$F(\tau) = F^+(\tau) - F^-(\tau) = 2\pi \int_{-1}^{1} d\mu\ \mu I(\tau, \mu). \tag{6}$$

Using Eq. (6) in Eq. (4), we can express the right going flux in terms of the radiation temperature and the left going flux, i.e.,

$$F^+(\tau) = 2\sigma\theta^4(\tau) - F^-(\tau). \tag{7}$$

Similarly, using Eq. (7) in Eq. (6) we can express the net flux in terms of the radiation temperature and the left going flux, i.e.,

$$F(\tau) = 2[\sigma\theta^4(\tau) - F^-(\tau)]. \tag{8}$$

Equations (7) and (8) will be important in our discussion of a previously suggested treatment of a transport-diffusion interface, given in Section 5.

The diffusion description follows by using Eq. (3) in Eq. (1) and forming the first two angular moments. The result is:

$$-\frac{1}{3}\frac{\partial^2\theta^4(\tau)}{\partial\tau^2} + [1 - \tilde{\omega}(\tau)]\,\theta^4(\tau) = [1 - \tilde{\omega}(\tau)]\,T^4(\tau). \tag{9}$$

We require boundary conditions on Eq. (9). We assume there is a right hand boundary at $\tau = 0$, with a known angular distribution incident upon the system given by $\Gamma_-(\mu)$, i.e.,

$$I(0, \mu) = \Gamma_-(\mu), \qquad \mu < 0. \tag{10}$$

Thus the incident flux at $\tau = 0$, F_{inc}, is given by

$$F_{\text{inc}} \equiv 2\pi \int_{-1}^{0} d\mu\, |\mu|\, I(0, \mu) = 2\pi \int_{-1}^{0} d\mu\, |\mu|\, \Gamma_-(\mu). \tag{11}$$

This incident flux is just the left going flux at $\tau = 0$, previously denoted by $F^-(0)$ in Eq. (5). Thus we have

$$\sigma\theta^4(0) - \tfrac{1}{2}F(0) = F_{\text{inc}}, \tag{12}$$

or using Fick's law of diffusion in Eq. (12)

$$\theta^4(0) + \frac{2}{3}\frac{\partial\theta^4(0)}{\partial\tau} = \frac{F_{\text{inc}}}{\sigma}. \tag{13}$$

Equation (13) is the appropriate boundary condition at $\tau = 0$ for the diffusion equation. It is often referred to as the Marshak, or Milne, condition, particularly when $F_{\text{inc}} = 0$, i.e., no flux impinging upon the surface. In this case (a vacuum boundary), Eq. (13) gives the familiar diffusion result for the linear extrapolation distance, namely two-thirds of a mean free path. A similar boundary condition applies at the left hand boundary, say $\tau = a$. Equation (9), together with the boundary conditions at $\tau = 0$ and $\tau = a$, constitute the diffusion description of radiative transfer. This diffusion description is sometimes referred to as the two-temperature description since it involves the material temperature $T(\tau)$ as well as the radiation temperature $\theta(\tau)$. This is in contrast to the cruder diffusion approximation, called equilibrium, or one-temperature, diffusion in which one assumes local equilibrium between material and radiation, i.e.,

$$\theta(\tau) = T(\tau). \tag{14}$$

In this case, the radiative flux is simply given by

$$F(\tau) = -\frac{4\sigma}{3}\frac{dT^4(\tau)}{d\tau}. \tag{15}$$

We are concerned with two-temperature diffusion in this paper.

3. The Marshak Interface Condition

We now turn to the problem of formulating the interface conditions at a transport-diffusion interface. We take this interface to be at $\tau = 0$. To the left of the interface ($\tau \leqslant 0$) we assume the problem is described by the diffusion equation, namely Eq. (9) and to the right ($\tau \geqslant 0$) we assume a transport description according to the equation of transfer, Eq. (1). A straightforward application of the boundary conditions described in the last section gives the connecting conditions for these two descriptions at $\tau = 0$.

We first consider the diffusion region. The boundary condition at $\tau = 0$ is given by Eq. (13). The incident flux F_{inc} will just be the flux leaving the transport region. We call this F_{tran} (to emphasize that it arises from the transport region), and thus we have as the diffusion boundary condition at $\tau = 0$

$$\theta^4(0) + \frac{2}{3}\frac{\partial\theta^4(0)}{\partial\tau} = \frac{F_{\text{tran}}}{\sigma}, \tag{16}$$

where F_{tran} is given by

$$F_{\text{tran}} = 2\pi\int_{-1}^{0} d\mu \mid \mu \mid I(0, \mu). \tag{17}$$

Here $I(0, \mu)$ is the radiative intensity as computed for $\tau \geqslant 0$ in the transport region.

The boundary condition at $\tau = 0$ for the transport region is given by Eq. (7). The incident intensity $\Gamma_+(\mu)$ at $\tau = 0$ is due to the leakage from the diffusion region into the transport region. This leakage is just $F^+(0)$, given by Eq. (4), i.e.

$$F^+(0) = \sigma\theta^4(0) + \tfrac{1}{2}F(0), \tag{18}$$

or, using Fick's law of diffusion,

$$F^+(0) = \sigma\left[\theta^4(0) - \frac{2}{3}\frac{\partial\theta^4(0)}{\partial\tau}\right]. \tag{19}$$

Here $\theta^4(0)$ and $\partial\theta^4(0)/\partial\tau$ are the fourth power of the radiation temperature and its derivative as computed for $\tau \leqslant 0$ in the diffusion region. For the boundary condition on the transport region, we need specify not only the flux entering the system, but also its angular distribution. If we assume an isotropic distribution in the forward hemisphere, we then have as the boundary condition on the transport region

$$I(0, \mu) = \frac{F^+(0)}{\pi} = \frac{\sigma}{\pi}\left[\theta^4(0) - \frac{2}{3}\frac{\partial\theta^4(0)}{\partial\tau}\right], \qquad \mu > 0. \tag{20}$$

This assumption of hemispherical isotropy is reasonable for several reasons. In the first place, it is the simplest angular distribution. Secondly, it is consistent with the diffusion region exit angular distribution in the limit of a vanishing small net flux at $\tau = 0$ (only in this limit is the diffusion approximation rigorously accurate). In addition, in the important limit of the diffusion region radiating as a black body this assumption of hemispherical isotropy is exact since black bodies radiate isotropic radiation. Finally, it should be noted that the overall solution in the transport region is relatively insensitive to the angular distribution of the incoming radiation. The important parameter is the incoming flux, which Eq. (20) gives correctly.

A slightly more complex alternative to Eq. (20) is

$$I(0, \mu) = \frac{\sigma}{\pi}\left[\theta^4(0) - \mu\frac{\partial\theta^4(0)}{\partial\tau}\right], \qquad \mu > 0, \tag{21}$$

which utilizes the full diffusion theory angular dependence. Equation (21) would obviously be more appropriate if the transport-diffusion interface were placed several mean free paths into the diffusion region. For reasons already mentioned, such a placement is generally impractical. If one accepts as a practical necessity the placement of the transport-diffusion interface at a material boundary, then Eq. (20), which gives the proper black body angular distributoin, seems preferable. The choice of either Eq. (20) or (21) does not affect the discussion to follow concerning the boundary condition on the diffusion region, which is the main concern of this paper.

Equations (16) and (20) or (21) are the interface conditions that arise naturally from the Marshak–Milne condition at the transport-diffusion interface. One property that these matching conditions, together with the transport and diffusion equations, must satisfy if they are to constitute a reasonable calculational scheme is the equilibrium property. That is, they must give the correct equilibrium solution for an infinite medium at a constant material temperature T. This equilibrium solution is the Planck distribution, $B(\nu, T)$, at all points, and this must be the case for arbitrary material properties, i.e., for $\tilde{\omega}(\tau)$ an arbitrary function of τ. It is easily verified that these equations possess this property.

We note that the diffusion description, Eqs. (9) and (16), can be written in an alternate, but equivalent, way. Since these equations are linear in $\theta^4(\tau)$, the solution can be decomposed into two components, one corresponding to the emitted radiation associated with the material temperature, and one corresponding to the incident flux F_{tran}. That is, Eqs. (9) and (16) are entirely equivalent to writing

$$\theta^4(\tau) = \theta_1^4(\tau) + \theta_2^4(\tau), \tag{22}$$

where $\theta_1(\tau)$ satisfies the inhomogeneous equation

$$-\frac{1}{3}\frac{\partial^2\theta_1^4(\tau)}{\partial\tau^2} + [1 - \tilde{\omega}(\tau)]\,\theta_1^4(\tau) = [1 - \tilde{\omega}(\tau)]\,T^4(\tau), \tag{23}$$

with the homogeneous boundary condition

$$\theta_1^4(0) + \frac{2}{3}\frac{\partial\theta_1^4(0)}{\partial\tau} = 0, \tag{24}$$

and $\theta_2(\tau)$ satisfies the homogeneous equation

$$-\frac{1}{3}\frac{\partial^2\theta_2^4(\tau)}{\partial\tau^2} + [1 - \tilde{\omega}(\tau)]\,\theta_2^4(\tau) = 0, \tag{25}$$

with the inhomogeneous boundary condition

$$\theta_2^4(0) + \frac{2}{3}\frac{\partial\theta_2^4(0)}{\partial\tau} = \frac{F_{\text{tran}}}{\sigma}. \tag{26}$$

That these equations are correct is clear physically, and is easily demonstrated mathematically. Adding Eqs. (23) and (25) gives Eq. (9), and adding Eqs. (24) and (26) gives Eq. (16). This alternate description gives, of course, the proper equilibrium solution since it is entirely equivalent to the composite description, Eqs. (9) and (16).

In general, the transport and diffusion problems must be solved simultaneously since the solution in one region contributes the boundary condition to the other. As a concrete example of our considerations, however, we consider a problem where a decoupling of the transport and diffusion solutions occur and, further, where each solution can be obtained analytically. Specifically, we consider two semi-infinite halfspaces with a common interface at $\tau = 0$. The right halfspace ($\tau \geqslant 0$) is a pure absorber or blackbody ($\tilde{\omega} = 0$) with a constant fixed temperature T_+. This halfspace is described by transport theory. The left halfspace ($\tau \leqslant 0$) contains scattering

($\tilde{\omega} \neq 0$), but the single scattering albedo, $\tilde{\omega}$, is independent of τ. In this left halfspace, described by diffusion theory, we assume a different constant and fixed temperature T_-.

For this problem, the transport solution for $\mu < 0$ can be computed without reference to the rest of the problem. Having this one can compute the exit flux from the transport region, F_{tran}, which is required to specify the boundary condition on the diffusion region. The diffusion region can then be solved completely, including the boundary ($\tau = 0$) values for θ^4 and $\partial\theta^4/\partial\tau$ needed for the transport boundary condition. With the transport boundary condition in hand, one can complete the solution in the transport region (i.e., obtain the solution for $\mu > 0$). It should be noted that the exact transport solution (i.e., treating both regions as transport regions) for this problem is available in the literature. In particular, if one is interested in the net flux transmitted from the left halfspace to the right halfspace, we have

$$F(0) = \epsilon\sigma(T_-^4 - T_+^4), \tag{27}$$

where ϵ is the emissivity of the left halfspace ($\epsilon = 1$ for the right half-space since by assumption it is a blackbody, i.e., $\tilde{\omega} = 0$). We shall return to Eq. (27) shortly.

Omitting the straightforward algebraic detail, we find that the solution in the diffusion region is given by

$$\begin{aligned} \theta^4(\tau) &= \theta_1^4(\tau) + \theta_2^4(\tau) \\ &= T_-^4 + (T_+^4 - T_-^4)\left(1 + \frac{2\kappa}{3}\right)^{-1} e^{\kappa\tau}. \end{aligned} \tag{28}$$

In particular, the flux leaving the diffusion region, $F^+(0)$, is then given by Eq. (19) as

$$F^+(0) = \sigma\left[T_-^4 + \left(1 - \frac{2\kappa}{3}\right)\left(1 + \frac{2\kappa}{3}\right)(T_+^4 - T_-^4)\right]. \tag{29}$$

The solution in the transport region is

$$I(\tau, \mu) = \begin{cases} \dfrac{\sigma T_+^4}{\pi}, & \mu < 0, \\ \dfrac{\sigma T_+^4}{\pi}(1 - e^{-\tau/\mu}) + \dfrac{F^+(0)}{\pi} e^{-\tau/\mu}, & \mu > 0. \end{cases} \tag{30}$$

In constructing this solution, we have used Eq. (20) as the transport boundary condition.

It is easily verified, when $T_+ = T_-$, i.e., when the entire problem has a fixed, uniform, temperature, that the solution just constructed is the proper equilibrium solution. This is consistent with our earlier observation that the Marshak interface conditions lead, in general, to the proper thermodynamic equilibrium solution. Computing the net flux across the interface at $\tau = 0$, we find

$$F(0) = F^+(0) - F^-(0) = \sigma\left(\frac{4\kappa}{3}\right)\left(1 + \frac{2\kappa}{3}\right)^{-1}(T_-^4 - T_+^4). \tag{31}$$

Comparing this with the exact transport result, Eq. (27), we see that $\bar{\epsilon}$, defined as

$$\bar{\epsilon} = \left(\frac{4\kappa}{3}\right)\left(1 + \frac{2\kappa}{3}\right)^{-1}, \tag{32}$$

is just an approximation to emissivity for the left halfspace. It is an approximation because it was obtained by using a diffusion, rather than the correct transport, description in the left halfspace.

The emissivity as a function of $\tilde{\omega}$ is available, from numerical transport calculations, in the literature [2]. Table 1 compares ϵ and $\bar{\epsilon}$ as a function of $\tilde{\omega}$. We see that $\bar{\epsilon}$, the diffusion approximation for the emissivity, is somewhat larger than the exact value. As expected, for $\tilde{\omega}$ near unity, $\bar{\epsilon}$ is most accurate (since the diffusion description is most accurate for highly scattering media). Unfortunately, in most practical problems, the diffusion region is almost always a highly absorbing medium ($\tilde{\omega} \approx 0$). In particular, for a blackbody ($\tilde{\omega} = 0$), we see $\bar{\epsilon} = 1.072$, which implies that a diffusion calculation overestimates the radiation from a blackbody by 7.2%. In the next section, we suggest a modification to the Marshak (Milne) interface conditions which corrects this deficiency of diffusion theory.

Before doing this, however, we discuss this problem with the Marshak boundary condition from another point of view which is closely tied to the numerical implementation of these equations. Specifically, the decomposition of the diffusion equation into two components, $\theta_1(\tau)$ and $\theta_2(\tau)$, suggests an attractive way to proceed numerically. Consider, for simplicity of argument, a purely absorbing diffusion region ($\tilde{\omega} = 0$). Since Eqs. (25) and (26) for $\theta_2(\tau)$ are the diffusion description corresponding to an incoming flux F [illegible] incident upon a zero temperature region, they suggest intuitively that their solution would correspond to absorbing the incoming photons into the diffusion region according to the diffusion kernel $\exp(-\sqrt{3}\mid\tau\mid)$. In this way the incoming photons would contribute to the material field. Equation (23) and (24) for $\theta_1(\tau)$ then dictate a diffusion solution with the established material field in the diffusion region with a homogeneous (vacuum) boundary condition at $\tau = 0$. One finds, however, that this numerically attractive procedure is not equivalent to solving the equations as stated. In particular, a numerical experiment which applied this procedure to a problem initially at thermodynamic equilibrium (and which, physically, should remain at thermodynamic equilibrium) gave the result that this equilibrium was not maintained. A new steady state was established which exhibited a radiation energy gradient in the vicinity of the transport-diffusion interface. This physically incorrect behavior is traced back to the fact that the inhomogeneous boundary condition, Eq. (26) does not correspond to the intuitive procedure of absorbing all of the incident photons in a purely absorbing medium according to $\exp(-\sqrt{3}\mid\tau\mid)$. The absorption, as predicted by Eqs. (25) and (26) is, in fact, greater than the incident flux. Since diffusion theory conserves energy, this excess absorption leads to a negative reflected flux. That is, the diffusion description, Eq. (25) with the usual Marshak (Milne) boundary condition, Eq. (26), does not lead to the physically correct result of absorption of all photons incident upon a blackbody. Another manifestation of this basic error of diffusion theory with the Marshak boundary condition was noted earlier; namely a black body will radiate, according to this diffusion description given by Eqs. (23) and (24), in excess of the physical blackbody limit. This excess radiation precisely cancels the negative reflected flux referred to above, so that the composite equations (i.e., those of $\theta^4 = \theta_1^4 + \theta_2^4$) do give the proper equilibrium solution, i.e., a hemispherical flux in each direction at $\tau = 0$ of σT^4. However, upon breaking the right going flux into its two components (corresponding to θ_1 and θ_2), one finds, as noted above, that each component is in error, with the errors being of equal magnitude (7.2 %), but differing in sign. Thus, with the Marshak interface condition, it is incorrect to apply the intuitive procedure of depositing all the flux incident upon the diffusion region. For consistency with the equations, one must deposit 1.072 times the incident flux, a procedure unappealing to one's physical intuition.

In the next section we suggest a modification to the Marshak interface condition with corrects this error in each component. This allows a numerical scheme to be based upon the intuitive notion, referred to above, of depositing the photons incident upon the diffusion region according to $\exp(-\sqrt{3} \mid \tau \mid)$, and having this procedure to be entirely equivalent to solving the diffusion equation with the modified boundary condition. The second component of the radiation field, namely that corresponding to a heated body radiating into a vacuum, will then exhibit, with the modified boundary condition, the correct behavior of radiating a flux given by σT^4 in the blackbody limit.

4. A Modification to the Marshak Interface Condition

We assume we wish to retain the diffusion equation as the description of the left halfspace. We also assume that the quantity of prime interest is the net flux crossing the boundary at $\tau = 0$, the diffusion-transport interface. We modify the interface conditions at $\tau = 0$ to improve the accuracy of $F(0)$ which, as we have seen, is measured by the emissivity of the left halfspace.

We assume, in order to keep the modified boundary condition simple, that in most practical problems the diffusion region is highly absorbing (almost a blackbody). Thus our scheme will be to modify the interface conditions so that in the limit of a blackbody, the diffusion description will predict an emissivity of unity. The resulting interface conditions, while "normalized" to give exact results for a blackbody, are meant to apply generally to any $\tilde{\omega}$ and any geometric configuration and temperature distribution. As a test of this general applicabliity, we compute, in this modified diffusion description, the emissivity as a function of $\tilde{\omega}$.

The Marshak interface conditions of the previous section followed from the basic Marshak expressions for $F^+(\tau)$ and $F^-(\tau)$, given by Eqs. (4) and (5), evaluated at $\tau = 0$, i.e.,

$$F^+(0) = \alpha\sigma\theta^4(0) + \beta F(0), \tag{33}$$

$$F^-(0) = \gamma\sigma\theta^4(0) - \delta F(0), \tag{34}$$

where

$$\alpha = \gamma = 1; \qquad \beta = \delta = 1/2. \tag{35}$$

Our procedure will be to ignore Eq. (35), and choose α, β, γ, and δ to improve the accuracy of the diffusion description. In particular, we wish to obtain an emissivity value of unity for $\tilde{\omega} = 0$.

To determine these four constants, we require, in addition to the constraint that $\epsilon = 1$ for $\tilde{\omega} = 0$, that: (i) energy is conserved, and (ii) the proper equilibrium solution is obtained. These two conditions, together with the requirement that ϵ $(\tilde{\omega} = 0) = 1$, uniquely determine α, β, γ, and δ. Considering first energy conservation, we note that the net flux, $F(0)$, is just the difference of $F^{+}(0)$, i.e.,

$$F(0) = F^{+}(0) - F^{-}(0). \tag{36}$$

If we require that our interface conditions conserve energy, Eqs. (33), (34), and (36) yield

$$\beta + \delta = 1. \tag{37}$$

We now consider equilibrium, by which we mean an infinite medium at a uniform material temperature T. The specific intensity in this case is given by

$$I(\tau, \mu) = \frac{\sigma T^4}{\pi}, \tag{38}$$

and the flux in any 2π solid angle is then given by

$$F(\tau)\,|_{\text{any } 2\pi} = \sigma T^4, \tag{39}$$

the blackbody flux. In particular, $F^{+}(0)$ and $F^{-}(0)$ must obey Eq. (39), and since the net flux $F(0) = 0$, Eqs. (33) and (34) give

$$\alpha = \gamma = 1. \tag{40}$$

Using Eqs. (37) and (40), Eqs. (33) and (34) become

$$F^{+}(0) = \sigma\theta^4(0) + (1 - \delta)\, F(0), \tag{41}$$

$$F^{-}(0) = \sigma\theta^4(0) - \delta F(0). \tag{42}$$

We determine the remaining unknown δ by demanding that $\epsilon(\tilde{\omega} = 0) = 1$. We note that in the Marshak treatment $\delta = 1/2$.

Rewriting Eqs. (41) and (42) in the manner previously employed in going from

Eqs. (4) and (5) to Eqs. (16) and (20), we find that the modified boundary condition on the transport region is

$$I(0, \mu) = \frac{\sigma}{\pi}\left[\theta^4(0) - \frac{4}{3}(1-\delta)\frac{\partial\theta^4(0)}{\partial\tau}\right], \qquad \mu > 0, \tag{43}$$

and the modified boundary condition on the diffusion region is

$$\theta^4(0) + \frac{4}{3}\delta\frac{\partial\theta^4(0)}{\partial\tau} = \frac{F_{\text{tran}}}{\sigma}, \tag{44}$$

with the constant δ still to be determined from the condition $\epsilon(\tilde{\omega} = 0) = 1$. The similar modification to Eq. (21) yields

$$I(0, \mu) = \frac{\sigma}{\pi}\left[\theta^4(0) - 2(1-\delta)\,\mu\,\frac{\partial\theta^4(0)}{\partial\tau}\right], \qquad \mu > 0. \tag{45}$$

Applying Eq. (43) and (44) to the problem previously considered (two semi-infinite halfspaces with a common interface at $\tau = 0$, and each with a fixed, constant temperature), we find for the net flux at $\tau = 0$, omitting the algebraic details,

$$F(0) = \sigma\hat{\epsilon}(T_-^4 - T_+^4), \tag{46}$$

where the emissivity, $\hat{\epsilon}$, is given by

$$\hat{\epsilon} = \left(\frac{4\kappa}{3}\right)\left(1 + \frac{4\kappa\delta}{3}\right)^{-1}. \tag{47}$$

For $\tilde{\omega} = 0$ (a blackbody), we have $\kappa = \sqrt{3}$, and thus the requirement that $\hat{\epsilon}(\tilde{\omega} = 0) = 1$ gives

$$\delta = 1 - \frac{\sqrt{3}}{4} = 0.5670. \tag{48}$$

This is to be compared with $\delta = 1/2$ for the usual Marshak treatment.

Table 1 compares $\hat{\epsilon}$, as given by Eq. (46) with δ fixed (independent of $\tilde{\omega}$) according to Eq. (48), with the exact transport emissivity. We see that the modified interface condition gives quite accurate results for the emissivity, and hence the net flux at $\tau = 0$, for all values of $\tilde{\omega}$. We could have forced exact agreement, in our model problem, for all $\tilde{\omega}$ by allowing δ to be a function of $\tilde{\omega}$, but this complexity is probably not warranted. If we had allowed δ to depend upon $\tilde{\omega}$ in this way, it would not be clear what value to assign to $\tilde{\omega}$ in the general case of $\tilde{\omega}$ depending upon position, and in addition we would have no assurance of exact results when the temperature profile depended upon position.

TABLE I

Comparison of the Exact Emissivity with Two Approximate Formulations

$\hat{\omega}$	κ	$\bar{\epsilon}$	$\hat{\epsilon}$	ϵ
0	1.732	1.072	1.000	1.000
0.1	1.643	1.046	0.977	0.979
0.2	1.549	1.016	0.951	0.954
0.3	1.449	0.983	0.922	0.926
0.4	1.342	0.944	0.888	0.892
0.5	1.225	0.890	0.848	0.854
0.6	1.095	0.844	0.799	0.805
0.7	0.949	0.775	0.737	0.744
0.8	0.775	0.681	0.651	0.658
0.9	0.548	0.535	0.516	0.522
0.92	0.490	0.492	0.477	0.482
0.94	0.424	0.441	0.428	0.433
0.96	0.346	0.375	0.366	0.369
0.98	0.245	0.281	0.276	0.278
0.99	0.173	0.207	0.204	0.205
1.00	0.000	0.000	0.000	0.000

Use of Eq. (48) in Eq. (44) in the case of no incident flux, i.e., $F_{\text{tran}} = 0$, gives

$$\theta^4(0) + 0.7560 \frac{\partial \theta^4(0)}{\partial \tau} = 0, \tag{49}$$

which implies an "extrapolated endpoint" or "linear extrapolation distance" of 0.756 mean free paths, as contrasted to the value of 2/3 as predicted by the Marshak condition, and the classic value of 0.7104 for the transport solution of the Milne problem (a purely scattering halfspace with a source at infinity).

Since this modification to the interface conditions was obtained by requiring that the diffusion predicted emissivity be unity for a black-body, one can now solve these equations in the intuitive manner referred to at the end of the last section. That is, the incident flux is deposited into the diffusion region according to the diffusion kernel $\exp(-\sqrt{3} \mid \tau \mid)$, and the contribution to the radiation field arising from the non-zero temperature in the diffusion region is found by solving the diffusion equation subject to the modified vacuum boundary condition, Eq. (49). This "deposition" method of solution, convenient from a numerical point of view, is entirely equivalent to solving the diffusion equation, together with the modified boundary conditions, as stated. The numerical experiment mentioned previously was redone using these

[redacted]

In closing this section, we mention that for the model problem we solved analytically to obtain Eq. (47), the modified interface conditions lead to exact transport results for $I(\tau, \mu)$ in the transport region.

5. The Brockway Interface Condition

Brockway [3] has earlier suggested a treatment of the connecting conditions at a transport-diffusion interface. The Brockway conditions are currently being used to connect transport and diffusion regions in large radiative transfer problems. He basically used the Marshak expressions for F^+ and F^- as given by Eqs. (4) and (5), but in a particular finite difference, rather than the differential equation, setting. By straightforward algebraic manipulation, he arrived at the equations

$$F(0) = S(\sigma\theta_{zc}^4 - F_{\text{tran}}), \tag{50}$$

$$F^+(0) = S\sigma\theta_{zc}^4 + RF_{\text{tran}}. \tag{51}$$

Here θ_{zc} is the radiation temperature at the zone center of the first diffusion zone, and the coefficients S and R are given by

$$S = \frac{4/3}{2/3 + \Delta\tau}, \tag{52}$$

$$R = 1 - S = \frac{\Delta\tau - 2/3}{2/3 + \Delta\tau}, \tag{53}$$

where $2\Delta\tau$ is the optical thickness of the first diffusion zone. Because of the position of these coefficients S and R in Eqs. (50) and (51), Brockway argued that S plays the role of a transmission coefficient, and R plays the role of a reflection coefficient. He then concluded that a transport-diffusion boundary can be treated by: (i) emit a flux $S\sigma\theta_{zc}^4$ from the boundary into the transport region, and (ii) when a photon from the transport region reaches the boundary, absorb (transmit) an amount SF_{tran} into the diffusion region and reflect (or re-emit) an amount RF_{tr} back into the transport region. As suggested by this wording, Brockway's considerations were within the context of a Monte Carlo transport treatment.

We note that in the limit $\Delta\tau = 0$ (i.e., the differential equation limit), Brockway's equations reduce to the Marshak equations given in Section 2, namely Eqs. (7) and (8) evaluated at $\tau = 0$, noting that $F^-(0) = F_{\text{tran}}$. Since our considerations of Section 3 were also based upon those same Marshak equations, there must be a close correspondence between Brockway's scheme and our (unmodified) scheme. We address this point very shortly.

We note that in this limit $\Delta\tau = 0$, we have, from Eqs. (52) and (53),

$$S = 2; \qquad R = -1. \tag{54}$$

That is, the transmission coefficient becomes two, and the reflection becomes minus one. Clearly the interpretation of these quantities as probabilities leads to conceptual difficulties in the diffusion equation limit ($\Delta\tau = 0$). Numerically, this negative reflection has been handled by using a portion of the positive flux emitted from the surface, namely $S\sigma\theta_{zc}$, to "cancel" the negative reflection, RF_{tran}, and thereby, in effect, emitting only the difference. This numerical procedure, which works well, gives the resolution to this apparent conceptual difficulty. There is no need to interpret each term in Eqs. (50) and (51) as a reflected or transmitted flux (although there may, for large $\Delta\tau$, be some heuristic value in such an interpretation). Those equations only require that the net flux $F(0)$ and the positive direction flux $F^+(0)$ each be given by the sum of two terms. Giving each of these two terms a separate physical significance is unnecessary. The numerical cancelation is, in fact, entirely consistent with these two equations.

We conclude that the conceptual difficulty of the Brockway scheme is more apparent than real, and that this scheme, since is based on the same Marshak equations, is entirely equivalent to the scheme we presented in Section 3 (with the obvious distinction of course, that the Brockway equations are a certain finite difference representation of the differential interface conditions). This observation also leads to the conclusion that the modified interface conditions of the last section could be implemented either by the deposition scheme previously discussed or by extending the Brockway finite difference approach to incorporate the modifications we have suggested in the differential equation context.

Using Eqs. (41) and (42) as the starting point and following the algebraic approach of Brockway, one finds that the modified finite difference equations are again of the Brockway form, Eqs. (50) and (51), but in this case the quantities S and R are given by (we prefer not to call these quantities transmission and reflection coefficients for reasons already mentioned),

$$S = \frac{4/3}{(4\delta/3) + \Delta\tau}, \tag{55}$$

$$R = 1 - S = \frac{\Delta\tau - 4(1-\delta)/3}{(4\delta/3) + \Delta\tau}. \tag{56}$$

Since Brockway's considerations are not available in the literature, we sketch the detail which leads to Eqs. (55) and (56). Equations (41) and (42), together with Eq. (6), can be rewritten

$$F(0) = F^+(0) - F_{\text{tran}}, \tag{57}$$

$$F^+(0) = \sigma\theta_B^4 + (1-\delta)\,F(0), \tag{58}$$

where we have use $F^-(0) = F_{\text{tran}}$ and set $\theta(0) = \theta_B$, the boundary value of the radiation temperature. Eliminating $F^+(0)$ between Eqs. (57) and (58) gives

$$F(0) = \frac{1}{\delta}\,(\sigma\theta_B^4 - F_{\text{tran}}). \tag{59}$$

Now, a finite difference form of Fick's law is

$$F(0) = \left(\frac{4\sigma}{3\Delta\tau}\right) (\theta_{zc}^4 - \theta_B{}^4), \tag{60}$$

where θ_{zc} is the radiation temperature at the center of the first diffusion zone. Equating Eqs. (59) and (60) gives

$$\theta_B{}^4 = \left[\frac{4\delta/3}{(4\delta/3) + \Delta\tau}\right] \theta_{zc}^4 + \left[\frac{\Delta\tau}{(4\delta/3) + \Delta\tau}\right] \frac{F_{\text{tran}}}{\sigma}, \tag{61}$$

which gives the boundary temperature in terms of the zone-centered temperature. Use of Eq. (61) in Eq. (59) gives

$$F(0) = \left[\frac{4/3}{(4\delta/3) + \Delta\tau}\right] (\sigma\theta_{zc}^4 - F_{\text{tran}}), \tag{62}$$

and use of Eq. (62) in Eq. (58) gives

$$F^+(0) = \left[\frac{4/3}{(4\delta/3) + \Delta\tau}\right] \sigma\theta_{zc}^4 + \left[\frac{\Delta\tau - 4(1 - \delta)/3}{(4\delta/3) + \Delta\tau}\right] F_{\text{tran}}\,. \tag{63}$$

Equations (62) and (63) correspond to the Brockway forms, Eqs. (50) and (51), with S and R given by Eqs. (52) and (53).

Which of these two equivalent interface treatments (i.e., the deposition scheme as discussed in the last section or the modified Brockway scheme just presented) is better, in the practical sense of numerical efficiency in solving real problems, has yet to be determined. Undoubtedly, the answer to this question depends upon the details of the numerical approach used, and may well be problem dependent as well. In this regard, it should be noted that the finite difference equations of Brockway, or our modification, resulted from one particular finite difference approach, namely Eq. (60). Other finite difference forms are obviously also possible.

6. Concluding Remarks

In this paper we have suggested the use of a coupled transport and diffusion treatment for certain radiative transfer problems. Specifically we addressed the treatment of the boundary (connecting) conditions at a transport-diffusion interface. The straightforward extension of the Marshak (Milne) boundary condition at an exterior (vacuum) boundary led to a self-consistent mathematical description of the interface problem. However, it was shown that this boundary treatment overestimates the radiation from a blackbody. A manifestation of this basic discrepancy in the Marshak treatment is, in addition to this excess blackbody radiation, a negative reflection of photons from a blackbody. These observations led us to modify the Marshak boundary conditions in such a way that the emissivity of a blackbody, as predicted by diffusion theory, is unity, and the reflection from a black-body is accordingly zero.

The Brockway finite difference boundary conditions, previously suggested as the interface conditions, were shown to correspond to a certain finite difference representation of our unmodified differential equation considerations. In the limit of infinitely small zones (the differential equation limit), Brockway's scheme and our modification to it are equivalent to the Marshak considerations, including the modification, presented here.

We have preliminarily tested these connecting conditions, both analytically and numerically, and find them to behave as expected. In particular, for problems involving optically thin regions, analytic calculations have shown that this transport-diffusion description can be significantly more accurate than a pure diffusion solution. Numerically, both the deposition approach and the Brockway equations have been used successfully in test problems. As mentioned earlier, we have numerically confirmed that the pure Marshak connecting conditions do not lead to the proper thermodynamic equilibrium in the deposition method, while the modified Marshak conditions do.

At this time we do not have a definitive recommendation as to the best way to implement these interface conditions into general purpose radiative transfer codes. Such an implementation will, of course, depend heavily upon the details of the finite difference or other numerical approximations contained in a given code. Because of this, the "best" numerical treatment of these interface conditions will be code dependent, and undoubtedly much experimentation will be required to find the optimum treatment for a given code. In any event, it seems probable that improved accuracy will result for a wide class of problems from the use of the modified Marshak conditions discussed here. This should be the case if the modified Marshak treatment is used in the transport-diffusion context, or at a vacuum boundary in a pure diffusion calculation.

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