The transport equation in optically thick media ⋆

Abraham Szőke * Eugene D. Brooks III

University of California, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550, USA

Abstract

The photon transport equation is transformed into a new form by considering the deviation of the specific intensity from the local equilibrium field. We call the new form of the equations the difference formulation. It is rigorously equivalent to the original transport equation. The difference formulation is particularly suited for thick media, where the radiation field approaches local equilibrium and the deviations from the Planck distribution are small. The difference formulation for photon transport also clarifies the diffusion limit. Preliminary results confirm our expectations of a substantial advantage for accurate numerical calculations in optically thick media.

Key words: difference formulation, radiation transport

1 INTRODUCTION

The transport of photons in thick media is of great importance in many fields of science. Radiation transport determines the temperature distribution in stellar interiors as well as the observable spectrum of stellar atmospheres. The temperature on the surface of the Earth depends on the amount of solar radiation reflected by clouds. Photon transport is the dominant cooling mechanism even in moderately hot bodies, with material opacities moderating the loss.

The natural way of deriving the transport equation is to follow the propagation of narrow beams of photons as they are emitted, propagate *in vacuo*, are

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* Corresponding Author:
Email address: szoke1@llnl.gov (Abraham Szőke).

scattered and, finally, are absorbed by matter [1], [2]. In transparent media the absorption, emission and scattering of photons is weak and the transport equation describes the overall propagation very well. Mathematically, the equations of propagation are hyperbolic partial differential equations and their numerical solution is relatively easy and stable in optically thin media.

In optically thick media, however, the probability that a photon propagates in a straight line, unhindered, is very small; radiation transport is dominated by many scattering, absorption and re-emission events. As a result, the solution of the transport equation in thick media is not straightforward. An important example is hot, dense matter with a high absorption coefficient. It results in conditions of local thermodynamic equilibrium (LTE) and very strong emission of photons. The emitted photons, in turn, are quickly re-absorbed, heating the medium locally. The net emission (or absorption) is then a small difference between two large terms. The process leads to stiffness of the transport equation: the local temperature relaxes much faster than any excess energy is transported away. In any numerical method that uses explicit differencing to balance spontaneous emission with absorption, the stiffness can cause instability, as well as a significant increase in noise for Monte Carlo methods. If the scattering coefficient is high a photon does not propagate in a straight path. This poses a difficulty for methods that are highly dependent upon efficient streaming of photons.

More generally, in thick systems the radiation tends to be nearly isotropic and, eventually, close to local equilibrium with the matter temperature. The computational burden of performing transport calculations in this regime is so high that the radiation diffusion equation [3] is often solved instead, in order to efficiently obtain an approximate solution to the problem of interest.

In this paper we transform the transport equation in a new way. The transformation is achieved by considering the difference between the radiation field and the local equilibrium field at each point in the problem domain. The local equilibrium field is a function of the matter temperature, and therefore a function of both space and time. This makes the transformation a function of both space and time. One might suspect that it would lead to a transport equation that is difficult to deal with. In fact, however, the resulting equation contains only quantities that are small when the system is thick. In particular, the large emission term and its (almost) compensating absorption term are replaced by a pure absorption term for the "difference field". The only sources for it come from the variation of the material temperature in space and time. We call the resulting formulation for radiation transport the *difference formulation*.

Why is the difference formulation interesting? To summarize, the equations are written in terms of quantities that are "natural" in thick media. (The traditional formulation is written in terms of variables that are natural in thin media.) In hot, dense matter the terms describing the nearly equal emission and absorption of photons are eliminated and only the small, *net* transport terms appear in the equation. We expect that this change of variables will aid in its numerical solution: it will make it less stiff, more numerically stable, and it will reduce the noise in Monte Carlo methods. In fact, preliminary results on a very simple model system confirm our expectations. Derivation of the diffusive behavior of the transport equation in thick media is simplified and clarified by the difference formulation. As the difference equation is able to satisfy the correct physical boundary conditions, we hope to find a fast and accurate alternative to the radiation diffusion equation. Finally, the new formalism might lead to the development of new numerical methods.

The rest of this paper is organized as follows: In Section 2, the traditional formulation for transport is presented, along with a discussion of the parameters that become small for thick media. We introduce the difference formulation in Section 3, first in a context without scattering where the new source terms are easily understood. We analyze the source terms in some detail. We show how the difference difference formulation leads to a simplified discussion of the diffusion limit. We then write down the general equations and develop them for the case of coherent scattering. In Section 4 we present preliminary results, applying the difference formulation to Monte Carlo calculations for a simple two-level system. We end with a discussion. Higher order treatment of asymptotic expansions are considered in an Appendix.

2 Radiation transport in LTE

2.1 Traditional formulation

Radiation transport and its coupling to matter is described by the equations of radiation hydrodynamics. In their general form, they consist of the equations of hydrodynamics coupled to those of radiation transport and to the interaction of radiation with matter. Excellent treatises have been written by Pomraning, [4], Mihalas [2] and Castor [1].

In this paper we deal only with a subset of those equations. They are the radiation transport equation, the material energy balance equation and the conservation equation for the sum of the radiation and material energy. Furthermore we assume local thermodynamic equilibrium (LTE) - *i.e.* that the material has a well defined temperature - it emits radiation thermally. We also assume that the material is at rest or that it moves with constant velocity. In real hydrodynamic cases, where different parts of the material move at different velocities, the "co-moving frame transformation" has to be used and proper account has to be given to kinetic energy and hydrodynamic work [1]. When the local acceleration of the material is significant, general relativity has to be invoked [5]. Our equations are written in the rest frame of the material, assumed to be an inertial frame. Otherwise, the scattering terms would have a more complicated angle and frequency dependence.

The transport equation describes the propagation of the radiation field in terms of the specific intensity, $I(\mathbf{x}, t; \nu, \mathbf{\Omega})$, where $\mathbf{x}, t$ are the space and time variables, ν is the radiation frequency and $\mathbf{\Omega}$ is a unit vector in the direction of propagation.

$$\frac{1}{c}\frac{\partial I(\mathbf{x}, t; \nu, \mathbf{\Omega})}{\partial t} + \mathbf{\Omega}\cdot\nabla I(\mathbf{x}, t; \nu, \mathbf{\Omega}) = \sigma_a'(\nu, T(\mathbf{x}, t))[B(\nu, T(\mathbf{x}, t)) - I(\mathbf{x}, t; \nu, \mathbf{\Omega})] + Q(I) \tag{1}$$

$B(\nu, T)$ is the thermal (Planck) distribution at the material temperature, $T(\mathbf{x}, t)$, and c is the speed of light. The absorption coefficient, σ_a', and the scattering term, $Q(I)$, will be defined below. The specific intensity is related to the photon distribution function $f(\mathbf{x}, t; \nu, \mathbf{\Omega})$ by

$$I(\mathbf{x}, t; \nu, \mathbf{\Omega}) = ch\nu f(\mathbf{x}, t; \nu, \mathbf{\Omega}) \quad , \tag{2}$$

where $h\nu$ is the photon energy.

In Eq. (1), all the variables, I, σ_a', B are functions of the independent variables, $\mathbf{x}, t; \nu, \mathbf{\Omega}$ and/or $T(\mathbf{x}, t)$. In the following, the independent variables will mostly be suppressed.

The emission function and the absorption cross sections, corrected for stimulated emission, are

$$B(\nu, T) = \frac{2h\nu^3}{c^2}\left(e^{h\nu/kT} - 1\right)^{-1} \quad , \tag{3}$$

$$\sigma_a'(\nu, T) = \sigma_a(\nu, T)\left(1 - e^{-h\nu/kT}\right) \quad , \tag{4}$$

with σ_a being the "ordinary" absorption coefficient, per unit distance.

The scattering terms are denoted by $Q(I)$

$$Q(I) = \int_0^\infty d\nu' \int_{4\pi} d\mathbf{\Omega}' \frac{\nu}{\nu'}\sigma_s(\nu' \to \nu, \mathbf{\Omega}\cdot\mathbf{\Omega}')I(\nu', \mathbf{\Omega}')\left[1 + \frac{c^2 I(\nu, \mathbf{\Omega})}{2h\nu^3}\right]$$

$$
-\int_0^\infty d\nu' \int_{4\pi} d\mathbf{\Omega}' \sigma_s(\nu \to \nu', \mathbf{\Omega}\cdot\mathbf{\Omega}') I(\nu, \mathbf{\Omega}) \left[1 + \frac{c^2 I(\nu', \mathbf{\Omega}')}{2h\nu'^3}\right] \quad , \tag{5}
$$

where the $\mathbf{x}, t; T$ dependence of σ_s has been suppressed. In LTE there are thermodynamic relations among the partial scattering cross sections in Eq. (5). These follow from the observation that the radiation field reduces to the black body spectrum no matter what the scattering cross sections are. See Eq. (30) below.

The zeroth moment of the intensity gives the radiation energy density

$$
E_{rad} = \frac{1}{c} \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\, I \tag{6}
$$

and its first moment is the radiation flux vector

$$
\mathbf{F}_{rad} = \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\; \mathbf{\Omega}\, I \quad . \tag{7}
$$

Interaction of radiation with matter is expressed by the conservation law

$$
\frac{\partial E_{mat}}{\partial t} = \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\, \sigma_a'[I - B(\nu, T)] - \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\, Q(I) + G \quad , \tag{8}
$$

where E_{mat} is the energy per unit volume of the material and G is a volume source of energy.

In the absence of hydrodynamic work terms or thermal conductivity, the total energy of the radiation field and the material are conserved

$$
\frac{\partial(E_{mat} + E_{rad})}{\partial t} + \nabla\cdot\mathbf{F}_{rad} = G \quad . \tag{9}
$$

2.2 Thick media

We all have a common-sense concept of a thick medium; we attempt to clarify it here. One property of radiation in thick media is that its distribution is almost isotropic. Another property of thick media is that the transport of energy by radiation is severely hindered.

In the spirit of the first property we define a streaming parameter, ϵ_{stream}; it is the ratio of the magnitude of the actual radiation flux, $|\mathbf{F}_{rad}|$, to the maximum possible one

$$\epsilon_{stream} := \frac{|\mathbf{F}_{rad}|}{c\,E_{rad}} \quad . \tag{10}$$

It is clear that $0 \leq \epsilon_{stream} \leq 1$ and that $\epsilon_{stream} = 1$ only if the radiation streams in one well-defined direction. In thick media, ϵ_{stream} is a small parameter: $\epsilon_{stream} \ll 1$.

In the spirit of the second property, we look at the ratio of the photon mean free path, l_{rad} and some scale length, L. The scale length defines the distance of significant variation in the properties of the material. We define

$$\epsilon_{space} := \frac{4}{3}\frac{l_{rad}}{L} \quad . \tag{11}$$

In thick media $\epsilon_{space} \ll 1$.

In thick media that strongly absorbs and emits radiation, far from any boundary layer, the diffusion approximation is valid. In the diffusion limit, the photon mean free path is determined by the Rosseland mean opacity, $l_{rad} = 1/\sigma_R$ and the scale length is set by the rate of change in the temperature: $1/L = (1/4T^4)|\nabla(T^4)|$. In the diffusive regime the radiation energy density is that of a black body, $E_{rad} = a\,T^4$ and the diffusion flux is $\mathbf{F}_{rad} = -(ac/3\sigma_R)\nabla(T^4)$. (Both of the preceding formulas are valid to first order in the small parameter ϵ_{space}.) Simple algebra shows that in the interior of a thick, strongly absorbing and emitting region, without scattering, the two approaches give the same result

$$\epsilon_{space} \approx \epsilon_{stream} \quad . \tag{12}$$

The time rate of change of conditions in thick media can be estimated in a similar manner. We define a small parameter that is the ratio of the free flight time of a photon to the time rate of change of the temperature

$$\epsilon_{time} := \frac{1}{c\,\sigma_R}\frac{1}{T^4}\frac{\partial T^4}{\partial t} \quad . \tag{13}$$

Heating of the material results from radiation transport. Using the smallness of the energy flux, $\epsilon_{stream} \ll 1$, from the energy balance in a small volume we get the estimate

$$\epsilon_{time} \approx \epsilon_{space}^2 \frac{3E_{rad}}{E_{rad} + \partial E_{mat}/\partial(T^4)} \quad . \tag{14}$$

The parameters ϵ_{stream}, ϵ_{space} and ϵ_{time} are not small in some boundary layers and in the leading edge of thermal waves.

3 The difference formulation

In the introduction we discussed the difficulties of solving the transport equation, Eq. (1), in thick media. In the previous section we identified the streaming parameter, ϵ_{stream}, that is small in thick media. We now show a very simple transformation of the transport equation so that it is written in terms of variables that are small in thick media. We call the result of the transformation the "difference formulation." In the following we show the transformation in a simple case and discuss its remarkable properties.

3.1 The difference formulation without scattering

We start by repeating the transport equation, Eq. (1), without scattering

$$\begin{aligned}\frac{1}{c}\frac{\partial I(\mathbf{x},t;\nu,\mathbf{\Omega})}{\partial t} + \mathbf{\Omega}\cdot\nabla I(\mathbf{x},t;\nu,\mathbf{\Omega}) = \\ -\sigma_a'(\nu,T(\mathbf{x},t))[I(\mathbf{x},t;\nu,\mathbf{\Omega}) - B(\nu,T(\mathbf{x},t))] \quad . \end{aligned} \tag{15}$$

The equation is written in terms of the specific intensity carried by photons, $I(\mathbf{x},t;\nu,\mathbf{\Omega})$. The left-hand side of the equation describes their unhindered propagation, the first term on the right-hand side describes their attenuation. The two terms on the left-hand side and the first term on the right-hand side constitute a homogeneous equation. The last term on the right-hand side, $\sigma_a'B$, is a "source term" that makes the full equation inhomogeneous. It describes the emission of radiation by matter. From our considerations in the previous section, we expect that the difference between the two terms on the right-hand side is of the order of ϵ_{stream} in thick media, even though each term by itself is of the relative order unity.

We introduce now a "difference intensity"

$$D(\mathbf{x},t;\nu,\mathbf{\Omega}) := I(\mathbf{x},t;\nu,\mathbf{\Omega}) - B(\nu,T(\mathbf{x},t)) \tag{16}$$

and subtract $(1/c)(\partial B/\partial t) + \mathbf{\Omega}\cdot\nabla B$ form both sides of Eq. (15).

$$\frac{1}{c}\frac{\partial D(\mathbf{x},t;\nu,\mathbf{\Omega})}{\partial t} + \mathbf{\Omega}\cdot\nabla D(\mathbf{x},t;\nu,\mathbf{\Omega}) = -\sigma_a'(\nu,T(\mathbf{x},t))D(\mathbf{x},t;\nu,\mathbf{\Omega})$$

$$-\frac{1}{c}\frac{\partial B(\nu,T(\mathbf{x},t))}{\partial t} - \ \mathbf{\Omega}\cdot\nabla B(\nu,T(\mathbf{x},t)) \qquad (17)$$

Let us rewrite it with the independent variables suppressed for clarity.

$$\frac{1}{c}\frac{\partial D}{\partial t} + \ \mathbf{\Omega}\cdot\nabla D = -\sigma_a' D - \frac{1}{c}\frac{\partial B}{\partial t} - \ \mathbf{\Omega}\cdot\nabla B \qquad (18)$$

It should be emphasized that Eq. (18) and Eq. (15) are completely equivalent. In particular, they are able to satisfy equivalent initial and boundary conditions. The positivity constraint, $I \geq 0$, translates into $D \geq -B$.

It is important to investigate the properties of the new equation, (18), comparing it to its traditional counterpart, Eq. (15) and, by extension, to Eq. (1). The terms on the left-hand side and the first term on the right-hand side of Eq. (18) are completely analogous to those in Eq. (15): they describe the straight line propagation and the attenuation of the difference intensity, D. We conclude that the intensity I and the difference intensity D propagate the same way. In particular, their Green's functions (propagators) are the same.

In contrast, the inhomogeneous source terms have been changed drastically. The source term in Eq. (15) is $\sigma_a' B \approx B/l_{rad}$, while the last source term in Eq. (18) is $\mathbf{\Omega}\cdot\nabla B \approx B/L$. In thin media, where $l_{rad} \gg L$, the first version of the source term is small, while in thick media, where $l_{rad} \ll L$, it is the other way around. In addition to the question of asymptotic behavior, the source terms in the difference formulation are smooth in the frequency domain as they do not involve a factor of σ_a'.

The formulas in the previous section can be used to estimate the orders of the terms in Eq. (18) in optically thick regions. Let us divide the equation by $\sigma_a' B$ and consider the D/B term as the unknown. In thick media, the dominant source term is $|\mathbf{\Omega}\cdot\nabla B|/\sigma_a' B \approx \epsilon_{space}$; therefore we conclude that $D/B \approx \epsilon_{space}$. We can then estimate that the other terms $(1/c)(\partial B/\partial t)/\sigma_a' B \approx \epsilon_{time} \approx \epsilon_{space}^2$ and $\mathbf{\Omega}\cdot\nabla D/\sigma_a' B \approx \epsilon_{space}^2$. Finally, the $(1/c)(\partial D/\partial t)/\sigma_a' B$ term is of order ϵ_{space}^3.

Another significant difference between Eqs. (15) and (18) is in the angular dependence of the source terms. The source term in the traditional formulation is $\sigma_a' B$; it is spherically symmetric, *i.e.* of P_0 symmetry. The dominant source term in the difference formulation is $\mathbf{\Omega}\cdot\nabla B$; it is antisymmetric in angle; more accurately it is of P_1 symmetry. In the difference formulation there is also a small source term, $(1/c)(\partial B/\partial t)$ of P_0 symmetry. While the $\sigma_a' B$ term adds energy to the radiation field, in the difference equation the dominant source term, $\mathbf{\Omega}\cdot\nabla B$, only transports the difference intensity; it adds nothing to the total energy of the radiation field. That task is relegated to the small $(1/c)(\partial B/\partial t)$ term.

The source term in the traditional formulation for photon transport, $\sigma_a' B$, accounts for spontaneous emission and is balanced by absorption in a thick system. In the difference formulation, the reference value for the radiation field is B, not zero. This reference value is a function of the local temperature, $T(\mathbf{x}, t)$, and is therefore a function of both space and time. The new source terms in the difference formulation have a straightforward, intuitive interpretation. The term involving the time derivative of B can be understood from energy conservation. If the local temperature changes, the resultant change in B, all else remaining constant, must be accounted for by a change in the difference field, D, in order to maintain (locally) the energy in the radiation field.

The term involving the space derivative of B is more interesting. To understand this term, consider transport in one-dimensional slab geometry where this term is now written $\mu\, dB/dx$; the direction cosine of the propagation direction is $\mu = \mathbf{\Omega}\cdot\hat{\mathbf{x}}$, where $\hat{\mathbf{x}}$ is a unit vector perpendicular to the slab. If the temperature is uniform, dB/dx is zero and there are no sources. Consider, however, the case where there is a positive step in the value of B, of magnitude b, at the origin. The source term, $\mu\, dB/dx$, is now $\mu\, b\, \delta(x)$. The difference field has a source term only at the origin, with a negative source for positive μ and a positive source for negative μ. The right-moving negative source is interpreted as the missing photons that would have been streaming across the origin if the step in B did not exist. The negative sources are "photon holes", borrowing a term from solid state physics. The left-moving positive source is simply the photons being emitted from the hotter region into the cooler region. More succinctly, the $\mu\; dB/dx$ term generates the transport between the hotter and cooler regions that would otherwise not occur. The total "photon" energy emitted at the origin integrates to zero.

For completeness, we write the radiation energy density and its first moment, the radiation flux vector, in terms of D

$$E_{rad} = \frac{1}{c}\int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega} I = \frac{1}{c}\int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}(D+B) \quad , \tag{19}$$

$$\mathbf{F}_{rad} = \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\; \mathbf{\Omega}\, I = \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\; \mathbf{\Omega}\, D \quad , \tag{20}$$

and the coupling of the radiation to the material, from Eq. (8)

$$\frac{\partial E_{mat}}{\partial t} = \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega} \sigma_a' D + G \quad . \tag{21}$$

The energy conservation equation, (9), is unchanged.

3.2 The diffusion limit, without scattering

In thick media, in LTE, far from boundaries, after sufficient time, radiation tends to the diffusion limit. This is a well established result of asymptotic analysis; nevertheless even very recently a reanalysis was published by Morel [6]. We show now how the difference formulation leads to the diffusion limit. In fact we will show it in two different ways. First, we formally integrate the transport equation; second, we show that the traditional asymptotic expansion yields the same result to first order. It has to be emphasized that we show the diffusion limit of the exact transport equation; therefore it includes all terms, it is able to satisfy boundary conditions correctly and it includes the treatment of boundary layers.

3.2.1 Formal solution

Equation (18) has a formal solution. We define a path variable, s, by

$$\mathbf{x} = \mathbf{x_0} + \mathbf{\Omega}\, s \quad ; \qquad t = t_0 + s/c \quad . \tag{22}$$

It is easy to see that Eq. (18) can be written as

$$\frac{dD}{ds} = -\sigma'_a D - \frac{dB}{ds} \quad , \tag{23}$$

giving the formal solution

$$\begin{aligned} D(s) = D(0) exp\left[-\int_0^s \sigma'_a(s')ds' \right] \\ - \int_0^s ds' \frac{dB(s')}{ds'} exp\left[-\int_{s'}^s \sigma'_a(s'')ds'' \right] \quad . \end{aligned} \tag{24}$$

The formal solution shows that the boundary condition, $D(0)$, decays in a few absorption lengths. Deep in the material σ'_a varies slowly. In fact both σ'_a and dB/ds are constant to first order in ϵ_{stream}. Eq. (24) can then be integrated. The result is

$$D(s) = \left[D(0) + \frac{1}{\sigma'_a}\frac{dB}{ds} \right] exp[-\sigma'_a s] - \frac{1}{\sigma'_a}\frac{dB}{ds} \quad . \tag{25}$$

It shows that

$$D(s) = -\frac{1}{\sigma'_a(s)}\frac{dB(s)}{ds} \tag{26}$$

is the steady-state solution of Eq. (24) and that any boundary value of $D(0)$ decays to it in a few absorption lengths. A result that is correct to second order in ϵ_{stream} is sketched in the Appendix. It uses the mean value theorem of integration.

3.2.2 Asymptotic expansion

The relative orders of various terms in the transport equation, Eq.(18), in thick media were estimated in Section 2.2. The estimation is valid far from boundary layers and time transients. To first order in ϵ_{stream}, there are only two terms

$$0 = -\sigma'_a D - \mathbf{\Omega}\cdot\nabla B \quad , \tag{27}$$

giving the solution

$$D = -\frac{1}{\sigma'_a}\,\mathbf{\Omega}\cdot\nabla B = -\frac{1}{\sigma'_a}\frac{\partial B}{\partial T^4}\,\mathbf{\Omega}\cdot\nabla(T^4) \quad . \tag{28}$$

The radiation flux, from Eq. (20), is

$$\mathbf{F}_{rad} = -\left[\int_0^\infty d\nu \frac{1}{\sigma'_a}\frac{\partial B}{\partial T^4}\right]\frac{1}{3}\nabla(T^4) = -\frac{ac}{3\sigma_R}\nabla(T^4) \quad . \tag{29}$$

This is the correct diffusion limit of the transport equation. We also recovered the correct definition of the Rosseland mean opacity, σ_R; see [1], [2]. To first order Eq. (29) is identical to Eq. (25). It confirms the first order accuracy of the diffusion flux [6]. Note the utter simplicity of the derivation.

An expansion in higher orders of ϵ_{stream} can also be carried out. The results are similar to those of Morel [6], but they are slightly different and more consistent. A short discussion is given in the Appendix.

3.3 The difference formulation, in LTE, with scattering

3.3.1 The scattering term

The scattering term was displayed in Eq. (5). In LTE, the Planck distribution at the material temperature is stationary and it also satisfies detailed balance. This imposes thermodynamic conditions on the scattering cross sections

$$\begin{aligned}\frac{\nu}{\nu'}\,\sigma_s(\nu'\to\nu,\mathbf{\Omega}{\cdot}\mathbf{\Omega}')B(\nu')\left[1+\frac{c^2B(\nu)}{2h\nu^3}\right] \quad &= \\ \sigma_s(\nu\to\nu',\mathbf{\Omega}{\cdot}\mathbf{\Omega}')\,B(\nu)\left[1+\frac{c^2B(\nu')}{2h\nu'^3}\right] \quad &, \end{aligned} \tag{30}$$

where the $\mathbf{x},t;T$ dependence of σ_s and B has been suppressed. After some algebra we get the surprising result

$$\begin{aligned} Q(D) = &\int_0^\infty d\nu' \int_{4\pi} d\mathbf{\Omega}' \frac{\nu}{\nu'}\sigma_s(\nu'\to\nu,\mathbf{\Omega}{\cdot}\mathbf{\Omega}')D(\nu',\mathbf{\Omega}')\left[1+\frac{c^2D(\nu,\mathbf{\Omega})}{2h\nu^3}\right] \\ &-\int_0^\infty d\nu' \int_{4\pi} d\mathbf{\Omega}' \sigma_s(\nu\to\nu',\mathbf{\Omega}{\cdot}\mathbf{\Omega}')D(\nu,\mathbf{\Omega})\left[1+\frac{c^2D(\nu',\mathbf{\Omega}')}{2h\nu'^3}\right] \quad . \end{aligned} \tag{31}$$

We would like to stress that Eq. (31) is valid only in LTE. Otherwise the stimulated scattering terms cannot be written in terms of D alone.

If scattering does not change the radiation energy, *e.g.* in Thomson scattering, the stimulated emission terms in Eq. (5) cancel identically and an isotropic distribution is stationary under those conditions. In fact, we define, as usual

$$J(\mathbf{x},t;\nu) := \frac{1}{4\pi}\int_{4\pi} d\mathbf{\Omega}\, I(\mathbf{x},t;\nu,\mathbf{\Omega}) \quad . \tag{32}$$

Then $I = J$ is stationary and Eq. (5) can be written as

$$\begin{aligned} Q_{mono}(I-J) = &\int_{4\pi} d\mathbf{\Omega}'\,\sigma_s\left(\nu,\mathbf{\Omega}{\cdot}\mathbf{\Omega}'\right)\left[I(\nu,\mathbf{\Omega}')-J(\nu)\right] \\ &-\int_{4\pi} d\mathbf{\Omega}'\,\sigma_s\left(\nu,\mathbf{\Omega}{\cdot}\mathbf{\Omega}'\right)\left[I(\nu,\mathbf{\Omega})-J(\nu)\right] \quad . \end{aligned} \tag{33}$$

In the scattering terms, Eqs. (5), (31), (33), both $\sigma_s(\nu'\to\nu,\mathbf{\Omega}{\cdot}\mathbf{\Omega}')$ and $I(\nu,\mathbf{\Omega})$ or $D(\nu,\mathbf{\Omega})$ can be expanded in spherical harmonics [7]. The integrals are then reduced to relaxation equations for the spherical harmonic components of D, or $I - J$, respectively. In particular, if the scattering is isotropic, Eq. (33) reduces to

$$Q_{mono}(I - J) = \sigma_s(\nu)(I - J) \quad . \tag{34}$$

Finally, we note that the scattering terms are always proportional to

$$\sigma_s(\nu) = \int_{4\pi} d\mathbf{\Omega}' \, \sigma_s \left(\nu, \mathbf{\Omega}\cdot\mathbf{\Omega}'\right) \quad , \tag{35}$$

and to the analogous expressions in Eqs. (5), (31).

3.3.2 The full equations

The full equations in the difference formulation, in LTE, are obtained by adding the right-hand side of Eq. (31) to the right-hand side of Eq. (17). As the change of the radiation energy caused by scattering comes from the matter, the integral of Eq. (31) over frequency has to be subtracted from Eq. (21), in analogy to Eq. (8). They have to be solved together with the conservation equations, Eq. (9). In the more general case they have to be solved together with the full set of equations of radiation hydrodynamics [1], [2], [4].

Rather than presenting the formal development of the equations, we will sketch their simplified version that gives some insight into the relaxation behavior of the radiation intensity. We start by rewriting Eq. (1) in terms of the path variable, s, as defined in Eq. (22). We also take liberties with the scattering term; we tacitly assume it to be monochromatic and isotropic, as in Eq. (34).

$$\frac{dI}{ds} = -\sigma_a'(I - B) - \sigma_s(I - J) \quad . \tag{36}$$

Simple rearrangement gives

$$\frac{dI}{ds} = -\sigma_a'(J - B) - (\sigma_a' + \sigma_s)(I - J) \quad . \tag{37}$$

In parallel to our development of the difference formulation, we subtract dB/ds from both sides of the equation, to give

$$\frac{d(I - J)}{ds} + \frac{d(J - B)}{ds} = -\sigma_a'(J - B) - (\sigma_a' + \sigma_s)(I - J) - \frac{dB}{ds} \quad . \tag{38}$$

With the further assumption of $dB/ds = 0$ and the constancy of σ'_a and σ_s along the radiation path, it is easy to verify that Eq. (38) has the solution

$$J - B = [J(0) - B(0)]exp[-\sigma'_a s] \quad , \tag{39}$$

$$I - J = [I(0) - J(0)]exp[-(\sigma'_a + \sigma_s)s] \quad . \tag{40}$$

We note at this point that the material relaxation equation, Eq. (8), can always be written as

$$\frac{\partial E_{mat}}{\partial t} = 4\pi \int_0^\infty d\nu \sigma'_a (J - B) + G \quad , \tag{41}$$

so $J - B$ is a natural variable to consider.

We emphasize again that our derivation of the solution of Eq. (38) was highly simplistic. In particular it did not take into account material relaxation and the possibility of scattering with change of photon frequency, *e.g.* Compton scattering [1]. We hope to report later on further developments along these lines.

4 Preliminary Numerical Results

A detailed study of a Monte Carlo method for the numerical solution of the difference formulation will be presented elsewhere [10]. We offer here preliminary results that confirm our expectation that the difference formulation provides a significant performance advantage in optically thick media. This advantage arises from the fact that the local equilibrium field is treated deterministically, in addition to the quantitatively different character of the source terms that lead to substantial noise reduction for a Monte Carlo solution of a thick system.

We have implemented the difference formulation for the simple two-level line transport problem discussed in [9], specifically for a collisionally pumped slab problem. We made the additional simplification of the gray approximation (square line shape) in order to avoid the need to switch to the standard formulation in the wings of the line. The slab was started cold, the pump was turned on, and the evolution followed close to equilibrium. In the table below, we show the variance in the optical thickness at the end of the problem run for a large number of independent Monte Carlo runs, where the absorption coefficient has been adjusted to produce a nominal (average) equilibrium optical thickness for the finite slab of 10, 100, and 1000, respectively. Twenty one equally spaced zones were used for the first case with a total optical thickness of 10. Twenty one geometrically spaced zones, with the surface zone on each side of the finite slab being one mean free path thick, were used for other two cases.

The Monte Carlo particle count was chosen so that the nominal execution time was three minutes, reaching a fixed point in time for the evolution of the system close to equilibrium. The column labeled DIFF, in Table 1 below, is the variance in the optical thickness of the slab for the difference formulation for a large number of independent problem runs. The column labeled SIMC is the variance in the optical thickness of the slab for the standard formulation described in [9]. In the last column the ratio of the variances provides an estimate of the advantage in the execution speed for the difference formulation, compared to the standard formulation.

Table 1
Comparison of variance for the difference and standard formulations, respectively, as a function of optical thickness for a finite slab.

optical depth	DIFF	SIMC	RATIO
10	1.19×10^{-6}	1.96×10^{-5}	1.6×10^{1}
100	1.15×10^{-6}	7.88×10^{-3}	6.9×10^{3}
1000	1.31×10^{-6}	8.64×10^{-1}	6.6×10^{5}

The performance advantage for the difference formulation is clear. The variance for the runs using the difference formulation is independent of optical thickness, in sharp contrast to the standard formulation. The ratio of the variances, giving the performance advantage for the difference formulation, grows rapidly as the optical depth is increased. Of course, the average results are the same for the two formulations.

5 Summary and conclusions

We have introduced a new analytical formulation for the transport equation. The new formulation is for the transport of the difference between the specific intensity and the local black body equilibrium radiation at the matter temperature, at any point in space, time and direction. Appropriately, we call the new transport equation the difference formulation to distinguish it from the traditional formalism. We have shown that the difference formulation is expressed in terms of quantities that become small in optically thick media. The transformation is a simple one and results in a completely equivalent system of equations, without approximation.

The most important distinction between the two formulations is in the source terms. In the traditional formulation, the source term is the spontaneous emission of the medium. It is small in optically *thin* regions, resulting in straight line propagation of photons. The traditional formulation is well suited for this regime. In the difference formulation, the source term is the space-time gradient of the Planck function at the material temperature. The latter gets small in optically *thick* regions. In addition to this important difference in asymptotic behavior, the two formulations differ in that the spontaneous emission depends upon the absorption cross sections for the emitting medium, while the source term in the difference formulation depends only upon the temperature of the medium, as a function of space and time. The two formulations are able to satisfy equivalent boundary conditions and initial conditions.

Even the largest terms in the difference formulation are of the order of ϵ_{space}, *i.e.* the ratio of the photon mean free path to the gradient length. In optically thick regions this ratio is a small quantity. We have shown that the equations reduce to the diffusion limit in the proper circumstances. We have also discussed briefly the extensions needed when scattering is important.

In all practical problems the transport equation has to be solved numerically. Numerical solutions require discretization of the equations in space and time. These issues will be discussed elsewhere.

We believe that the difference formulation will help in numerical solutions of the equations of radiation hydrodynamics in optically thick regions. We expect that it will be useful regardless of the numerical method employed, be it a deterministic method, for example S_n and P_n, or a Monte Carlo method, for example the Symbolic Implicit Monte Carlo (SIMC) method of Brooks [8]. The source of instability for Monte Carlo methods, the spontaneous emission term, is removed in the difference formulation and replaced by terms that are small in thick systems. Because of this, the well known stability problem for Monte Carlo methods in thick systems may, in fact, be removed. We will report on this possibility in future work. We would like to note that the Symbolic Implicit Monte Carlo method is well suited for dealing with the $(1/c)(\partial B/\partial t)$ term, should it be a source of instability. Preliminary results show that the efficiency for Monte Carlo methods in thick systems will be improved, due to the removal of the balance between emission and absorption in a zone that produces a relatively noisy estimate for the difference.

A similar treatment may be useful in other transport problems. Neutron transport near criticality has many of the same properties as photon transport in optically thick regions. Similarly, the success of radiation therapy depends on accurate model of particle transport in the presence of strong absorption and scattering. We hope to be able to extend our treatment to some of those applications in the future.

6 Appendix

The first order approximation of the transport equation in thick media shows both the boundary layer and the diffusion limit. We have shown in the paper how easy it is to get those limits in the difference formulation. Here we go to the next order in the expansion of the formal solution and to higher order in the asymptotic expansion of the transport equation. We stay with the assumption of no scattering. There is no difficulty to include scattering, but the equations get really complicated.

6.1 Formal solution

The first order approximation to the formal solution of the difference formulation of the transport equation, Eq. (24), was obtained in Eq. (25). We sketch here the steps to obtain a higher order approximation. First, the integrals in the exponential terms are approximated using the mean value theorem, giving

$$D(s) = D(0) exp[-\sigma'_a(s_1)s] - \int_0^s ds' \frac{dB(s')}{ds'} exp[-\sigma'_a(s_2)(s-s')] \quad , \tag{42}$$

where $0 \leq s_1 \leq s$, $s' \leq s_2 \leq s$. Next, we approximate $\sigma'_a(s_2) \approx \sigma'_a(s) + (d\sigma'_a(s)/ds)(s_2 - s)$. We note that
$0 \leq |(d\sigma'_a(s)/ds)|(s-s_2)(s-s') \leq |(d\sigma'_a(s)/ds)|(s-s')^2 \ll 1$, where the last inequality is reasonable for optically thick media, if $s \ll L$ where L is the scale length of the medium. It allows the estimate $exp[-(d\sigma'_a(s)/ds)(s-s_2)(s-s')] \approx 1-(d\sigma'_a(s)/ds)(s-s')^2$. Using this approximation, the second integral in Eq. (43) can be carried out, giving the final result

$$\begin{aligned} D(s) = &\left[D(0) + \frac{1}{\sigma'_a(s)}\frac{dB(s_3)}{ds}\right] exp[-\sigma'_a(s_1)s] - \frac{1}{\sigma'_a(s)}\frac{dB(s_3)}{ds} \\ &- \frac{1}{\sigma'_a(s)}\frac{dB(s_3)}{ds}\left[\frac{d\sigma'_a(s)}{ds}\left(s^2 + \frac{2s}{\sigma'_a(s)}\right.\right. \\ &\left.\left. + \frac{2}{\sigma'_a(s)^2}\left(1 - exp[-\sigma'_a(s)s]\right)\right)\right] \quad . \end{aligned} \tag{43}$$

We remind the reader that s_1 and s_3 are appropriate points in the interval, $0 \leq s_1, s_3 \leq s$ and $dB(s_3)/ds$ denotes the value of the derivative at $s = s_3$.

The maximum error in the first order solution, Eq. (25), can be estimated by comparing it with Eq. (43). It is easy to verify that it is of second order in ϵ_{stream}.

In Section 2.2 we discussed the smallness of the parameters ϵ_{stream} and ϵ_{time}. In traditional asymptotic analysis one multiplies the relevant terms in the equations with the correct orders of an artificial parameter, ϵ. The original equations are then recovered when the parameter is set to unity. Our treatment here again neglects scattering. It is similar to that of Morel [6], but more general by including non-grey opacities.

The relevant equations to solve are Eqs. (18), (9), (21). We write them down here with the proper powers of ϵ.

$$\frac{\epsilon^2}{c}\frac{\partial D}{\partial t} + \epsilon\, \mathbf{\Omega}\cdot\nabla D = -\sigma_a' D - \frac{\epsilon^2}{c}\frac{\partial B}{\partial t} - \epsilon\, \mathbf{\Omega}\cdot\nabla B \tag{44}$$

$$\epsilon^2 \frac{\partial(E_{mat} + E_{rad})}{\partial t} + \epsilon\nabla\cdot\mathbf{F}_{rad} = 0 \tag{45}$$

$$\epsilon^2 \frac{\partial E_{mat}}{\partial t} = \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\sigma_a' D \tag{46}$$

For completeness, we repeat Eqs. (19), (20)

$$E_{rad} = \frac{1}{c}\int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}(D + B) = \frac{1}{c}\int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega} D + a\,\theta \quad ,$$

$$\mathbf{F}_{rad} = \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}(\mathbf{\Omega} I) = \int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}(\mathbf{\Omega} D) \quad ,$$

where we defined $\theta := T^4$ and used the radiation constant, a, in its usual meaning.

Next we note that $\nabla B = (\partial B/\partial\theta)\nabla\theta$. Similarly, $\partial B/\partial t = (\partial B/\partial\theta)\partial\theta/\partial t$ and $\partial E_{mat}/\partial t = (dE_{mat}/d\theta)\partial\theta/\partial t$. Next, we expand the variables in power series in ϵ

$$\theta = \theta^{(0)} + \epsilon\theta^{(1)} + \epsilon^2\theta^{(2)} + \ldots \tag{47}$$

$$D = \epsilon D^{(1)} + \epsilon^2 D^{(2)} + \ldots \tag{48}$$

The definitions of θ and D are substituted into the equations and we demand that the equations be satisfied order by order in ϵ. We list now the results.

To order ϵ^0 we get

$$E_{rad}^{(0)} = a\theta^{(0)} \quad , \tag{49}$$

where a is the radiation constant. In other words, to zeroth order the radiation is that of a black body in equilibrium with the material.

To first order in ϵ we recover our Eqs. (28), (20)

$$D^{(1)} = -\frac{1}{\sigma'_a}\,\mathbf{\Omega}\cdot\nabla B = -\frac{1}{\sigma'_a}\frac{\partial B}{\partial\theta}\,\mathbf{\Omega}\cdot\nabla\theta^{(0)} \quad , \tag{50}$$

$$\mathbf{F}_{rad}^{(1)} = -\left[\int_0^\infty d\nu \frac{1}{\sigma'_a}\frac{\partial B}{\partial\theta}\right]\frac{1}{3}\nabla\theta^{(0)} = -\frac{ac}{3\sigma_R}\nabla\theta^{(0)} \quad , \tag{51}$$

and find

$$E_{rad}^{(1)} = a\theta^{(1)} \quad . \tag{52}$$

To order ϵ^2 we find from Eq. (44),

$$\mathbf{\Omega}\cdot\nabla D^{(1)} = -\sigma'_a D^{(2)} - \frac{1}{c}\frac{\partial B}{\partial\theta}\frac{\partial\theta^{(0)}}{\partial t} - \frac{\partial B}{\partial\theta}\,\mathbf{\Omega}\cdot\nabla\theta^{(1)} \quad , \tag{53}$$

and from energy conservation, Eq. (45), we get

$$\left(\frac{dE_{mat}}{d\theta} + a\right)\frac{\partial\theta^{(0)}}{\partial t} = \nabla\cdot\int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\,\mathbf{\Omega}\,D^{(1)} \quad . \tag{54}$$

Substituting for $D^{(1)}$ from Eq. (50), we find that $\theta^{(0)}$ satisfies the diffusion equation

$$\left(\frac{dE_{mat}}{d\theta} + a\right)\frac{\partial\theta^{(0)}}{\partial t} = -\nabla\cdot\left[\frac{ac}{3\sigma_R}\nabla\theta^{(0)}\right] \quad . \tag{55}$$

Among the equations of order ϵ^3 we consider only the one for conservation of energy. It is

$$\left(\frac{dE_{mat}}{d\theta} + a\right)\frac{\partial\theta^{(1)}}{\partial t} + \frac{1}{c}\int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\frac{\partial D^{(1)}}{\partial t} = \nabla\cdot\int_0^\infty d\nu \int_{4\pi} d\mathbf{\Omega}\,\mathbf{\Omega}\,D^{(2)} \quad . \tag{56}$$

Equations (53), (56) can be solved for the pair of unknowns $\theta^{(1)}$ and $D^{(2)}$. Algebraic manipulations show that $\theta^{(1)}$ satisfies a diffusion equation identical to the one satisfied by $\theta^{(0)}$, Eq. (55). We conclude that $\theta^{(1)} = 0$ is a consistent solution of the transport equation to second order in ϵ_{space}. This conclusion agrees with Morel's and confirms the second order accuracy of the diffusion approximation under the proper conditions. The solution for $D^{(2)}$ follows from Eq. (53), it is

$$D^{(2)} = -\frac{1}{\sigma'_a}\,\mathbf{\Omega}\cdot\nabla D^{(1)} - \frac{1}{c}\frac{1}{\sigma'_a}\frac{\partial B}{\partial\theta}\frac{\partial\theta^{(0)}}{\partial t} \quad . \tag{57}$$

The first term on the right-hand side has a P_2 symmetry and the last one is spherically symmetric. We note that both terms contribute to E_{rad} and modify the Eddington tensor. When the last term is added to the formula for $D^{(1)}$, the expression agrees with the $(1/\sigma'_a)(dB/ds)$ source term of Eq. (26).

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