The Non-Equilibrium Diffusion Equation
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by

B. E. Freeman
ABSTRACT

The system of equations describing the diffusion of radiation through material is discussed from the point of view of the formulation for numerical solution. These equations, which are more general than the equilibrium diffusion equation, contain terms describing (a) cooling of material by radiation in optically thin systems, (b) diffusion of radiation through material with or without energy exchange with the material, and (c) an approximation to the free streaming of radiation. Consequently, they are applicable to a much wider range of radiation transport phenomena than the equilibrium diffusion equation.

The several regions of applicability are examined from the point of view of the structure of the equations and the frequency dependence. Finally, the general non-equilibrium diffusion equations are discussed regarding appropriate mean absorption coefficients for frequency groups. Spatial and time dependences of the difference equations are also considered.
Introduction

The radiation diffusion equation containing the Rosseland mean absorption coefficient results from several independent approximations which need not be made simultaneously. The purpose of this report is to display and discuss the equation resulting from approximation of the angular dependence of the radiation intensity by two terms of an expansion in Legendre polynomials about the isotropic distribution,

\[ I = I_0 + I_1 P_1(\mu) \]  

(1)

In this approximation the radiation energy density \( E(\text{erg sec/cm}^3) \) is

\[ E = 2\pi \int_{-1}^{1} I d\mu = 4\pi I_0 \]

and the net radiative flux \( F(\text{ergs/cm}^2) \) is

\[ F = 2\pi c \int_{-1}^{1} I \mu d\mu = \frac{4\pi}{3} c I_1 \]

The role of additional approximations will be noted subsequently. Interaction of the radiation with the material consists of (1) pure absorption in the LTE approximation for which the absorption coefficient corrected for induced emission is \( \mu'_a(\text{cm}^{-1}) \) and (2) the Thomson limit of Compton scattering by free electrons giving a total scattering coefficient \( \mu_s = 8\pi/3 r_0^2 N_e \text{(cm}^{-1}) \), where \( r_0 = \text{classical electron radius} \) and \( N_e = \text{free electron density} \).
In the diffusion approximation the transport equation becomes [Eq. (2) of Ref. 1]

$$\frac{1}{c} \frac{\partial I_0}{\partial t} + \frac{1}{3r} \frac{\partial}{\partial r} (r^{\alpha} I_1) = \mu'_a (B - I_0)$$

and

$$\frac{1}{c} \frac{\partial I_1}{\partial t} + \frac{\partial I_0}{\partial r} = -(\mu'_a + \mu_s) I_1,$$  \hspace{1cm} (2)

a result which is also obtained for the total intensity when photon polarization is included [Eq. (6) of Ref. 1]. In these equations $\alpha = 0$ gives the slab geometry result while $\alpha = 2$ gives the equations for radial diffusion in a sphere. The dependence of source function, absorption coefficient, and intensity on frequency has been suppressed.

Equations (2) also contain the material temperature through the absorption coefficient $\mu'_a$ and Planck function $B$. To complete the system of equations it is necessary to describe how the material temperature changes. In addition to the effect of hydrodynamic motions the material energy $E_m$ (ergs/cm$^3$) can change in the above approximations through the spontaneous emission of radiation and the absorption and induced emission of radiation. Scattering in the Thomson limit occurs without energy change. When supplemented with an equation of state the temperature change is determined by the following equation:

$$\frac{dE_m}{dt} = - p \frac{dT}{dt} - c \int_0^\infty dv \mu'_a (\mu B - E).$$  \hspace{1cm} (3)

Transcribing Eqs. (2) in terms of $E$ and $F$ gives
\[ \frac{\partial E}{\partial t} + \nabla \cdot F = c \mu' (4\pi B - E) \]

and

\[ \frac{1}{c} \frac{\partial F}{\partial t} + \frac{c}{\beta} \nabla E = - (\mu'_a + \mu_s) F \]  \( \text{(4)} \)

Comparisons of the solutions of these equations with the transport equation solutions in plane geometry indicate a much wider region of applicability than for the equilibrium diffusion equation. Equations (4) written in terms of the divergence and gradient operators are more widely applicable than the original derivation indicates. Equations (3) and (4), together with the material equation of state and the equation of hydrodynamic motion, form a system for the evolution of the radiation field and material temperature. The frequency of the photons enters through the Planck function and the coefficient of pure absorption and, in general, does not permit a grey atmosphere solution.

The several regions of applicability of Eqs. (3) and (4) are examined below from the point of view of the structure of the equations and their frequency dependence. Appropriate mean absorption coefficients for frequency groups are introduced, and spatial and time dependences of the difference equations are considered.

**Radiation Streaming**

In special cases the equations take a simpler form, however. When the radiation streams through the system without appreciable interaction with the material \((\mu'_s = \mu_s = 0)\) the radiation energy equation becomes

\[ \frac{\partial^2 E}{\partial t^2} - \frac{c^2}{\beta^2} \nabla \cdot \nabla E = 0 \]  \( \text{(5)} \)

This wave equation describes the propagation of disturbances traveling
with the speed \( \pm c/\sqrt{3} \) corresponding to an average direction of many oblique waves as described by the diffusion approximation. The integral of Eq. (5) over frequency can be performed to give an identical equation for the total radiation energy. The inclusion of the \( \delta F/\delta t \) term, therefore, adds the ability to describe the streaming of radiation signals without interaction with the material, albeit with a very crude approximation to the angular distribution of the propagating wave.

The Diffusion Equation

Neglecting this term Eqs. (4) become

\[
\frac{\partial E}{\partial t} = \frac{c}{3} \nabla \cdot \left( \mu_A + \mu_E \right) \nabla E + c \mu_A' \left( 4\pi B - E \right),
\]

(6)

a diffusion equation in which radiation energy changes, in addition, due to material absorption and emission. It is necessary now, of course, to include Eq. (3) to determine how the matter temperature changes and affects the radiation propagation. Introducing the total radiation energy \( E_R \) (ergs/cm\(^3\)) and net flux \( F_R \) (ergs/cm\(^2\) sec),

\[
E_R = \int_0^\infty E \, dv
\]

and

\[
F_R = \int_0^\infty F \, dv
\]

the frequency integrated Eq. (6) with Eq. (3) is
\[
\frac{dE_m}{dt} + \frac{dE_R}{dt} = -\mathbf{v} \cdot \mathbf{F}_R - \mathbf{p} \frac{d\mathbf{r}}{dt}
\]

and

\[
F_R = -\frac{c}{3} \int_0^\infty dv \frac{1}{\mu_a + \mu_s} \mathbf{v} E.
\]  

(7)

The first equation of Eqs. (7) is just the total energy conservation equation as solved in the regular radiation diffusion equation. The second equation for the net flux is also closely related to the regular diffusion equation except for the form of the radiation energy. To obtain the standard form it is necessary to make an additional assumption that the radiation energy is in local equilibrium with the material and thus has a Planck distribution corresponding to the local temperature. Then it is possible to perform the frequency integration independently of the energy gradient since the spatial dependence occurs only through the material temperature \(T_m\). The familiar result is

\[
F_R = -\frac{ca}{3} \lambda_R v_0^l T_m,
\]

where

\[
\int_0^\infty \mu_B dv = a\theta_m^l,
\]

\(\lambda_R\) is the Rosseland mean free path,

\[
\lambda_R = \int_0^\infty \frac{1}{\mu_a + \mu_s} \frac{\partial B}{\partial v} dv 
\]

\[
\int_0^\infty \frac{\partial B}{\partial v} dv
\]

(8)

and \(a\) is the radiation energy constant.
Matter-Radiation Equilibration

The radiation equilibrium assumption is appropriate only when certain criteria are satisfied which insure that the interaction between radiation and material has had time to effect equilibration. For example, in an enclosure in which no inhomogeneities exist the radiation energy changes with time as

\[ E(t) = \int_0^t \mu'_a \, dt = \frac{4\pi}{c} \int_0^t \mu'_a B \, e^{\frac{-\mu'_a t}{c}} \, dt + E_0. \]

Since the total energy is conserved the temperature will change as the radiation energy changes so that the integrands above depend on time. If \( E_R \ll E_m \) during the equilibration history, however, then \( B \) and \( \mu'_a \) remain substantially constant and

\[ E = 4\pi B + (E_0 - 4\pi B) e^{-\frac{\mu'_a t}{c}}. \]

The characteristic time \( \tau_R \) for the radiation energy to relax to the equilibrium value \( 4\pi B \) is \( \tau_R = \frac{1}{c \mu'_a} \), which depends on the temperature and the frequency. When the radiation field is heated solely by emission the relevant absorption coefficient frequency average is given by

\[ E_R = a_0^h \left[ 1 - S(ct) \right], \]

where the transmission function \( S \) is given by

\[ S(s) = \frac{4\pi}{a_0^h} \int_0^\infty dv Be^{-\frac{\mu_a s}{a}}, \]

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For early times the relevant frequency average gives the Planck mean absorption coefficient. If, on the other hand, \( E_R \gg E_m \) during the equilibration and the radiation spectrum is Planckian with temperature \( \theta_r \), the material energy will change; but \( E_R \) will remain approximately constant,

\[
\frac{\partial E_m}{\partial t} = 4\pi c \int_0^\infty dv \mu_a [B(\theta_r) - B(\theta_m)].
\]

Introducing a two-temperature Planck mean absorption coefficient,

\[
\mu_p(\theta_m, \theta_r) = \frac{\int_0^\infty \mu_a(\theta_m)B(\theta_r)dv}{a\theta_r^4},
\]

the equation becomes

\[
\frac{\partial E_m}{\partial t} = ca [\theta_r^4 \mu_p(\theta_m, \theta_r) - \theta_m^4 \mu_p(\theta_m, \theta_m)].
\]

The quantitative result is complicated by the dependence of quantities on the changing \( \theta_m \), but an estimate of the characteristic relaxation time \( \tau_m \) for the material to reach the radiation temperature is

\[
\tau_m = \frac{1}{ca \mu_p(\theta_r, \theta_r) a\theta_r^4} E_m(\theta_r).
\]

If the temperature changes appreciably in the time intervals \( \tau_R \) or \( \tau_m \), deviations from local radiative equilibrium will occur. Factors increasing the deviation are (1) low density and (2) high radiation frequency or temperature, which make \( \mu_p \) small.
Scattering Diffusion

When the radiation is diffusing in a medium having a very small absorption coefficient but in which the scattering coefficient is appreciable, the radiation equation becomes

\[ \frac{\partial E}{\partial t} = \frac{c}{\delta} \nabla \left( \frac{1}{\mu_s} \right) \nabla E . \]

Since the scattering coefficient is frequency independent, photons diffuse without changing frequency. It is clear that in this approximation an initially inhomogeneous blackbody distribution of radiation will evolve to a non-blackbody distribution through merging of spectra and dilution of the photon energy density. Consequently, in this case it is necessary to follow portions of the spectrum in separate calculations if spectral resolution is desired. The total radiation energy, however, can be found by solving the single equation

\[ \frac{\partial E_R}{\partial t} = \frac{c}{\delta} \nabla \left( \frac{1}{\mu_s} \nabla E_R \right) . \] (10)

Scattering Diffusion with an Emission Source

In both the diffusion and material energy equations the spontaneous emission term can be integrated in frequency in terms of the Planck mean. More generally, for a frequency interval \( \nu_j \leq \nu \leq \nu_{j+1} \) the partial Planck mean may be introduced,

\[ \mu \pi \int_{\nu_j}^{\nu_{j+1}} \mu_a B \, d\nu = \mu_p(\theta, \nu_j, \nu_{j+1}) \, b_a \theta^4 . \] (11)
where the normalized Planck integral

\[ b_j = \frac{15}{4} \int_{\frac{h \nu_j}{\theta_m}}^{u_{j+1}} du \frac{u^3}{e^u - 1} , \]

\[ u_j = \frac{h \nu_j}{\theta_m} , \]

and

\[ \mu_p(\theta_m, \nu_j, \nu_{j+1}) = \frac{\int_{u_j}^{u_{j+1}} \frac{\mu_a u^3}{e^u - 1} du}{\int_{u_j}^{u_{j+1}} \frac{u^3}{e^u - 1} du} . \]

If \( \mu_s \gg \mu_a' \) so that \( \mu_a' \) is negligible in the diffusion term and \( \frac{h \nu B}{E} \gg E \) so that \( E \) is negligible in the coupling term (as in a hot optically thin medium), then Eqs. (3) and (6) can be integrated over frequency to give

\[ \frac{dE_R}{dt} = \frac{c}{2} \left( \frac{1}{\mu_s} \nabla E_R \right) + \alpha c \mu \theta \frac{h}{\rho m} \]

and

\[ \frac{dE_m}{dt} = -p \frac{dt}{\mu_p} - \alpha c \mu \theta h \rho_m , \tag{12} \]

where \( \mu_p \) is the total Planck mean

\[ \mu_p(\theta_m) = \sum_j b_j \mu_p(\theta_m, \nu_j, \nu_{j+1}) . \]
Equations (12) with the equation of state describe the cooling of the material and the diffusion of the radiation by scattering after emission by the material.

Non-Equilibrium Diffusion

If either of the two approximations above is not satisfied, it is necessary to retain information about the radiation frequency dependence because the material and radiation energies are then coupled together in a way dependent on the spectrum. In the material equation the heating by absorption depends on the frequency dependence of \( E \) as does the corresponding radiation energy cooling term. In addition, the frequency dependence of \( \mu_a' \) makes the diffusion term dependent on the frequency spectrum. Neglecting the streaming term, the equations are

\[
\frac{\partial E}{\partial t} = \frac{c}{\gamma} \nabla \left( \frac{1}{\mu_a' + \mu_s} \nabla E \right) + c \mu'_a (4\pi B - E)
\]

and

\[
\frac{\partial E}{\partial t} = -c \int_0^\infty d\nu \mu'_a (4\pi B - E) \tag{13}
\]

Introducing frequency groups \( v_j \leq \nu \leq v_{j+1} \), within which the absorption coefficients take mean values, Eqs. (13) are approximated by

\[
\frac{\partial E_j}{\partial t} = \frac{c}{\gamma} \nabla \left( \lambda_j \nabla E_j \right) + ca \theta_{mb} \mu_j - c \mu'_j E_j, \; j = 1, 2, \cdots J
\]

and

\[
\frac{\partial E_m}{\partial t} = -c \sum_j (a \theta_{mb} \mu_j - \mu'_j E_j) \tag{14}
\]
Different frequency means appear in the various terms of Eqs. (14). In the material emission term the correct mean in the partial Planck, \( \mu_j = \mu_p(\theta_m, \nu_j, \nu_{j+1}) \), is defined in Eq. (11). For the absorption term the correct value given by the Chandrasekhar mean cannot be formed. Clearly, it should depend on parameters associated with the radiation spectrum but should reduce to the partial Planck mean when the radiation and material are in equilibrium. Such a quantity, containing only a single radiation parameter, is the two-temperature Planck mean absorption coefficient introduced in Eq. (9). The corresponding partial mean is

\[
\mu_p(\theta_m, \theta_r, \nu_j, \nu_{j+1}) = \frac{4\pi \int_{\nu_j}^{\nu_{j+1}} \mu_a(\theta_m) B(\theta_r) \, d\nu}{a\theta_r b_j(\theta_r)} ,
\]

which may be used for \( \mu_j' \). The diffusion term contains a mean free path which, in the equilibrium diffusion approximation, becomes the Rosseland mean free path of Eq. (8). A satisfactory mean for this term must have this limiting behavior and also contain parameters characterizing the radiation field when it deviates from equilibrium. A quantity containing one such radiation parameter is the two-temperature Rosseland mean which for the frequency group is defined as

\[
\lambda_R(\theta_m, \theta_r, \nu_j, \nu_{j+1}) = \frac{\int_{\nu_j}^{\nu_{j+1}} \frac{1}{\mu_a(\theta_m) + \mu_s \frac{\partial B}{\partial \theta_r} (\theta_r)} \, d\nu}{\int_{\nu_j}^{\nu_{j+1}} \frac{\partial B}{\partial \theta_r} (\theta_r) \, d\nu} ,
\]

which may be used for \( \lambda_j \). Both of the above quantities contain the parameter \( \theta_r \) which represents the shape of the radiation spectrum for
the frequency group in question. Since the frequency dependence within a group is unknown it must be inferred by examining all available information. This information may be derived, for example, from the nature of the source or from variation in intensity between neighboring frequency groups.

The absorption coefficients entering Eqs. (4) also can be calculated in the way described above. Consequently, the term limiting to the wave equation can be included to give a system of equations which is capable of accounting for all of the phenomena discussed above.

The Difference Equations

Assuming that appropriately averaged frequency group absorption coefficients are available, the remaining step is to devise difference equations in space and time. To simplify the spatial difference equations, a problem in plane geometry is chosen for illustration; other geometries can also be calculated, however, quite analogously with the equilibrium diffusion equation. Retaining the streaming term, the difference equations corresponding to Eqs. (3) and (4) are

\[
\begin{align*}
\frac{E_{n+1}^{i+1/2,j} - E_{n+1}^{i+1/2,j}}{\Delta t_n} &+ \frac{F_{n+1}^{i+1,j} - F_{n+1}^{i,j} + F_{i+1,j}^{n+1} - F_{i,j}^{n}}{2 \Delta x_{i+1/2}^n} \\
&= c \left\{ a_{i+1/2,j}^{n+1/2} + b_{i+1/2,j}^{n+1/2} \left[ (g_{n+1/2}^{i+1/2})^4 + (g_{n+1/2}^{i+1/2})^4 \right] \right. \\
&\left. - \mu_{i+1/2,j}^{n+1/2} \left( E_{i+1/2,j}^{n+1} + F_{i+1/2,j}^{n} \right) \right\}, \tag{17}
\end{align*}
\]
In Eqs. (17), (18), and (19) the subscript \(i\) denotes the spatial position. The flux \(F_i\) is evaluated at interfaces between zones having thickness \(\Delta x_i\). The half-integer subscripts (as for the energy \(E_{i+1/2}\)) denote quantities evaluated at zone centers. Material thermodynamic properties are associated with zone centers so that absorption coefficients are most easily formed at \(i + 1/2\). The quantities \(\lambda_i\) and \(\Delta x_i\) are to be obtained by judicious averages of neighboring zone quantities. The material temperature has been denoted by \(\theta\) in Eqs. (17) and (19), dropping the subscript \(m\).

The solution is contained in the simultaneous equations for \(E_{n+1}^{i+1/2}\), \(F_{n+1}^i\), and \(g_{n+1}^i\), which involve adjacent spatial points. The flux can be eliminated between these first two equations, however, to give

\[
A_{i+1/2}E_{i-1/2}^{n+1} - B_{i+1/2}E_{i+1/2}^{n+1} + C_{i+1/2}E_{i+3/2}^{n+1} + D_{i+1/2} = 0 ,
\]

where, dropping the frequency subscripts, the coefficients have the values
Equation (20) is in suitable form for solution by the well known algorithm for the tri-diagonal matrix. It is coupled, however, with the energy equation, Eq. (19). Consequently, an iteration is required to make the two equations consistent. Temperature dependent coefficients may be improved in the iteration also.

In the event that a single frequency group is sufficient to describe the frequency dependence the equations may be linearized either in $\theta$ or $\theta^4$. 

\[
A_{i+1/2} = -\frac{c}{12\Delta x_{i+1/2}} \frac{1}{\Delta x_i} \left( \frac{1}{c\Delta t_n} - \frac{1}{2\lambda_i} \right),
\]

\[
B_{i+1/2} = \frac{1}{\Delta t_n} + \frac{c\mu_{i+1/2}}{2} + \frac{c}{12\Delta x_{i+1/2}} \left( \frac{\Delta x_{i+1}}{c\Delta t_n} - \frac{\Delta x_i}{2\lambda_i} \right),
\]

\[
C_{i+1/2} = -\frac{c}{12\Delta x_{i+1/2}} \frac{1}{\Delta x_{i+1}} \left( \frac{1}{c\Delta t_n} - \frac{1}{2\lambda_{i+1}} \right),
\]

\[
D_{i+1/2} = -\frac{c}{2} \left\{ a_{i+1/2} b_{i+1/2} \left[ \left( \theta_{i+1/2}^{n+1} \right)^4 + \left( \theta_{i+1/2}^{n} \right)^{4} \right] - \mu_{i+1/2} E_{i+1/2}^{n} \right\} - \frac{E_{i+1/2}^{n}}{\Delta t_n}
\]

\[
+ \frac{F_{i+1} - F_{i}}{2\Delta x_{i+1/2}} + \frac{c}{12\Delta x_{i+1/2}} \left( \frac{E_{i+1/2}^{n} - E_{i-1/2}^{n}}{\Delta x_i} - \frac{E_{i+3/2}^{n} - E_{i+1/2}^{n}}{\Delta x_{i+1}} \right)
\]

\[
+ \frac{1}{2\Delta x_{i+1/2}} \left[ 2 \left( \frac{1}{c\Delta t_n} + \frac{1}{2\lambda_{i+1}} \right) - F_{i} \left( \frac{1}{c\Delta t_n} - \frac{1}{2\lambda_i} \right) \right] - F_{i+1} \left( \frac{1}{c\Delta t_n} + \frac{1}{2\lambda_i} \right).
\]
and solved simultaneously. To do this, the material energy may be expressed as

$$
\frac{E_{m}^{n+1} - E_{m}^{n}}{\Delta t^{n}} = \frac{c^{n+1/2}}{4\left(\delta_{i+1/2}\right)^{3}} \frac{(\delta_{i+1}^{n+1})^{4} - (\delta_{i}^{n})^{4}}{\Delta t^{n}}
$$

for the fourth power case. Solving the resulting Eq. (19) for \((\delta_{i+1/2}^{n+1})^{4}\), the temperature term in Eq. (17) can be eliminated. The resulting equation for \(E\) has the same form as Eq. (20), but the coefficients \(B\) and \(D\) are modified,

$$
E'_{i+1/2} = \frac{1}{\Delta t^{n}} + \frac{c^{'i+1/2}}{2} + \frac{c}{12\Delta x_{i+1/2}^{2}} \left( \frac{1}{\Delta x_{i}^{2}} + \frac{1}{\Delta x_{i+1}^{2}} \right)
$$

$$
+ \frac{c^{2}a_{i+1/2}}{\left(\delta_{i+1/2}^{n+1/2}\right)^{3}} \frac{2c_{vi+1/2}}{2c_{vi+1/2}}
$$

$$
p'_{i+1/2} = -\frac{c}{2} \frac{2a_{i+1/2}}{\left(\delta_{i+1/2}^{n+1/2}\right)^{4}} \frac{\mu_{i+1/2}^{n+1/2}}{\Delta t^{n}}
$$

$$
- \frac{E_{i+1/2}^{n}}{\Delta t^{n}} + \frac{F_{i+1}^{n} - F_{i}^{n}}{2\Delta x_{i+1/2}^{2}} + \frac{c}{12\Delta x_{i+1/2}^{2}} \left( \frac{E_{i+1/2}^{n} - E_{i-1/2}^{n}}{\Delta x_{i}^{2}} - \frac{E_{i+3/2}^{n} - E_{i+1/2}^{n}}{\Delta x_{i+1}^{2}} \right)
$$

$$
+ \frac{1}{2\Delta x_{i+1/2}^{2}} \left[ F_{i+1}^{n} \left( \frac{1}{\Delta x_{i}^{2}} + \frac{1}{\Delta x_{i+1}^{2}} \right) - F_{i}^{n} \left( \frac{1}{\Delta x_{i}^{2}} + \frac{1}{\Delta x_{i+1}^{2}} \right) \right].
$$

The resulting equation still contains time dependent coefficients whose centering may require improvement by iteration.
REFERENCES

