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SOME APPROXIMATIONS IN THE NUMERICAL TREATMENT OF RADIATION TRANSPORT
THROUGH MEDIA WITH FREQUENCY-DEPENDENT ABSORPTION COEFFICIENTS

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The Nuclear/Chemical Pulse Reaction Propulsion Project

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SOME APPROXIMATIONS IN THE NUMERICAL TREATMENT OF RADIATION TRANSPORT
THROUGH MEDIA WITH FREQUENCY-DEPENDENT ABSORPTION COEFFICIENTS

I. INTRODUCTION

The investigation¹ into the properties of a numerical treatment of the transport of radiation through slabs of material is extended. Although the integral formulation of the energy change equation is retained, the method is made applicable to a medium having a frequency-dependent absorption coefficient rather than the frequency-independent one assumed in the grey-atmosphere approximation. In other respects the formulation is identical to that previously described. The proposed extension relies on the possibility of making a valid approximation to the absorption coefficient of the form:

$$\sigma(\nu, T, \rho) = \sigma_1(\nu) \sigma_2(T, \rho) \quad , \quad (1)$$

which permits a separation of the spatial and frequency-dependent parts of the calculation.

Replacing the exponential integral tables required in the previous formulation are new tables. These new functions are obtained by performing integrations over the frequency spectrum of certain functions of the absorption coefficient which single out the Rosseland or Planck mean absorption coefficient under appropriate limiting conditions.

II. APPROXIMATE FREQUENCY DEPENDENCE

While in (I) $\sigma_2(x')$, was assumed to be independent of ν and to depend only on x' , in fact real materials display a strong dependence on frequency as typified by the absorption coefficients of low- z materials in the partially ionized state.² Not only are the discontinuities at the

¹GAMD-2874, B. E. Freeman, "A Numerical Method for the Radiation Transport Equation in Plane Geometry". (Called I in following text.)

²GA-2528, J. C. Stewart and K. D. Pyatt, Jr., "Theoretical Study of Optical Properties".

photoelectric edges in evidence but the broadened lines may add a great deal of structure to the spectrum.

As the temperature and density of a material are changed the absorption coefficient changes both in magnitude and in spectral shape. Over limited ranges of temperature and density it is sometimes permissible to single out the changes in magnitude of the spectrum and disregard the changes in spectral shape so that:

$$\sigma(\nu, T, \rho) = \sigma_1(\nu) \sigma_2(T, \rho) \quad .$$

This factorization of the absorption coefficient will form the starting point for subsequent treatment of the frequency-dependent case.

III. THE RADIATION FLUX

The expression for the radiation flux as developed in Equation (8) of (I) is:

$$\begin{aligned} \phi(x) = 2\pi C \int_0^\infty d\nu \left[-\int_x^\infty B_\nu(x') \sigma_\nu(x') E_2 \left(\int_x^{x'} \sigma_\nu dx'' \right) dx' \right. \\ \left. + \int_{-\infty}^x B_\nu(x') \sigma_\nu(x') E_2 \left(\int_{x'}^x \sigma_\nu dx'' \right) dx' \right] \quad , \end{aligned} \quad (2)$$

where

$$B_\nu = \frac{2h}{c^3} \frac{\nu^3}{e^{h\nu/KT} - 1}$$

Equation (2) takes the form of Equation (16) of (I) provided σ is not a function of ν . Introduction of the factorization assumption, Equation (1), allows the frequency integration to be carried out inside the spatial integral:

$$\begin{aligned} \phi(x) = 2\pi C \left\{ -\int_x^\infty \sigma_2(x') dx' \int_0^\infty B_\nu(x') \sigma_1(\nu) E_2 \left[\sigma_1 \int_x^{x'} \sigma_2 dx'' \right] d\nu \right. \\ \left. + \int_{-\infty}^x \sigma_2(x') dx' \int_0^\infty B_\nu(x') \sigma_1 E_2 \left[\sigma_1 \int_{x'}^x \sigma_2 dx'' \right] d\nu \right\} \quad . \end{aligned} \quad (3)$$

Introducing the average optical depth, τ , defined in terms of the spatial part of the absorption coefficient σ_2 ,

$$\tau = \int_0^x \sigma_2 dx' \quad , \quad (4)$$

the flux from Equation (3) takes the form:

$$\begin{aligned} \phi(x) = \frac{Ca}{2} & \left[- \int_{\tau}^{\infty} d\tau' T^4(\tau') \mathcal{E}_2(T(\tau'), \tau - \tau') \right. \\ & \left. + \int_{-\infty}^{\tau} d\tau' T^4(\tau') \mathcal{E}_2(T(\tau'), \tau - \tau') \right] \quad . \quad (5) \end{aligned}$$

In Equation (5) the new kernel $\mathcal{E}_2$ has been defined as follows:

$$\mathcal{E}_2(T, x) = \frac{\int_0^{\infty} d\nu B_\nu(T) \sigma_1 \mathcal{E}_2(\nu, x)}{\int_0^{\infty} d\nu B_\nu(T)} \quad . \quad (6)$$

In case $\sigma_1 = 1$, $\mathcal{E}_2 = E_2(x)$ as required by the grey approximation.

The essential simplification introduced by factorizing the absorption coefficient occurs in the argument of the E_2 function permitting a single optical depth to enter as a parameter there. The function $\mathcal{E}_2$ as defined in Equation (6) depends on two parameters. The argument x is the optical depth from source to point at which the flux is being evaluated. In addition, T , the temperature at the source point, will change $\mathcal{E}_2$ if the frequency dependence differs strongly from constant over the range of the weighting function.

IV. NUMERICAL INTEGRATION

In order to evaluate the integral in Equation (5) numerically, it may be desirable to assume that the temperature is constant within a zone. This amounts in Equation (3) to assuming a spatially constant source through the zone. Carrying out the integral over each zone and summing all of the zone contributions gives the results:

$$\phi(x_j) = 2\pi C \left\{ -\sum_{i=j}^{\infty} \int_0^{\infty} d\nu B_\nu(x_{i+1/2}) \left[E_3(\tau_1 \int_{x_j}^{x_{i+1}} \sigma_2 dx) - E_3(\tau_1 \int_{x_j}^{x_{i+1}} \sigma_2 dx) \right] \right. \\ \left. + \sum_{i=-\infty}^{j-1} \int_0^{\infty} d\nu B_\nu(x_{i+1/2}) \left[E_3(\tau_1 \int_{x_{i+1}}^{x_j} \sigma_2 dx) - E_3(\tau_1 \int_{x_{i+1}}^{x_j} \sigma_2 dx) \right] \right\} \quad (7)$$

The zones have been chosen in the same way as in (I) with the flux being evaluated at an interface between zones. In terms of the optical depth τ of Equation (4):

$$\phi(x_j) = \frac{Ca}{2} \left\{ -\sum_{i=j}^{\infty} T^4(\tau_{i+1/2}) \left[\mathcal{E}_3(T(\tau_{i+1/2}), \tau_i - \tau_j) \right. \right. \\ \left. \left. - \mathcal{E}_3(T(\tau_{i+1/2}), \tau_{i+1} - \tau_j) \right] \right. \\ \left. + \sum_{i=-\infty}^{j-1} T^4(\tau_{i+1/2}) \left[\mathcal{E}_3(T(\tau_{i+1/2}), \tau_j - \tau_{i+1}) - \mathcal{E}_3(T(\tau_{i+1/2}), \tau_j - \tau_i) \right] \right\}, \quad (8)$$

where

$$\mathcal{E}_3(T, x) = \frac{\int_0^{\infty} d\nu B_\nu(T) E_3(\tau_1 x)}{\int_0^{\infty} d\nu B_\nu(T)} \quad (9)$$

When τ_1 is independent of frequency Equation (8) reduces to the exact form proposed in (I) in zones removed from the point at which the flux is being evaluated. While the prescription indicated above is suitable for optically thin zones and for optically thin material, a more refined description of the temperature between zones is required to obtain the proper limiting behavior for optically thick zones and material. The next order of refinement is to express the source function as a linear function of optical depth in the neighborhood of the point at which the flux is being evaluated:

$$B(x') = \alpha_j + \beta_j (\tau - \tau_j) \quad (10)$$

$$\alpha_j = B(\tau_j) = \frac{(\tau_j - \tau_{j-1}) B_{j+1/2} + (\tau_{j+1} - \tau_j) B_{j-1/2}}{\tau_{j+1} - \tau_{j-1}}$$

$$\beta_j = \frac{\partial B}{\partial \tau_j} = \frac{\partial B}{\partial T^4} \frac{\partial T^4}{\partial \tau_j} = \frac{2 \partial B}{\partial T^4} \frac{T_{j+1/2}^4 - T_{j-1/2}^4}{\tau_{j+1} - \tau_{j-1}}$$

The contribution of the two zones adjacent to the interface at which the flux is evaluated is replaced by that obtained by assuming the distribution of Equation (10):

$$\begin{aligned} \phi(x_j) = 2\pi c \int_0^\infty d\nu & \left\{ \alpha_j \left[E_3(\nu, \tau_{j+1} - \tau_j) - E_3(\nu, \tau_j - \tau_{j-1}) \right] \right. \\ & + \frac{1}{\sigma_1} \beta_j \left[-\frac{2}{3} + E_4(\nu, \tau_{j+1} - \tau_j) + E_4(\nu, \tau_j - \tau_{j-1}) \right] \\ & + \sigma_1 (\tau_{j+1} - \tau_j) E_3(\nu, \tau_{j+1} - \tau_j) \\ & \left. + \sigma_1 (\tau_j - \tau_{j-1}) E_3(\nu, \tau_j - \tau_{j-1}) \right\} \quad (11) \end{aligned}$$

Carrying out the frequency integrations gives:

$$\begin{aligned} \phi(x_j) = \frac{ca}{2} & \left\{ \frac{\tau_j - \tau_{j-1}}{\tau_{j+1} - \tau_{j-1}} T_{j+1/2}^4 \left[\mathcal{E}_3(T_{j+1/2}, \tau_{j+1} - \tau_j) \right. \right. \\ & \left. \left. - \mathcal{E}_3(T_{j+1/2}, \tau_j - \tau_{j-1}) \right] \right. \\ & \left. + \frac{\tau_{j+1} - \tau_j}{\tau_{j+1} - \tau_{j-1}} T_{j-1/2}^4 \left[\mathcal{E}_3(T_{j-1/2}, \tau_{j+1} - \tau_j) - \mathcal{E}_3(T_{j-1/2}, \tau_j - \tau_{j-1}) \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + 2 \frac{T_{j+1/2}^4 - T_{j-1/2}^4}{\tau_{j+1} - \tau_{j-1}} \left[-\frac{2}{3\sigma_R(T_j)} + \mathcal{E}_4(T_j, \tau_{j+1} - \tau_j) \right. \\
& + \mathcal{E}_4(T_j, \tau_j - \tau_{j-1}) \\
& \left. + (\tau_{j+1} - \tau_j) \mathcal{E}'_3(T_j, \tau_{j+1} - \tau_j) + (\tau_j - \tau_{j-1}) \mathcal{E}'_3(T_j, \tau_j - \tau_{j-1}) \right] \Bigg\}, \quad (12)
\end{aligned}$$

where

$$\sigma_R(T) = \left\{ \frac{\int_0^\infty \frac{d\nu}{\sigma_1} \frac{dB_\nu}{dT^4}}{\int_0^\infty d\nu \frac{dB_\nu}{dT^4}} \right\}^{-1} = \left[+3 \mathcal{E}_4(T, 0) \right]^{-1}.$$

$$\mathcal{E}_4(T, x) = \frac{\int_0^\infty \frac{d\nu}{\sigma_1} \frac{dB_\nu}{dT^4} E_4(\sigma_1 x)}{\int_0^\infty d\nu \frac{dB_\nu}{dT^4}},$$

$$\mathcal{E}'_3(T, x) = \frac{\int_0^\infty d\nu \frac{dB_\nu}{dT^4} E_3(\sigma_1 x)}{\int_0^\infty d\nu \frac{dB_\nu}{dT^4}}.$$

Equation (12) is more complex than the corresponding one for the grey atmosphere approximation but reduces precisely to it when σ_1 is independent of ν . In that case $\mathcal{E}_3 = \mathcal{E}'_3 = E_3$, so that only two functions, E_3 and E_4 , are required. It is possible that the difference between $\mathcal{E}_3$ and $\mathcal{E}'_3$ is of secondary importance. The Planck mean, σ_R , of the frequency dependent factor is the leading term of the expression. Since the linear interpolation is important only for optically thick zones the contributions of $\mathcal{E}'_3$ and $\mathcal{E}_4$ are small. It is likely that either $\mathcal{E}'_3$ could be replaced by $\mathcal{E}_3$ or the interpolation could be modified to achieve the replacement. Whether simplification of these terms is possible is to be determined by test calculations yet to be performed.

In order to carry out the calculation it is proposed that tables of $\mathcal{E}_3$, $\mathcal{E}_4$ and $\mathcal{E}_3'$ be prepared to be used instead of E_3 and E_4 . The table preparation, while a bigger job than finding the Rosseland and Planck means, can be computed with relatively little difficulty and computer time before the time-dependent part of the transport calculation is performed.

V. PROPERTIES OF THE FUNCTIONS

The $\mathcal{E}$ -functions entering the frequency-dependent formulation display properties which depend on various means of the absorption coefficient as a function of frequency.

The emission of energy from an optically thin region will depend on the $\mathcal{E}_3$ function. The value of $\mathcal{E}_3$ for small argument is:

$$\mathcal{E}_3(T, x) = 1/2 - x\sigma_p(T) \quad , \quad (13)$$

where σ_p is the Planck frequency mean of the frequency factor σ_1 of the absorption coefficient. In the case of very transparent material Equation (8) for the flux out of the material reduces with Equation (13) to a sum of terms. Each term represents the Planck emission of a zone of the material and contains the frequency dependence correctly through the Planck mean.

For regions of material which are optically very thick the corrections given in Equation (12) are applicable. The leading term and the only one which survives for very thick zones is:

$$\phi(x_j) = -\frac{Ca}{3} \frac{1}{\sigma_R} \frac{\partial T^4}{\partial \tau} \quad , \quad (14)$$

which is the diffusion approximation to the radiation flux containing the Rosseland mean of the frequency factor. The next term $\mathcal{E}_4$ is a generalization of the Rosseland mean which weights even more strongly the regions of small absorption coefficient. However, it and the $\mathcal{E}_3$ terms will be relatively small in the diffusion regime by virtue of the exponentially decreasing character of the E_3 and E_4 functions of large argument. The $\mathcal{E}_3'$ function contains the derivative of the Planck function as does $\mathcal{E}_4$ but contains E_3

and has no σ_1 appearing outside the E_3 argument. In this sense, it represents a combination of optically thin and thick properties. Its role is not yet understood.

VI. SUGGESTIONS FOR FUTURE DEVELOPMENT

The method proposed offers the possibility of treating frequency dependence by a numerical treatment with the equivalent of a single frequency group, having very mild stability restrictions, and giving reasonable accuracy. It is attractive as compared to alternatives which call for solution of the intensity equations with attendant large storage requirements, possibly small time steps associated with photon transit, angular groups, and frequency groups. In particular, the latter has appeared to require a large proliferation of the calculation in order to adequately treat the complexity presented by the absorption coefficients of real materials.

However, the approximation Equation (1) upon which the frequency treatment rests may require refinement to treat general problems. Several possibilities, none of which has been investigated to any degree, suggest themselves as being relatively easy and inexpensive extensions of the present method:

1. Divide the spectrum into coarse groups, in each of which the factorization is assumed to hold but with different spatial dependence.
2. Express the absorption coefficient as a sum of factored terms, the spatial dependence being different in each term.
3. Expand the dependence of absorption coefficient on temperature and density about a central value and retain the constant and linear terms.