A Multi-Source Full Spectrum K-Distribution Method for 1-D Inhomogeneous Media

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Abstract. The k-distribution method for treating the spectral properties of an absorbing-emitting medium represents an alternative to line-by-line calculations which reduces the number of RTE evaluations from the order of a million to the order of ten without any significant loss of accuracy. For problems where an appropriate reference temperature can be defined, the k-distribution method is formally exact. However, when no appropriate reference temperature can be defined, the method results in errors. There have been several attempts to implement corrections to the k-distribution method to extend its application to inhomogeneous media by modelling the effects of temperature, pressure, and concentration gradient. Some of these techniques are very effective at reducing these errors, but none successfully extend the k-distribution method to inhomogeneous media in a way that retains the analytical guarantee of line-by-line accuracy. The Multi-Source Full Spectrum K-Distribution Method (MSFSK) introduced here manages to attain this goal for 1-dimensional domains with piecewise constant temperature distributions by applying the superposition principle to the original RTE before applying the k-distribution transformation to decompose the problem into a set of sub-problems each of which is able to be solved exactly via the ordinary or modified full spectrum k-distribution method.

1. Introduction
Heat transfer problems in general involve solving the conservation of energy equation. If convection is important, there is an associated fluid dynamics problem that is coupled to the energy equation that must be solved in order to determine the flow field. The general energy equation for a single-component translucent fluid including all three heat transfer modes is

\[
\rho c_p \frac{DT}{Dt} = \beta T \frac{DP}{Dt} + \nabla \cdot (k \nabla T - q_r) + q'' + \Phi_d
\]

(1.1)

where \(\beta\) is the thermal coefficient of volume expansion of the fluid, \(q_r\) is the radiant flux vector, \(q''\) is the local energy source, and \(\Phi_d\) is the energy production due to viscous dissipation [1].

In this paper, we are only concerned with calculating the radiant flux vector and its divergence. This term is neglected in many engineering applications. However, since the radiative term scales as \(T^3\), it becomes increasingly significant in high temperature applications. These applications could include analysis of the heat transfer in furnaces, glass melting and cooling, and spacecraft reentry. As advances in materials continue to be made, higher temperatures are becoming more common in a wider array of applications in turbo machinery as well. In addition to high temperature applications, radiation is dominant in atmospheric heating and cooling making it of special interest to
meteorologists. Regardless of the application, in order to find a solution to Equation (1.1) an expression for \( q \) is needed.

The integral formulation of the radiant flux divergence is found by analyzing the local radiative flux. The divergence of the radiative flux vector is equal to the rate of energy emitted locally by the medium minus the energy absorbed by the medium. This relation is valid at any location within the medium. Specifically, this quantity is defined by Equation (1.2).

\[
\nabla \cdot q_r(S) = 4\pi \int_{\lambda=0}^{\infty} \kappa_{\lambda}(\lambda, S) I_{\lambda b}(\lambda, S)d\lambda - \int_{\lambda=0}^{\infty} \int_{\Omega=0}^{\infty} \kappa_{\lambda}(\lambda, S) I_{\lambda}(\lambda, S, \Omega)d\Omega d\lambda
\]

(1.2)

Here, \( \kappa_\lambda \) is the local absorption coefficient as a function of wavelength, \( I_{\lambda b} \) is the blackbody intensity as a function of wavelength, and \( I_\lambda \) is the local incoming radiative intensity as a function of wavelength and solid angle, \( \Omega \). The subscript \( \lambda \) indicates the dependence of the quantity upon wavelength. The use of the absorption coefficient and the blackbody intensity in the definition of the emission term is dependent upon the assumption of local thermodynamic equilibrium or LTE. For the purposes of this review, this assumption will be presumed valid in every situation.

The intensities are both intrinsically dependent upon temperature. The local black-body intensity present in the emission term is dependent upon the local temperature. The incident intensity in the absorption term is dependent upon the global temperature field. The local incoming radiative intensity is also a function of scattering (if present) and is given by Equation (1.3). The spectral absorption coefficient includes a temperature dependence as well.

\[
I_{\lambda}(\tau_\lambda, \Omega) = I_{\lambda}(0, \Omega)e^{-\tau_\lambda} + \int_{\lambda}^{\tau_\lambda} \tilde{I}_{\lambda}(\tilde{\tau}_\lambda, \Omega)e^{-(\tau_\lambda - \tilde{\tau}_\lambda)}d\tilde{\tau}_\lambda
\]

(1.3)

where \( \tilde{I}_{\lambda}(\tilde{\tau}_\lambda, \Omega) \) is the source function and \( \tau_\lambda \) is the opacity or optical depth and is defined in Equation (1.4). This is the way in which scattering affects the incident intensity. While it does not directly account for emission or absorption it does decrease the effective mean free path within the medium.

\[
\tau_\lambda(S) = \int_{0}^{S} \left[ \kappa_{\lambda}(s) + \sigma_{\lambda a}(s) \right]ds
\]

(1.4)

In some situations, scattering can be neglected. If this is the case, the source function in Equation (1.3) is given simply as the local blackbody intensity, \( I_{\lambda b} \). In general however, the source function is more complicated and is given by

\[
\tilde{I}(\tau_\lambda, \Omega) = (1 - \omega_\lambda)I_{\lambda b}(\tau_\lambda) + \frac{\omega_\lambda}{4\pi} \int_{\Omega=0}^{4\pi} I_{\lambda}(\tau_\lambda, \tilde{\Omega})\Phi_{\lambda}(\Omega, \tilde{\Omega})d\tilde{\Omega}
\]

(1.5)

\( \omega_\lambda \) is the scattering albedo. The albedo is a generalized reflectivity of the medium and is defined as the ratio of the scattering coefficient (\( \sigma_{\lambda a} \)) to the extinction coefficient (\( \kappa_{\lambda} + \sigma_{\lambda a} \)). Basically, the scattering albedo defines the portion of attenuated radiation that is scattered rather than absorbed. This is an important quantity because it helps to determine which solution methods might be appropriate. Scattered energy continues to be tracked through the system until it is absorbed, so problems with a high scattering albedo generally require additional computational expense unless special methods developed just for those cases are utilized.

2. Solving the Spectral Radiative Transport Equation in Isothermal Media

Our goal is to determine the total radiative flux divergence. As is suggested by the definition, the radiative flux divergence may be found by solving Equation (1.3) for the spectral intensity and then integrating over all wavelengths. There are many methods that have been developed for solving Equation (1.3), each with its own advantages and disadvantages. Which method is used to solve the transport equation for any given application is not relevant to this paper. Here, we are focused on the
integration of the spectral intensity over all wavelengths and how to evaluate this integral numerically in a way that is both accurate and computationally efficient.

2.1. Line-by-line method
Calculation of the radiative flux divergence within a medium requires integration of the absorption coefficient and intensities over all wavelengths. The most direct and accurate method is line-by-line calculations. In a line-by-line scheme, the spectrum is divided into small spectral intervals over which the absorption coefficient and local black-body intensity may be assumed constant. In real gases these intervals must be extremely small in order to capture the many resonance peaks in the absorption coefficient spectrum. The RTE is then solved for local intensity within each wavelength interval. This is time consuming and expensive.

The spectral RTE along a given path neglecting scattering is given by Equation (2.1). The absorption coefficient is potentially a function of \(S\) since in inhomogeneous media the absorption coefficient varies spatially.

\[
\frac{dI_\lambda}{dS} = \kappa_\lambda (I_{\lambda \lambda} - I_\lambda)
\]

The total intensity is found by integrating the spectral intensity over all wavelengths as shown in Equation (2.2).

\[
I = \int_0^\infty I_\lambda d\lambda
\]

Evaluating this integral numerically can be very computationally expensive. In real gases hundreds of thousands or millions of spectral intervals may be required in order to accurately calculate the total intensity.

2.2. The k-distribution method
The k-distribution method represents an alternative to line-by-line calculations which reduces the number of RTE evaluations from the order of a million to the order of ten without any significant loss of accuracy for homogeneous media [2]. This requires the formulation of a weighted cumulative distribution function of the absorption coefficient where the weight function is the Planck function.

\[
g(\kappa) = \frac{\pi}{\sigma T^4} \int_{\lambda \text{ at } \kappa} I_{\lambda \lambda} d\lambda
\]

Figure 1 demonstrates graphically the regions over which the Planck distribution would be integrated in order to compute \(g\) for a particular value of the absorption coefficient, \(\kappa\) (or equivalently, the absorption cross section, \(C\)) for a narrow section of a representative spectrum.
C is directly proportional to κ. The constant of proportionality is the number density, N. Assuming ideal gas behavior, this relationship is expressed in Equation (2.4).

$$\kappa = C \cdot N \approx C \cdot \frac{P}{RT}$$

where P is the pressure, T is the temperature and R is the universal gas constant expressed in consistent units.

The cumulative distribution function, g, is a smooth monotonically increasing function of κ. In fact, g is bijective. Figure 2 shows an example of a k-distribution generated for a 10% mixture of CO$_2$ at 600K and 1 atm. Since g(κ) is a bijection, it is invertible and a unique function κ$_g$ or C$_g$ may be defined.

Figure 1: k-distribution Demonstration [3]

Figure 2: Example k-distribution for 10% CO$_2$ at 600K, 1 atm
We can then rewrite the radiative transport equation as a function of $g$ rather than $\lambda$.

$$\frac{dI_g}{dS} = \kappa_g (I_b - I_g) \quad (2.5)$$

Additionally, we can evaluate the total intensity by integrating over $g$ rather than $\lambda$.

$$I = \int \limits_0^1 I_g \, dg \quad (2.6)$$

As can be seen from Figure 2, $\kappa_g$ is a smoothly varying function of $g$ and consequently, $I_g$ is a smoothly varying function of $g$ as well. This allows for a much smaller number of quadrature points to achieve near-line-by-line accuracy. The integration over $g$ may be accomplished using any available quadrature rule. An 8 point Gaussian quadrature is found to provide good results in most cases although increased accuracy may be achieved by using higher order quadrature schemes.

In addition, it should be noted that for each value of $g$ we find the intensity by solving the RTE for a (potentially inhomogeneous) gray gas. This solution may be found by a number of methods ranging from highly accurate but computationally expensive to extremely fast with only first order accuracy. Which solution method is appropriate may be determined based upon the optical thickness for a given value of $g$.

There is an inherent problem with the method just described when analyzing non-isothermal media. The Planck distribution in Equation (2.3) is not only a function of wavelength, but of temperature as well. Choosing the appropriate temperature for use in defining the k-distribution function a priori is difficult for non-isothermal problems. For cases where temperature variations across the domain are relatively small, this temperature dependence is negligible and the full spectrum k-distribution method provides good results for any reasonable choice of reference temperature including but not limited to the maximum temperature in the system, the minimum temperature in the system, the volume averaged temperature, the Planck mean temperature, and the emission weighted temperature [4].

As the temperature variations become large, significant errors can develop as a result of this approximation [5]. One way to solve this temperature dependence problem is to model the absorption coefficient's dependence on the temperature as was done in the Multi-Group Full Spectrum k-distribution Method (MGFSK) [6].

The MGFSK method provides good results for inhomogeneous media and the accuracy may be increased by the inclusion of an increasing number of groups. However, the method remains approximate. A more accurate but more computationally expensive alternative is presented here. The multi-source full spectrum k-distribution method is capable of providing exact results for one dimensional geometries with piecewise constant temperature and absorption coefficient in the same way that the full spectrum k-distribution method is able to provide exact results for homogeneous media problems.

3. Solving the Spectral Radiative Transport Equation in Non-Isothermal Media

For treatment of non-isothermal media, various approximations must be made. It is not feasible to provide a continuous definition of the medium’s spectral properties as a function of temperature. As a substitute, the continuous temperature distribution within the slab is modeled as piecewise constant in what has been called a multilayer approach. Solovyov and Webb applied this method to the SLW and CW methods in 2008 and demonstrated that a relatively small number of layers is actually required in order to achieve good predictions of the radiative heat flux and flux divergence [7].

The non-isothermal slab is divided into $K$ layers. Each layer has a reference temperature, $T_k$, a spectral absorption coefficient, $\kappa^k\lambda$ and a width, $\Delta x_k = x_k - x_{k-1}$. Within each layer, the total integrated heat flux and flux divergence are sought. The multi-layer approximation is similarly applicable to inhomogeneous media with concentration gradients. If concentration gradients exist, layers should be
sufficiently thin so that the spectral absorption coefficient may be modeled as constant within each layer.

For isotropic scattering and diffuse boundary conditions, the directionally integrated spectral heat flux is only a function of optical depth and is given by Equation (3.1).

\[
q_{r,d}(\tau_{\lambda}) = 2\pi \left\{ I_{\lambda}^{r}(0)E_{\lambda}(\tau_{\lambda}) - I_{\lambda}^{r}(\tau_{Lx})E_{\lambda}(\tau_{Lx} - \tau_{\lambda}) + \cdots \right. \\
+ \left. \int_{0}^{\tau_{Lx}} I_{\lambda}^{r}(\tau_{\lambda})E_{\lambda}(\tau_{\lambda} - \tau_{\lambda})d\tau_{\lambda} - \int_{\tau_{Lx}}^{\tau_{x}} I_{\lambda}^{r}(\tau_{\lambda})E_{\lambda}(\tau_{\lambda} - \tau_{\lambda})d\tau_{\lambda} \right\} 
\]

(3.1)

Neglecting scattering, the source function is simply the black-body intensity and is piecewise constant. The spectral heat flux then becomes

\[
q_{r,d}(x) = 2\pi \left\{ I_{\lambda}^{r}(0)E_{\lambda}(\tau_{\lambda}(x)) - I_{\lambda}^{r}(Lx)E_{\lambda}(\tau_{Lx} - \tau_{\lambda}(x)) + \cdots \right. \\
+ \left. \sum_{i=1}^{K-1} I_{\lambda}^{r}(Ti) \left[ E_{3}(\tau_{\lambda}(x) - \tau_{\lambda}(x_{i})) - E_{3}(\tau_{\lambda}(x) - \tau_{\lambda}(x_{i-1})) \right] + \cdots \right. \\
+ \left. \sum_{i=k+1}^{K} I_{\lambda}^{r}(Ti) \left[ E_{3}(\tau_{\lambda}(x_{i}) - \tau_{\lambda}(x)) - E_{3}(\tau_{\lambda}(x_{i-1}) - \tau_{\lambda}(x)) \right] + \cdots \right. \\
+ \left. I_{\lambda}^{r}(T_{K}) \left[ E_{3}(\kappa_{\lambda}^{x}(x) - \kappa_{\lambda}^{x}(x_{K})) - E_{3}(\kappa_{\lambda}^{x}(x_{K}) - \kappa_{\lambda}^{x}(x)) \right] \right\} 
\]

(3.2)

Using the multilayer approach, the definition of the optical depth from Equation (1.4) may be simplified.

\[
\tau_{\lambda}(x) = \int_{0}^{x} \kappa_{\lambda}(\tilde{x})d\tilde{x} = \sum_{i=1}^{k-1} \kappa_{\lambda}^{x} \Delta x_{i} + \kappa_{\lambda}^{x}(x - x_{k-1}) 
\]

(3.3)

The k-distribution method may be applied within each layer in order to reduce the number of spectral evaluations required. In order to do this, a reasonable reference temperature should be established. It has been shown [8] that in general non-isothermal problems this is not always feasible and that errors associated with this choice are difficult if not impossible to quantify.
The form of Equation (3.2) suggests an alternative to the establishment of a global reference
temperature. The problem may be recast as 3K sub-problems, K of which includes emission from
exactly one layer at exactly one temperature. The other 2K sub-problems involve purely absorbing
media with a (complex) spectral boundary condition. The spectral heat flux at the layer boundaries is
found by performing a line-by-line solution on a significantly coarser spatial grid with only K points.
There is no additional assumption introduced here. The radiative transport equation is linear and we
are simply representing the solution as a superposition of solutions to simpler problems.

For simplicity of explanation, we will discuss the contributions to the spectral heat flux at layer
boundaries as being due to contributions from each individual layer. The total spectral heat flux is
found by summing the contributions from each of the individual layers. In the 1-dimensional problem,
these contributions may be written explicitly.

The contribution to the spectral heat flux due to emission from the \( k \)th layer is given by Equation
(3.4).

\[
q^k_{sl}(x) = 2\pi I_{sl} (T_k) \left[ E_3 \left( \tau_\lambda (x) - \tau_\lambda (x_k) \right) - E_3 \left( \tau_\lambda (x_k) - \tau_\lambda (x_{k-1}) \right) \right] \quad x_k \leq x \leq x_{k-1}
\]

In order to use the k-distribution method to simplify the numerical spectral integration, an
appropriate weighting function for the generation of the absorption line blackbody distribution
function (ALBDF) must be defined. Usually, a Planck distribution at a set reference temperature is
used as this weighting function. However, the method may be generalized by using a general
weighting function which can be defined for each problem.

Consider the K sub-problems representing the flux within a given layer due to emission from that same layer. For
the \( k \)th sub-problem of this type, the weighting function is simply the Planck distribution and is given
by Equation (3.6).

\[
w(\lambda) = I_{sl} (T_k)
\]

A database of k-distribution functions using these weighting functions has previously been
developed by Modest for CO\(_2\) and H\(_2\)O. There is no geometry information imbedded in Equation (3.6)
so these functions may be evaluated and inverted offline.

There are an additional K sub-problems representing the heat flux within a given layer due to emission from layers to the left of that layer. For these sub-problems the appropriate weighting
function is given by Equation (3.7). Note that the weighting functions presented here only equal the
spectral heat flux up to a multiplicative constant since any such constant is eliminated in the
normalization of \( g \) performed in Equation (3.5).

\[
w(\lambda) = \sum_{l=1}^{k-1} \kappa_{l,l} I_{sl} (T_l) \left[ E_3 \left( \tau_\lambda (x_l) - \tau_\lambda (x_k) \right) - E_3 \left( \tau_\lambda (x_k) - \tau_\lambda (x_{k-1}) \right) \right]
\]

The remaining K sub-problems represent the heat flux within a given layer due to emission from
layer to the right of that layer. The appropriate weighting function in these sub-problems is given by
Equation (3.8).

\[
w(\lambda) = \sum_{l=k+1}^{K} \kappa_{l,l} I_{sl} (T_l) \left[ E_3 \left( \tau_\lambda (x_{k+1}) - \tau_\lambda (x_l) \right) - E_3 \left( \tau_\lambda (x_l) - \tau_\lambda (x_{l-1}) \right) \right]
\]
The k-distribution method has the advantage that any standard quadrature rule may be employed to evaluate the spectral integral which has been transformed into an integral over \( g \). While it is theoretically possible to vary the quadrature rule used at different spatial points within the slab, it is generally not very reasonable to do so. From this point forward, our notation will assume that the same N-point quadrature rule is used at every spatial point.

Within each layer, Equation (3.5) is inverted to define a unique function \( \kappa_k \) which is constant within that layer in the same manner as \( \kappa_\lambda \) and \( T_k \). The modified wavenumber, \( g \), is in \([0,1]\) and the choice of quadrature rule defines a set of N transport equations that should be solved within each layer. Any appropriate solution technique may be used to determine the solution within each sub-problem. The solution method may be chosen on the basis of layer optical thickness.

The significant cost savings provided by this method relative to a full line-by-line solution stems from the significant computational savings and efficiency gained by the use of the k-distribution method. This decrease in cost comes at virtually no cost in accuracy besides that incurred due to the use of the multilayer approximation.

4. Computational Cost Comparison
We will compare the computational cost of the multi-source k-distribution method with the cost of a line-by-line solution and with a standard k-distribution method. The line-by-line solution requires \( N_{lbl} \) solutions of the gray radiative transport equation at \( M \) spatial locations. The cost of a single gray RTE solution scales as \( M^\alpha \) where \( \alpha \in [2,3] \) depends upon the RTE solution technique as well as the linear algebra package employed. The case where \( \alpha = 2 \) corresponds to the evaluation of the analytical solution expressed in (3.1). \( \alpha = 3 \) corresponds to the solution of a general dense matrix.

The cost of a line-by-line solution is therefore given by Equation (4.1).

\[
N_{lbl} M^\alpha
\]  

(4.1)

By contrast, the cost of a solution by the standard k-distribution method is given by Equation (4.2)

\[
N_{kdist} M^\alpha
\]  

(4.2)

where \( N_{kdist} \ll N_{lbl} \) is the number of quadrature points used in the k-distribution spectral integration. This commonly represents an up to 5 or 6 orders of magnitude improvement in computational cost over the line-by-line method. However, for non-isothermal media, this improvement comes at a cost in accuracy which can be large in some cases and has yet to be effectively bounded in general.

The cost of the multi-source k-distribution method is between the two and is given by Equation (4.3).

\[
N_{lbl} K^\alpha + 3N_{kdist} K \left( \frac{M}{K} \right)^\alpha
\]  

(4.3)

where \( K \) is the number of layers used in the multilayer approximation. For simplicity, it is assumed that the number of spatial points per layer is uniform. For this method to be viable, \( K \ll M \). Ideal applications for this method involve the desire for a high order of accuracy on a fine spatial grid.

5. Results and Discussion
Solovjov and Webb established the convergence and viability of the multilayer approach in their paper [7]. This establishes the legitimacy of approximating a slab with a continuous temperature distribution as having a piecewise constant temperature distribution as depicted graphically in Figure 3. The question remains how well the k-distribution method and the multi-source k-distribution method predict the radiative heat flux and flux divergence in slab geometries with piecewise constant temperature distributions.
As a limiting case, consider a large step change in temperature. The left half of the slab (50 cm) is at 1000 K. The right half is at 300 K. The medium is 10% CO$_2$ by mole and is at a uniform pressure of 1 atm. Spectral line data (centers, half-widths, and intensities) are acquired from the HITRAN 2004 database [9]. The line data is used to generate a high resolution absorption spectrum. Lorentz profiles are used for all line shapes. The same spectrum is used in both the line-by-line solution and in the generation of the k-distribution functions.

Figure 4: Heat Flux Distribution in a Non-Isothermal Medium Bounded by Cold Black Walls

Figure 4 shows the calculated heat flux using the full spectrum k-distribution method with a single reference temperature and using the multi-source k-distribution method. These results are compared to those generated using line-by-line calculations. Using a reference temperature of 300 K gives poor results. The majority of the radiative energy is emitted in the hotter left half of the slab. Using a reference temperature of 300 K is totally incorrect for this spatial region. For this reason, the heat flux is poorly represented in every part of the domain.

Using a reference temperature of 1000 K, the heat flux prediction is quite accurate in the left half of the domain. The fact that this model does a relatively poor job of predicting the behavior of energy emitted from the right half of the medium has little effect since the vast majority of the flux is due to the high temperature emission from the left half of the slab. However, this model also does a poor job of predicting the absorption of energy in the right half of the slab. This leads to potentially large relative errors in predicting the heat flux exiting the right boundary. The thicker the cold region becomes, the more significant this error becomes.

Modest and Zhang analyzed the effect of the length of the cold region on the error in the heat flux at the right wall for several different reference temperature models [4]. They used a higher temperature for the hot zone and a slightly different gas mixture. However, the general trends should hold true. Five different reference temperatures were used in this study and none were capable of achieving the kind of accuracy reported here using the Multi-Source method. Admittedly, this improvement in accuracy comes at a computational cost. However, for applications for which accuracy is paramount, the multilayer multi-source k-distribution method provides a more efficient alternative to line-by-line calculations.

This example highlights the difficulty of using the k-distribution method in non-isothermal media. The appropriate choice for a reference temperature is virtually impossible to determine a priori. Furthermore, the error associated with an incorrect choice of reference temperature is unknown. The correct value of the heat flux at any given spatial location is not guaranteed to be bounded by the heat flux calculated using the maximum system temperature as the reference temperature and the heat flux
calculated using the minimum system temperature as the reference temperature. To the authors’ knowledge, there has been no effective bound developed for the model error introduced in this way. As can be seen from Figure 4, this error can be substantial.

6. Conclusions
The multilayer approach as presented in this paper presents a significant increase in accuracy over other k-distribution based approaches while remaining significantly less computationally expensive than a standard line-by-line solution. It will require modification to be applicable in more general higher dimensional geometries. Additionally, the definitions of the appropriate weighting functions for the multi-source k-distribution method provided implicitly assume a slab geometry. It is unclear at this time what errors would be introduced when generalizing this method for use in two or three dimensional domains, and this is a topic undergoing further research.

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