Journal of Quantitative Spectroscopy & Radiative Transfer 197 (2017) 26–44

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

The rank correlated SLW model of gas radiation in non-uniform media

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ARTICLE INFO

Article history:
Received 1 October 2016
Received in revised form
17 December 2016
Accepted 29 January 2017
Available online 1 February 2017

Keywords:
Gas radiation
Rank correlation of gas absorption spectra
Generalized SLW Method
SLW reference approach
Rank correlated SLW model

ABSTRACT

A comprehensive theoretical development of possible reference approaches in modelling of radiation transfer in non-uniform gaseous media is developed within the framework of the Generalized SLW Model. The notion of absorption spectrum "correlation" adopted currently for global methods in gas radiation is critically revisited and replaced by a less restrictive concept of rank correlated spectrum. Within this framework it is shown that eight different reference approaches are possible, of which only three have been reported in the literature. Among the approaches presented is a novel Rank Correlated SLW Model, which is distinguished by the fact that *i*) it does not require the specification of a reference gas thermodynamic state, and *ii*) it preserves the emission term in the spectrally integrated Radiative Transfer Equation. Construction of this reference model requires only two absorption line blackbody distribution functions, and subdivision into gray gases can be performed using standard quadratures. Consequently, this new reference approach appears to have significant advantages over all other methods, and is, in general, a significant improvement in the global modelling of gas radiation. All reference approaches are summarized in the present work, and their use in radiative transfer prediction is demonstrated for simple example cases. Further, a detailed rigorous theoretical development of the improved methods is provided.

1. Introduction

Global methods in modelling of radiation transfer in high-temperature gases such as SLW (Spectral Line Weighted-sum-of-gray-gases), ADF (Absorption Distribution Function), FSK (Full Spectrum *k*-distribution), and MBWSGG (Moment-Based Weighted-Sum-of-Gray-Gases) methods, and the hybrid forms of the SLW model with other spectral models [1–12] are computationally the most efficient methods in modelling of gas radiation. These methods can provide high accuracy of prediction of radiation transfer, often comparable to that of the benchmark line-by-line (LBL) method but at significantly lower computational cost. Despite the seeming difference between SLW, ADF, and FSK methods, they all are based on the same fundamental principle in modelling of the gas absorption spectrum, and it has been shown that all of them can be described as particular cases of the recently published Generalized SLW Model [6]. The primary challenge of global methods is to extend the spectral modeling from uniform (isothermal, homogeneous) to non-uniform (non-isothermal, non-homogeneous) media, for which some additional assumptions regarding the gas absorption spectrum (e.g., assumption of correlated or scaled spectra) must be made. The existing approaches are based on assumptions that can yield large errors in the case of high spatial temperature gradients in the medium. Simply put, the reference approach to handling nonisothermal, nonhomogeneous media involves defining a reference state and correcting all local states relative to that reference state. The main drawback of the reference approach is the absence of a consistent recommendation for the choice of the gas reference state. Despite the interest in the reference approach in global methods, not all possible variations of the method have been discovered. The Generalized SLW Model provides a backdrop to reveal more possibilities for new versions of the reference approach.

The objective of the present paper is to develop and present all possible versions of the SLW reference approach, and investigate and compare their characteristics. The main result is the new Rank Correlated SLW Model which distinguishes itself from other approaches in that it is the only method *i*) which does not require the specification of a gas reference state, and *ii*) which preserves the emission term in the spectrally integrated Radiative Transfer Equation. This method is introduced in Section 3.5.1 to follow, and its detailed outline is presented in Section 3.7. Rigorous theoretical justification of properties for the Rank Correlated SLW model is given in Appendices 1–3. It can be shown that the development presented for the Rank Correlated SLW model in non-uniform

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http://dx.doi.org/10.1016/j.jqsrt.2017.01.034
0022-4073/

media is based on the more general co-monotonic spectral model of gas radiation in non-uniform media employing an arbitrary probability distribution, and is a particular case of its application.

2. The SLW method

2.1. Spectral radiative transfer equation

Propagation of radiation in absorbing and emitting gaseous media along a path length s in a direction. $\boldsymbol{\Omega}$ is characterized by the spectral radiation intensity $I_\eta(s, \boldsymbol{\Omega})$, which is governed by the Radiative Transfer Equation (RTE)

$$\frac{\partial I_\eta(s, \boldsymbol{\Omega})}{\partial s} = -\kappa_\eta(s) I_\eta(s, \boldsymbol{\Omega}) + \kappa_\eta(s) I_{b\eta}\left[T(s)\right] \tag{1}$$

where η is the wavenumber, $I_{b\eta}\left[T(s)\right]$ is the spectral Planck blackbody intensity at the local gas temperature $T(s)$, and the local spectral absorption coefficient is defined as $\kappa_\eta(s) = N(s)Y(s)C_\eta(\phi(s))$, $\left[1/m\right]$ where $C_\eta(\phi(s))$, $\left[m^2/mol\right]$ is the gas absorption cross-section, and $\phi(s) = \left\{T(s), Y(s), p(s)\right\}$ is a symbolic vector notation for the definition of the local gas thermodynamic state at temperature $T(s)$, total pressure $p(s)$, and mole fraction $Y(s)$. High resolution spectral databases such as HITRAN and HITEMP are used to compile the spectral gas absorption cross-section $C_\eta(\phi)$.

The Line-by-Line (LBL) method solves the spectral RTE for each wavenumber η, following which the total intensity of radiation may be obtained by spectral integration over all wavenumbers. The narrow band approximation requires solution of the RTE at hundreds of thousands of spectral points η_i in the numerical integration:

$$I(s, \boldsymbol{\Omega}) = \int_0^\infty I_\eta(s, \boldsymbol{\Omega}) d\eta \approx \sum_i I_{\eta i}(s, \boldsymbol{\Omega}) \Delta\eta_i \tag{2}$$

The SLW model is a particular case of the so-called global family of methods in modeling gas radiation which, in contrast to the Line-by-Line method, starts first with spectral integration of the RTE, and then solves it directly for the spectrally integrated intensity $I(s, \boldsymbol{\Omega})$ for a finite number of discrete values of the absorption cross-section (rather than wavenumber). To determine total radiative properties it may be said that the SLW method integrates over absorption cross-section rather than wavenumber.

2.2. Characterization of the gas absorption cross-section – ALBDF and inverse ALBDF

A brief tutorial on the Generalized SLW model is presented here to provide context for the reference approaches identified in sections to follow. The spectral integration of the RTE in the SLW model is made efficient by application of the direct and inverse Absorption Line Blackbody Distribution Function (ALBDF).

The ALBDF $F\left(C, \phi_g, T_b\right)$ of the absorption cross-section C at a given gas thermodynamic state $\phi_g = \left\{T, Y, p\right\}$ describes the fraction of the total blackbody radiation power $E_b\left(T_b\right) = \sigma T_b^4$ emitted at temperature T_b that lies in the part of the spectrum where the gas absorption cross-section $C_\eta\left(\phi_g\right)$ is below the prescribed value C:

$$F\left(C, \phi_g, T_b\right) = \frac{1}{E_b\left(T_b\right)} \int_{\left\{\eta: C_\eta(\phi_g) < C\right\}} E_{b\eta}\left(T_b\right) d\eta = \int_0^\infty H\left(C_\eta(\phi) - C\right) \frac{E_{b\eta}\left(T_b\right)}{E_b\left(T_b\right)} d\eta \tag{3}$$

Here, H is the Heaviside unit-step function. The ALBDF is a strictly increasing function varying between 0 and 1 with respect to the variable C, and therefore, it is invertible. The inverse ALBDF $C\left(F, T_g, T_b\right)$ of the variable F is defined such that

$$C\left[F\left(C, \phi_g, T_b\right), \phi_g, T_b\right] = C \text{ , and } F\left[C\left(F, \phi_g, T_b\right), \phi_g, T_b\right] = F \tag{4}$$

The inverse ALBDF can be interpreted as a reordered gas absorption cross-section. The ALBDF is calculated in advance from the high-resolution gas absorption cross-section, and has recently been presented in tabulated form or mathematical correlations [5,6] using the most up-to-date spectral database, HITEMP 2010. The values of the inverse ALBDF may be obtained by inversion of the ALBDF tabulated data, or by polynomial interpolation of mathematical correlations with the help of the method of moments [6].

2.3. The SLW Method – spectral integration of RTE in uniform media

Consider a uniform gaseous medium at a specified thermodynamic state $\phi = \left\{T, Y, p\right\}$. The spectral gas absorption coefficient at this state is given as $\kappa_\eta(\phi) = NYC_\eta(\phi)$, where $C_\eta(\phi)$ is the gas spectral absorption cross-section.

2.3.1. SLW histogram spectrum

As shown in Fig. 1, the continuous line absorption coefficient $C_\eta(\phi)$ is modelled in the SLW method by a histogram spectrum in the following way. First, define a set of supplemental absorption cross-sections $\tilde{C}_j$ spaced between chosen limiting values $C_{\min}$ and $C_{\max}$ which effectively span the entire range of gas absorption spectrum. As an example, logarithmic spacing has been previously used as $\tilde{C}_j = C_{\min}\left(C_{\max}/C_{\min}\right)^{j/n}$, $j = 0, 1, \ldots, n$, where n is the number of gray gases in the model. The gray gas absorption cross-sections C_j can be chosen arbitrarily in the interval $\tilde{C}_{j-1} < C_j < \tilde{C}_j$, for example, as a geometric mean $C_j = \sqrt{\tilde{C}_{j-1}\tilde{C}_j}$. Then the gray gas absorption coefficients are $\kappa_j = NYC_j$, and the clear gas is defined as $\kappa_0 = 0$. The supplemental cross-sections define the gray gas and the clear gas spectral intervals:

$\Delta_j = \left\{\eta: \tilde{C}_{j-1} < C_\eta(\phi) < \tilde{C}_j\right\}$, $\Delta_0 = \left\{\eta: C_\eta(\phi) < \tilde{C}_0\right\}$

Then the SLW histogram spectrum is defined as

$\kappa_\eta(\phi) = \kappa_j$, $\eta \in \Delta_j$, $j = 0, 1, \ldots, n$

2.3.2. Spectral integration of the RTE

Integration of the spectral RTE over the gray gas spectral intervals Δ_j, $j = 0, 1, \ldots, n$ yields the following expression:

$$\int_0^\infty \frac{\partial I_\eta(s, \boldsymbol{\Omega})}{\partial s} d\eta = -\int_0^\infty \kappa_\eta(s) I_\eta(s, \boldsymbol{\Omega}) d\eta + \int_0^\infty \kappa_\eta(s) I_{b\eta}\left[T(s)\right] d\eta \tag{5}$$

Because the spectral gray gas intervals are fixed for all spatial locations in a uniform medium, the order of differentiation and integration on the left-hand side of the equation can be interchanged. That yields the gray gas RTEs:

$$\frac{\partial I_j(s, \boldsymbol{\Omega})}{\partial s} = -\kappa_j I_j(s, \boldsymbol{\Omega}) + a_j \kappa_j I_{b\eta}(T) \tag{6}$$

where

$$I_j(s, \boldsymbol{\Omega}) = \int_{\Delta_j} I_\eta(s, \boldsymbol{\Omega}) d\eta \tag{7}$$

is defined as the gray gas intensity, and

$$a_j = F\left(\tilde{C}_j, \phi_g = \phi, T_b = T\right) - F\left(\tilde{C}_{j-1}, \phi_g = \phi, T_b = T\right) \tag{8}$$

are the gray gas weights. After solution of the gray gas RTEs, the total intensity can be found by a summation over all gray gases: