Non-dimensional wavenumber in full-spectrum k-distribution computations with or without a reference state

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ABSTRACT

In the full spectrum k-distribution method, the k-distributions are Planck function weighted. These k-distributions depend on temperature, which varies with location in nonisothermal media. Consequently, in order to apply the method to nonuniform media, k-distributions evaluated at different local temperatures are correlated by a k-distribution evaluated at an arbitrarily chosen reference blackbody temperature. On the other hand, in the original band method, the k-distributions are directly related to spectral locations. Such k-distributions can replace Planck function weighted k-distributions computed at a reference temperature. This approach was employed by Maurente et al. [1] in order to deal with gas mixtures in non-equilibrium media. In this paper the formulation is presented for the equilibrium case. The proposed formulation simplifies the application of the FSK method to nonuniform media, and brings new directions to k-distribution issues. It can be employed with a reference state, but not a reference temperature, with reference state and temperature, as in the traditional FSK, and without any reference state, being in this case the continuous limit of the recently developed Rank Correlated SLW [2]. Results were obtained for test cases considering one-dimensional, nonuniform media, constituted by CO_2 and inert gases, and compared to line-by-line solutions.

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1. Introduction

Exact line-by-line solution of radiation heat transfer in participating media is computationally expensive, and can become prohibitive in cases of coupled simulations in which radiation is combined with other heat transfer modes. Because of that, one of the major issues regarding computational simulation of radiation heat transfer concerns how to efficiently and accurately account for the spectral dependence of the radiative properties. Several spectral models have been proposed, which are generally classified into: band and global models. The band models characterize the line-behavior inside spectral bands, while the global models encompasses all spectral lines that are important for the problem to be solved. The early band models, *Elsasser* and *Goody*, were proposed in the last half of the past century [3]. Regarding the global models, the weighted-sum-of-gray gases (WSGG), introduced by Hottel [4], is possibly the most widely used. Recently, Dorigon et al. [5] and Centeno et al. [6] updated parameters of the WSGG using data from HITEMP2010 [7] and demonstrated that it can still provide accurate results when compared to current line-by-line solutions.

The k-distribution methods use a transformation of variables in which the spectral absorption coefficient is reordered into a smooth, monotonically increasing function. This allows one to take into account several spectral intervals at once while solving the radiative transfer equation. Such procedure can be applied to bands or the full spectrum, resulting in band k-distribution or global k-distribution methods. The k-distribution principle has been applied to state-of-the-art methods, as the full-spectrum k-distribution (FSK) [8,9], spectral-line-based-weighted-sum-of-gray gases (SLW) [10–13], cumulative wavenumber (CW) [14], absorption distribution function (ADF) [15,16] and spectral-line moment-based (SLMB) [17].

In spite of the important achievements in terms of accuracy and computational efficiency, there still exist issues that maintains a great research interest on k-distributions. Following are some examples which demonstrate the diversity of studies about k-distribution methods accomplished during the last decades and recent years. Wang et al. [18], Wang and Modest [19], Maurente et al. [20,21] and Maurente and França [22] used the FSK combined with the Monte Carlo method. Methodologies to apply the FSK to

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media at non-local-thermodynamic equilibrium were proposed by Bansal et al. [23] and Maurente et al. [1]. Ma et al. [24] applied the spectral collection method with the FSK. Tencer and Howell [25] quantified uncertainties related to the correlated-k assumption for FSK computations. Solovjov et al. [26] and Solovjov and Webb [27] presented respectively the SLW-1, with only one gray gas, and the exact SLW, when the number of gray gases approaches infinity. A generalized SLW, which uses the absorption-line-blackbody distribution function (ALBDF) and its inverse form, was presented by Solovjov et al. [28]. Cai and Modest [29] proposed an improved version of the FSK for nonhomogeneous media using a narrow-band database, and André et al. [30] presented an exact formulation for k-distribution methods in nonhomogeneous media and also a computationally less costly method based on a multi-spectral framework which approximates their exact solution.

Although there is apparent simplicity behind the reordering idea, global k-distribution methods become significantly more complex for nonuniform media, as compared to the case in which the media are homogenous and isothermal. This happens because the non-trivial relation between the reordered absorption coefficient and the cumulative k-distributions evaluated at different states. Thus, there exists an interest in simplifying k-distribution approaches for nonuniform media. An example is the recently developed Rank Correlated SLW (RC-SLW) model [2,31], which does not require a reference state.

In this research it is proposed a FSK formulation which does not use a reference temperature. Instead, it employs a cumulative k-distribution which is equivalent to fractions of a spectral interval. Such a cumulative k-distribution is defined as in the original narrow band k-distribution and acts as a non-dimensional wavenumber. In the proposed formulation this non-dimensional wavenumber works like an independent variable which provides a direct relation between properties and spectral locations, and thus is useful for correlating the full spectrum cumulative k-distributions (or ALBDFs) across different media states, and simplifies the FSK equations. As will be shown, the proposed formulation is well suited to be employed without any reference state, being in this case the continuous limit of the RC-SLW [2,31]. The formulation can also be applied with a reference state but no reference temperature, or with reference state and temperature, the latter falling in the case of the traditional FSK approach. The three approaches will be compared against line-by-line calculations for test cases considering one-dimensional, nonuniform medium slabs formed by CO_2 and inert gases.

2. The k-distribution method

For an absorbing-emitting, but non-scattering medium, the variation of intensity of a radiation ray traveling along a path within this medium is described by the following simplified form of the *Radiative Transfer Equation (RTE)*:

$$\frac{dI_\eta}{ds} = \kappa_\eta I_{b,\eta} - \kappa_\eta I_\eta \tag{1}$$

where I_η is the spectral intensity of radiation and the subscript η refers to the wavenumber, indicating spectral dependence; $I_{b,\eta}$ is the blackbody spectral intensity, given by the Planck function; κ_η is the absorption coefficient and *ds* is a differential element of length along the path of propagation of the radiation ray.

Computing radiation heat transfer requires that the RTE be solved for a sufficiently large number of spectral intervals, then integration over the entire spectrum to find the total intensity of radiation. The k-distribution method uses a transformation of variables to reduce the extent of the calculations. The method is
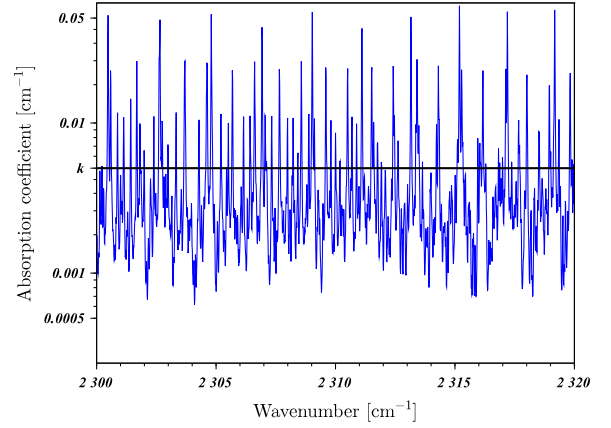

Fig. 1. Absorption coefficient, κ_η, of a medium constituted by 10% CO_2 and N_2, at 1500 K and 1 atm, in function of the wavenumber, η, in a narrow spectral region, which was computed using spectroscopic data from HITEMP [7].

based on the fact that for a small spectral portion corresponding to a narrow band the blackbody intensity does not vary significantly with the wavenumber and can be considered constant, while the absorption coefficient, κ_η, contains significant variations and repeats the same value, *k*, several times, as shown in the horizontal bold line in Fig. 1, which presents a narrow region of the spectrum of a medium constituted by 10% CO_2 and N_2, at 1500 K and 1 atm, computed using data from HITEMP2010 [7]. Thus, the intensity field can be computed only once for all the spectral locations where the absorption coefficient attains a specific same value.

In k-distribution computations, k-distributions themselves are not in fact necessary. It is more convenient to use the cumulative k-distributions, which are smoothly monotonically increasing functions and can be directly computed as

$$g(k) = \frac{1}{\Delta\eta} \int_{\Delta\eta} H(k - \kappa_\eta) d\eta \tag{2}$$

where *H* is the Heaviside function.

Although the narrow band k-distribution takes into account several spectral locations at once, the computational efficiency of the method is limited by the need of considering several small narrow band intervals. A more efficient version of the method is the full-spectrum k-distribution, presented by Modest and Zhang [8]. In this method the blackbody intensity is allowed to vary across the spectrum. In order to allow variation of the blackbody intensity, the cumulative k-distribution is defined as

$$F(k) = \frac{1}{I_b} \int_0^\infty I_{b,\eta} H(k - \kappa_\eta) d\eta \tag{3}$$

where I_b is the blackbody total intensity obtained integrating the Planck function over the entire spectrum.

The cumulative k-distribution computed with Eq. (3) gives the fraction of the blackbody intensity in the portions of the spectrum where the absorption coefficient is less than a prescribed value *k*, as depicted in Fig. 2. Such a function was previously defined by Denison and Webb [11] as the absorption-line-blackbody distribution function (ALBDF). The symbol *F* was used instead of *g* in order to distinguish the Planck function weighted cumulative k-distribution from that of the narrow band k-distribution method, which corresponds to fractions of the spectral interval $\Delta\eta$. For the sake of clarity, the cumulative k-distribution computed with Eq. (3) is from now on referred as ALBDF, and non-dimensional wavenumber is preferred for the wavenumber weighted cumulative k-distribution computed with Eq. (2).

The ALBDF, can be applied to reorder the RTE by grouping spectral segments which correspond to a same value of *k*. In the
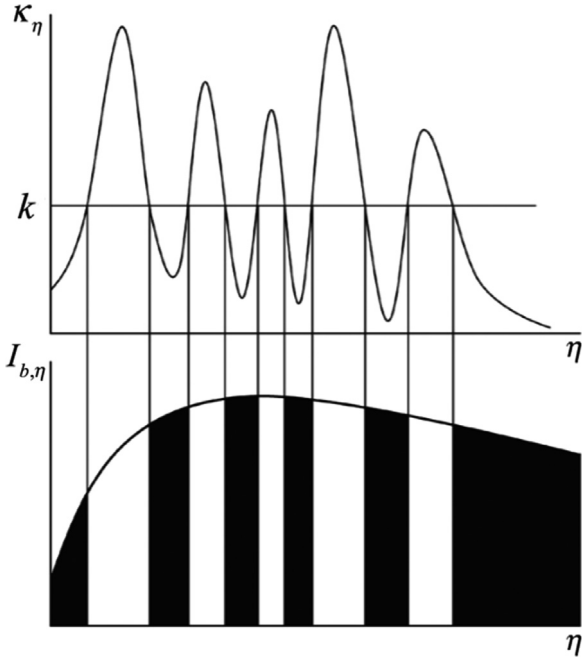
Fig. 2. Fraction of the blackbody energy in the spectral regions where $\kappa_\eta < k$.

case of a uniform non-scattering medium, the reordering process results in:

$$\frac{d}{I_F} ds = k I_b - k I_F \tag{4}$$

Eq. (4) can be solved to provide the intensity field, I_F. Then, the intensity for the entire spectrum, that is, the total intensity, is obtained by the following integration:

$$I = \int_0^1 I_F dF \tag{5}$$

The full-spectrum k-distribution method is exact for uniform media. However, when the state of the medium varies with location, the correlated-k assumption must be invoked. In this case, it is assumed that all wavenumbers that are associated to a same absorption coefficient value k_o at one state, are also associated to another single absorption coefficient value k at a different state, as depicted in Fig. 3. Since the spectra of real gases are not truly correlated, the FSK computations cannot be as accurate as line-by-line computations for nonuniform media.
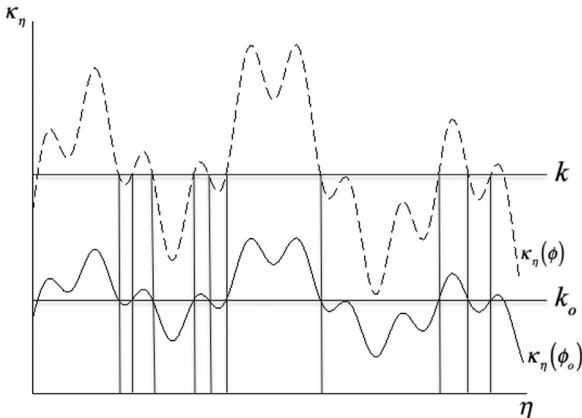
For correlated absorption coefficients,

Fig. 3. Example of correlated-k spectra.

$$F\big(T_b, \phi_o, k_o\big) = F\big(T_b, \phi, k\big) \tag{6}$$

where ϕ is the state vector of the medium, which includes temperature, pressure and mole fraction of the emitting/absorbing species, and the subscript o indicates reference state. The absorption coefficient k, evaluated at the state ϕ, is correlated to the absorption coefficient k_o, evaluated at ϕ_o.

Eq. (6) states that the fraction of the total blackbody intensity, I_b, within the spectral portions where $\kappa_\eta(\phi_o) < k_o$ is also the fraction of I_b where $\kappa_\eta(\phi) < k$, since both k_o and k are correlated and therefore associated to the same spectral locations. Such a relation holds only for ALBDFs evaluated at the same blackbody temperature, T_b. However, as the temperature of nonuniform media can vary with location, Modest and Zhang [8] proposed the use of a reference temperature, $T_{b,o}$, in order to obtain the following reordered RTE for full spectrum k-distribution computations in nonuniform media:

$$\frac{dI_F}{ds} = k(T_{b,o}, \phi, F_o)\big[a(T_b, T_{b,o}, F_o)I_b - I_F \big] \tag{7}$$

where $F_o = F(T_{b,o}, \phi_o, k_o)$ is the ALBDF computed using the reference temperature, and a is a factor which, according Solovjov et al. [28], can be computed as follows, if considering F_o as an independent variable:

$$a(T_b, T_{b,o}, F_o) = \frac{dF(T_b, \phi_o, k(F_o, \phi_o, T_{b,o}))}{dF_o} \tag{8}$$

For numerical solution Eq. (8) can be written in terms of finite increments, as presented by Wang et al. [33].

Assuming black walls, the boundary condition for Eq. (7) is

$$I_F = a(T_w, T_{b,o}, F_o)I_b(T_w) \tag{9}$$

where T_w is the wall temperature. This boundary condition applies also to the case of uniform media, where the wall temperature can be different of the medium temperature.

The intensity of radiation for the entire spectrum can be computed by integrating the intensity field I_F, from Eq. (7), over the entire F_o space:

$$I = \int_0^1 I_F dF_o \tag{10}$$

Radiation scattering and reflective surfaces were not considered in the above equations for simplicity. However, extending the formulation to include diffuse gray boundaries and media whose scattering coefficient and phase function are independent of the wavenumber is straightforward and does not change the characteristic k-distribution functions. Details about the derivation of the FSK formulation, which include diffuse gray boundaries and scattering can be found in [32].

3. The non-dimensional reordered wavenumber in FSK computations

The ALBDF, $F(T_b, \phi_o, k_o)$ varies with location in nonisothermal media, since the spectral distribution of the blackbody intensity depends on temperature. However, it must be always evaluated at the same considered spectral locations, where $k(T_{b,o}, \phi, F_o) = \kappa_\eta(\phi)$, as one solves Eq. (7) across the spatial locations. The factor $a(T_b, T_{b,o}, F_o)$ given by Eq. (8) correlates ALBDFs evaluated at the local temperature with the reference ALBDF, $F_o = F(T_{b,o}, \phi_o, k_o)$. Indirectly, $a(T_b, T_{b,o}, F_o)$ correlates ALBDFs evaluated at different local temperatures with the invariable spectral locations where $k(T_{b,o}, \phi, F_o) = \kappa_\eta(\phi)$.

In the proposed FSK formulation no reference temperature is

used. Instead, ALBDFs are directly related to spectral locations using wavenumber weighted cumulative k-distributions (or non-dimensional reordered wavenumbers) similar to that of the original band k-distribution, given by Eq. (2), although extended to the entire spectrum:

$$g(k) = \frac{1}{\eta_{\max}} \int_0^{\eta_{\max}} H(k - \kappa_\eta) d\eta \tag{11}$$

where $\eta_{\max}$ is such that the emission of radiation is negligible if $\eta > \eta_{\max}$.

The cumulative k-distribution computed using Eq. (11) gives the fraction of the spectrum where the absorption coefficient κ_η is lower than k. It is a non-dimensional reordered wavenumber for the entire spectrum, and varies from 0, when $k=0$, to 1, when $k = \kappa_{\eta,\text{peak}}$, where $\kappa_{\eta,\text{peak}}$ is the maximum (peak) value of the absorption coefficient. Using this non-dimensional wavenumber, the factor a can be simplified to

$$a(T, g) = \frac{dF(T, g)}{dg} \tag{12}$$

and the radiative transfer equation becomes:

$$\frac{dI_g}{ds} = k(\phi, g) \big[a(T, g) I_b - I_g \big] \tag{13}$$

Thus, the total intensity of radiation is obtained by integration of the intensity, I_g, over the non-dimensional reordered wavenumber g:

$$I = \int_0^1 I_g dg \tag{14}$$

If the medium spectra are correlated-k throughout the thermodynamic states, $g(\phi_1, k_1) = g(\phi_2, k_2) = g(\phi_o, k_o) = g(\phi, k)$, for any arbitrary state ϕ, the absorption coefficient, k, can be written as a function of the non-dimensional wavenumber, g, that is, $k = k(\phi, g)$. Also, for correlated-k spectra $F(T, \phi_o, k_o) = F(T, \phi, k)$. Therefore, $F(T, \phi, k)$ can be written as $F(T, g)$, by comparison with $g(\phi_o, k_o) = g(\phi, k)$, in order to simplify notation. A rigorous proof that $F(T, \phi_o, k_o) = F(T, \phi, k)$ for any state, ϕ, under the assumption of rank correlated spectrum, is presented by Solovjov et al. [2,31].

Observe that as g is a non-dimensional wavenumber it is well-suited for $F(T, g)$. With the proposed notation the fraction of the blackbody emitted energy is represented as a function of temperature and non-dimensional wavenumber, similar to the blackbody emissive power itself, which is a function of temperature and wavenumber.

In the traditional formulation, the dependence of quantities appearing in Eqs. (7) and (8) with respect to spectral locations is implicitly considered by the joint use of T_b, $T_{b,o}$, ϕ_o, k_o, F and F_o. Thus, the quantities depend on local properties and properties evaluated at a reference state. In the proposed formulation, the dependence of quantities with respect to the spectral locations is made explicit by the use of the non-dimensional wavenumber, g. Thus the quantities depend only on local properties and g, which is independent of the state. This simplifies notation, as can be verified by comparing Eqs. (7) and (8) with Eqs. (12) and (13). Moreover, looking at the method from a different viewpoint can lead to insights to provide new methodologies to solve FSK issues. The idea of using a wavenumber weighted cumulative k-distribution for the entire spectrum was first proposed by Maurente et al. [1] for applications to media at non-local thermodynamic equilibrium (non-LTE). In that case, the formulation was necessary to allow employing approximations for k-distributions of mixtures [34] along with the FSK for non-LTE method. In the present study the formulation was presented for the case of LTE media, thus becoming applicable to both LTE and non-LTE cases.

Next section presents two examples which demonstrate the application of the proposed formulation.

4. Example of application of the proposed FSK formulation

The proposed formulation is equivalent to the traditional one, and is expected to provide the same accurate results for uniform media or hypothetical nonuniform media with truly correlated absorption coefficients. However, in the case of real media, the correlated-k is an approximation, and the absorption coefficients evaluated at different states need to be computed based on some sort of assumption to be correlated. As presented in Section 3, in the traditional FSK, $k(T_{b,o}, \phi, F_o)$ are assumed correlated to $k_o(T_{b,o}, \phi_o, F_o)$. The proposed formulation suggests alternative assumptions for the computation of correlated absorption coefficients, as will be explained in this section.

Moreover, the proposed formulation can simplify the way one computes the data points for the numerical discretization of the cumulative k-distributions. The discretization procedure is important since the accuracy and computational efficiency of the FSK depends on the choice of the data points to represent the k-distribution functions and the respective reordered absorption coefficients. Large g values correspond to large k values, which tends to dominate radiative heat transfer. Thus, for the numerical solution it is advantageous to use a non-uniform discretization with more data points toward large values of g. Wang and Modest [35] presented high-accuracy, compact database for narrow band k-distributions of water vapor and carbon dioxide, and suggested two quadrature schemes for the computation of g data points. One of them is:

$$g = \cos\theta_n, \quad \theta_n = \frac{n\pi}{2N + 1} \quad (n = 1, 2, ..., N) \tag{15}$$

where N is the total number of data points used for the discretization of g. The scheme given by Eq. (15) has an open end at $g=0$, which is an advantage, since the $g=0$, corresponding to $k=0$, is not useful in k-distribution calculations. Such a scheme is used to compute the g data points for the considered examples.

Although Eq. (15) was proposed for narrow band cumulative k-distributions, it is used in traditional FSK computations through the following equations proposed by Modest and Riazzi [36]:

$$F(T_b, \phi_o, k) = \sum_{j=1}^{N_{\Delta\eta}} \frac{I_{b,j}}{I_b} g_j(k) \tag{16}$$

where

$$I_{b,j} = \int_{\Delta\eta_j} I_{b,\eta}(T_b) d\eta \tag{17}$$

is the Planck function integrated over narrow band $\Delta\eta_j$, $N_{\Delta\eta}$ is the number of bands, and $g_j(k)$ is the cumulative k-distribution of the narrow band, or the non-dimensional wavenumber of the band.

In order to compute ALBDFs using Eq. (16), it is necessary to consider several narrow band intervals, $N_{\Delta\eta}$, within which the blackbody intensity is approximated as constant, and the g_j must be computed to every one of these narrow bands. On the other hand, in the proposed formulation Eqs. (16) and (17) are not used. Instead, Eq. (15) can be directly employed to generate g data points for the entire spectrum, since the proposed formulation uses a non-dimensional wavenumber, g, for the full spectrum. After obtaining g data points from Eq. (15), the respective F and k are computed at any local state, as explained in the following example problems.
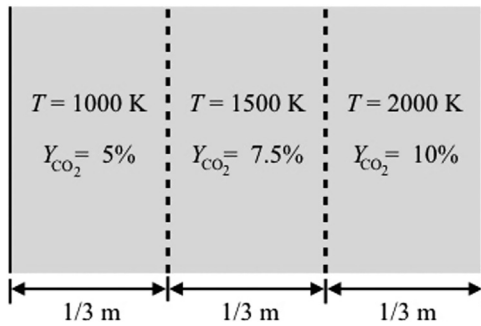
Fig. 4. One-dimensional slab of medium constituted by three different regions, considered in example 1.

4.1. Example 1

The considered problem consists of an one-dimensional non-uniform medium at 1 atm, composed of CO_2 and N_2, confined between two black cold walls. The medium has three different uniform regions, numbered as 1, 2 and 3, each 1/3 m thick. The temperature and CO_2 mole fraction in each of the three regions are shown in Fig. 4. The line-by-line absorption coefficients were computed using data from HITEMP2010 [7]. Lines from all CO_2 isotopes available in the database were taken into account, making a total of 11,193,608 lines distributed in the spectral range from 0 to 12,785 cm^{-1}. Considering wavenumber values higher than 12,785 cm^{-1} did not affect the LBL solution. Thus, $\eta_{max}=12{,}785$ cm^{-1} was assumed for the FSK solutions. Although the choice of η_{max} affects the $g(\phi, k)$ distribution, the formulation consistence relies on the relation between k, F and g. Thus, provided that all non-negligible regions of the spectrum be considered, a value higher than 12,785 cm^{-1} can be arbitrarily chosen for η_{max} without affecting the FSK radiative heat transfer solution. Nevertheless, η_{max} can have an effect on the numerical convergence. Thus, it is not desirable to chose for η_{max} a value far beyond that considered for the line-by-line spectrum.

The non-dimensional wavenumber data points were obtained for the entire spectrum with Eq. (15). Table 1 presents some ALBDFs, F, and reordered absorption coefficients, k, obtained with $N=30$ non-dimensional wavenumber data points. This number of data points was selected based on a convergence analysis performed for three 1 m thick uniform slabs with the temperature and CO_2 mole fraction of each uniform region of the medium shown in Fig Fig. 4. For $N=30$ the error associated with the numerical discretization was lower than 0.5%, which is considerably smaller than errors associated with the correlated-k.

The F and k are presented in Table 1 as functions of the non-dimensional wavenumber, g, whose values are associated with specific spectral locations. Therefore, the dependence of F and k

with respect to g, indicates dependence with respect to spectral locations. For example, in line 29 of Table 1, $g=0.995$ is a fraction of the spectrum, as computed with Eqs. (11), and also is associated to the spectral locations where $k=17.47$ cm^{-1} crosses $\kappa_\eta(\phi_1)$. For truly correlated spectra these spectral locations are also the same where $k=17.78$ cm^{-1} crosses $\kappa_\eta(\phi_2)$ and $k=17.22$ cm^{-1} crosses $\kappa_\eta(\phi_3)$. For a real spectrum it is an assumption in the proposed formulation, which is different from that adopted in the traditional FSK.

The formulation without reference state simplifies the application of the FSK, because F and k can be written as functions of the independent parameter, g, since only local properties are considered while solving the RTE. In this case, the proposed formulation becomes fundamentally identical to the continuous limit of the Rank Correlated SLW (RC-SLW) model [2,31], and can be understood as the extension of the theoretical foundation of RC-SLW to the FSK method.

Differently, in the usual assumption, a reference state, ϕ_o, must be chosen, and a Planck function is computed using the reference temperature, T_o; the reordered absorption coefficients, k, are computed for every considered state using the local absorption coefficients, $\kappa_\eta(\phi)$, and reference Planck function evaluated at T_o; finally, the ALBDFs are computed for every state using the absorption coefficient of the reference state, $\kappa_\eta(\phi_o)$, and Planck functions evaluated at local temperature. The F and k computed with such a procedure can be associated to non-dimensional wavenumbers so that the reordered RTE resulting from the proposed formulation, Eq. (13), can be employed. However, in this case the proposed formulation is exactly equivalent to the traditional formulation, which uses F_o instead of g.

A third procedure which uses an assumption close to the traditional one was also considered. It does not require a reference temperature; however, it uses a reference state. In this case, the ALBDFs are computed for every state using the absorption coefficient of the reference state, $\kappa_\eta(\phi_o)$, and Planck functions evaluated at local temperature.

For simplicity, from now on the approach which does not require any reference state will be referred as FSK-1; the approach which does use a reference state, but not a reference temperature will be referred as FSK-2; while the traditional approach will be referred as FSK-3. Some of the F and k obtained for the FSK-2 and FSK-3 are presented respectively in Tables 2 and 3. The reference state was chosen as that of the region with higher temperature.

Tables 1 and 2 differ only on the value of F, which in the FSK-1 approach is computed using local absorption coefficients, while in the case of FSK-2, it is computed using the absorption coefficient of the reference state. On the other hand, Table 3 differs from Table 2 only on the value of k, and from Table 1 on both F and k. The k are slightly different in Table 3 because they are weighted from a

Table 1

Data points for the FSK-1 solution: non-dimensional wavenumber (g), ALBDF (F), and reordered absorption coefficient (k).

N	g	Region 1		Region 2		Region 3	
		$k(\phi_1, g)$ [cm^{-1}]	$F(T_1, g)$	$k(\phi_2, g)$ [cm^{-1}]	$F(T_2, g)$	$k(\phi_3, g)$ [cm^{-1}]	$F(T_3, g)$
1	0.0257	1.89×10^{-7}	8.59×10^{-6}	1.16×10^{-7}	1.55×10^{-3}	8.32×1^{-8}	3.55×10^{-3}
2	0.0772	2.09×10^{-7}	2.78×10^{-5}	1.28×10^{-7}	5.54×10^{-3}	9.27×10^{-8}	1.18×10^{-2}
3	0.1284	2.50×10^{-7}	8.03×10^{-5}	1.53×10^{-7}	1.13×10^{-2}	1.11×10^{-7}	2.31×10^{-2}
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
28	0.988	4.47	0.958	7.33	0.956	9.11	0.982
29	0.995	17.47	0.981	17.78	0.980	17.22	0.992
30	0.999	46.92	0.995	42.55	0.995	30.87	0.998

Table 2
Data points for the FSK-2 solution: non-dimensional wavenumber (g), ALBDF (F), and reordered absorption coefficient (k).

N	g	Region 1		Region 2		Region 3	
		$k(\phi_1, g)$ [cm^{-1}]	$F(T_1, g)$	$k(\phi_2, g)$ [cm^{-1}]	$F(T_2, g)$	$k(\phi_3, g)$ [cm^{-1}]	$F(T_3, g)$
1	0.0257	1.88×10^{-7}	6.99×10^{-6}	1.15×10^{-7}	5.51×10^{-4}	8.33×10^{-8}	3.54×10^{-3}
2	0.0772	2.09×10^{-7}	2.98×10^{-5}	1.28×10^{-7}	1.99×10^{-3}	9.27×10^{-8}	1.18×10^{-2}
3	0.1284	2.487×10^{-7}	8.16×10^{-5}	1.54×10^{-7}	4.30×10^{-3}	1.11×10^{-7}	2.31×10^{-2}
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
28	0.988	4.46	0.954	7.33	0.971	9.11	0.982
29	0.995	17.48	0.979	17.76	0.987	17.22	0.992
30	0.999	46.93	0.995	42.60	0.997	30.87	0.998

Table 3
Data points for the FSK-3 solution: non-dimensional wavenumber (g), ALBDF (F), and reordered absorption coefficient (k).

N	g	Region 1		Region 2		Region 3	
		$k(\phi_1, g)$ [cm^{-1}]	$F(T_1, g)$	$k(\phi_2, g)$ [cm^{-1}]	$F(T_2, g)$	$k(\phi_3, g)$ [cm^{-1}]	$F_o = F(T_3, g)$
1	0.0257	1.89×10^{-7}	6.99×10^{-6}	1.15×10^{-7}	5.51×10^{-4}	8.32×10^{-8}	3.54×10^{-3}
2	0.0772	2.11×10^{-7}	2.98×10^{-5}	1.28×10^{-7}	1.99×10^{-3}	9.27×10^{-8}	1.18×10^{-2}
3	0.1284	2.51×10^{-7}	8.16×10^{-5}	1.54×10^{-7}	4.30×10^{-3}	1.11×10^{-7}	2.31×10^{-2}
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
28	0.988	4.06	0.954	7.17	0.970	9.11	0.982
29	0.995	17.14	0.979	17.87	0.987	17.22	0.992
30	0.999	47.56	0.995	42.60	0.997	30.87	0.998

reference ALBDF, F_o, while in FSK-1 and FSK-2 the k are weighted from the non-dimensional wavenumber g. The data presented in Table 3 can be employed with the traditional formulation, using Eq. (7), or with the proposed formulation, using Eqs. (13), and g in place of F_o. In this case, both formulations provide exactly the same results.

Table 4 presents results for the heat flux to the left and right walls obtained with FSK-1, FSK-2, FSK-3 and line-by-line. The table also shows the error of the FSK results with respect to the line-by-line solution. As expected, the results obtained with any of the FSK approaches presented some difference as compared to the line-by-line solution. However, the differences between the FSK results themselves were small.

In this example, the medium was composed by three distinct uniform regions. Such a simple problem is well suited for explain the proposed formulation. However, in real radiation heat transfer discontinuities as those of the considered example are unlikely to occur.

The next example considers a medium with continuous temperature variation.

Table 4
Results of example problem 1: heat flux to the left and right walls obtained with FSK-1, FSK-2, FSK-3 and line-by-line, and the error of the FSK with respect to the line-by-line solution.

	Heat flux		Error relative to line-by-line	
	Left wall	*Right wall*	*Left wall*	*Right wall*
Line-by-line	- 25.75 kW	48.96 kW	–	–
FSK-1	- 23.49 kW	48.79 kW	4.61%	-0.33%
FSK-2	- 24.11 kW	48.80 kW	3.35%	-0.32%
FSK-3	- 24.39 kW	48.66 kW	2.78%	-0.61%

4.2. Example 2

This second example consists of a one-dimensional slab of medium confined between two parallel cold walls. The medium is composed of 10% CO_2 and presents the following temperature profile proposed by Tencer and Howell [25]:

$$T(x) = 1250\cos(x/L) \tag{18}$$

where T is given in Kelvin, and L is the distance between the walls and its value is 1 m.

The finite volume method was used for the numerical solution. The slab was divided into 33 non-equal sized uniform volumes. Each volume was associated to one temperature and a respective spectral absorption coefficient obtained from the HITEMP2010 database [7], considering a spectral interval from 0 to 12,785 cm^{-1}. The k and F were obtained for each volume using the approaches FSK-1, FSK-2 and FSK-3 described above.

Fig. 5 presents the divergence of the radiative heat flux obtained with the three FSK approaches and line-by-line, and Fig. 6 shows similar results for the radiative heat flux. As can be seen, the FSK results presented good agreement with the line-by-line solution. To visualize with more detail the differences between the three FSK approaches, Fig. 7 shows the error of the heat flux obtained with the FSK with respect to the line-by-line, which was normalized by the maximum value of the heat flux to avoid division by zero. The errors associated to all three approaches were relatively low, the maximum difference was about 2.8% for the simplest FSK-1 approach, and occurred in the cold region of the gas where the heat transfer is less significant.

For the considered example problems, results obtained with the FSK-1, FSK-2 and FSK-3 presented good agreement with each other, indicating that the FSK-1 can provide results with accuracy comparable to that associated to the traditional FSK-3, with the
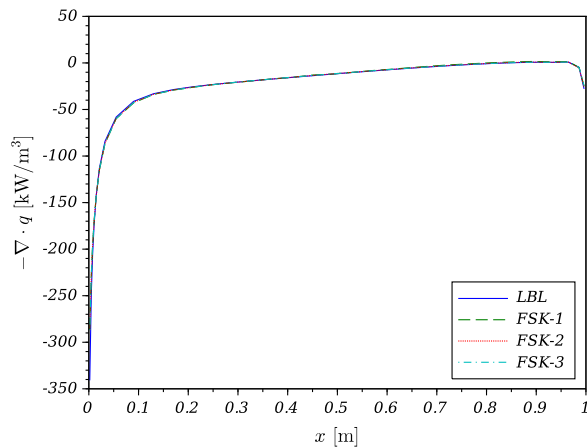
Fig. 5. Results of example problem 2: divergence of the radiative heat flux obtained with FSK-1, FSK-2, FSK-3 and line-by-line.
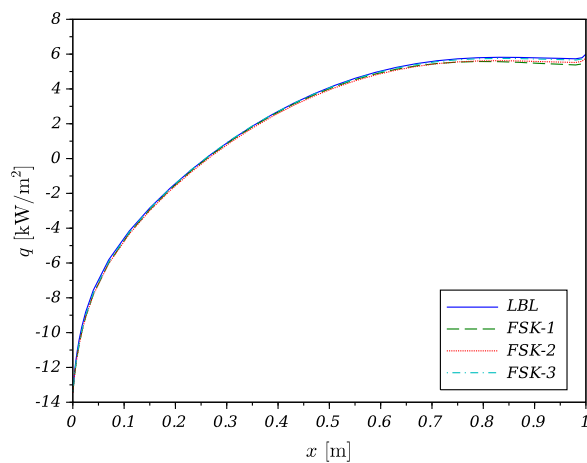

Fig. 6. Results of example problem 2: radiative heat flux obtained with FSK-1, FSK-2, FSK-3 and line-by-line.
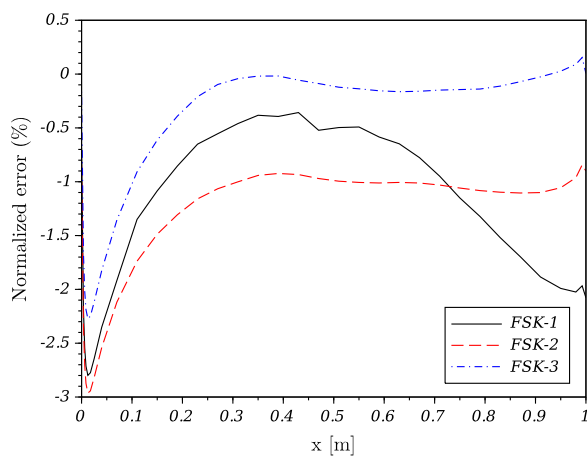

Fig. 7. Normalized error of the radiative heat flux obtained by FSK-1, FSK-2, FSK-3 approaches with respect to the line-by-line solution.

advantage of being significantly simpler, since it requires neither a reference temperature nor a reference state, and only local properties are considered.

5. Conclusions

A formulation for the full-spectrum k-distribution (FSK) which does not require the use of a reference blackbody temperature is presented. In place of a Planck function weighted reference cumulative k-distribution (or ALBDF of reference), the proposed formulation uses a cumulative k-distribution which is equivalent to fractions of a spectral interval, as in the original narrow band k-distribution, but extended over the entire spectrum. Such a cumulative k-distribution acts as a non-dimensional wavenumber and is independent of the state of the medium. This leads to some simplifications on the FSK equations: no arbitrary reference temperature is necessary, and the properties appearing in the reordered radiative transfer equation of the method are directly related to the non-dimensional wavenumber. The application of the proposed formulation was demonstrated through two example problems, where three different approaches regarding the use of the correlated-k were considered. The first one, referred as FSK-1, which corresponds to the continuous limit of the RC-SLW model, is the most well suited for applications with the proposed formulation and the simplest one, since it does not require any reference state, and only local properties are taken into account. The second approach uses a reference state, but not a reference temperature. The third approach uses a reference state and temperature falling into the case of the traditional FSK formulation.

Although the idea behind the FSK is apparently simple, the application of the method to solve problems involving nonuniform media can become complex, in part because of the implicit manner in which properties are related to spectral locations while solving the radiative transfer equation across different spatial locations at different states. Therefore, the proposed formulation can be very useful by simplifying the treatment of nonuniform media.

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