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Modeling the cumulative distribution of absorption coefficients of gases using the generalized *k*-moment method

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ABSTRACT

The generalized *k*-moment method is formulated in terms of Cutteridge–Devyatov polynomials (CDP). In this novel approach, the moments involved are spectral averages of integer powers of the logarithm of the absorption coefficient. The technique to obtain *k*-distributions from those generalized moments is detailed both theoretically and from a practical point of view. Its outputs are afterward assessed against reference data in several test cases of increasing complexity. Indeed, the first ones involve single lines in the Lorentz, Doppler and Voigt regimes. The most sophisticated situations investigated in this work concern applications of the method to high resolution LBL data for pure CO_2 at temperatures between 300 K and 2300 K and at atmospheric pressure. In any case, the CDP solution to the generalized *k*-moment problem is found to provide very accurate results. The present technique outperforms our previous approach to *k*-moment modeling of the cumulative distribution of absorption coefficients of gases that were based on first, second, first inverse and logarithmic moments, in all the situations investigated. Equations required to apply the model are provided in the paper, both over narrow bands and the full spectrum.

1. Introduction

Anyone who wants to solve a problem of radiative heat transfer in a gaseous medium has to manage two distinct challenging tasks [1]:

(i) The first one is related to the structure of the absorption spectra of gases. Indeed, gas–radiation interaction results from radiative transitions between energy levels of the molecules that are represented by spectral lines at high resolution. This problem can be solved accurately by the so-called Line-By-Line approach. Nevertheless, this technique is numerically too expensive to be applied in many situations. Consequently, approximate models are usually preferred in many applications. The choice of a particular model has to be done on the basis of the accuracy that one wants to reach and the calculation cost that one is ready to pay to achieve it. Several of them have been proposed during the past decades. Those models are based on spectral averaging techniques that can extend from a few cm^{-1}, as in narrow band models, up to the full spectrum [1,2].

(ii) The second one concerns the treatment of non-uniformities in terms of temperature and composition in the medium. Indeed, gaseous media usually encountered, whether they are related to heat transfer in planetary atmospheres or in combustion media, are rarely uniform (homogeneous and isothermal). This problem is complicated because gas spectra are

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Nomenclature

f	k-distribution, $(\mathrm{cm}^{-1})^{-1}$
g	cumulative k-distribution
$\overline{k}$	mean k value, $\mathrm{cm}^{-1}\,\mathrm{atm}^{-1}$
l_n, m_n	generalized k-moment at order n
L	uniform path length, cm
P	pressure, atm
T	temperature, K
T_P	blackbody weighting temperature, K
x	gas molar fraction

Greek symbols

κ_ν	spectral absorption coefficient, $\mathrm{cm}^{-1}\,\mathrm{atm}^{-1}$
ν	wavenumber, cm^{-1}
$\underline{\phi}$	composition variable, $\underline{\phi} = \{x \quad P \quad T\}$
$\Phi_p^{(n)}$	pth-Cutteridge–Devyatov polynomial for a maximum order n
τ	transmission function

Subscripts

b	blackbody weighted
max	maximum value
min	minimum value
ν	spectral

Superscript

$\Delta\nu$	spectral interval width, cm^{-1}

strongly dependent on the location in the medium via their local temperature and species concentrations. This, conjugated with the high resolution structure of gas spectra, makes any spectral averaging strategy delicate to apply in a general manner.

The aim of this paper is to propose a technique for the approximate modeling of cumulative k-distribution of gases, which is a key parameter in k-distributions approaches. This method was proposed in the 30s for modeling spectral gas radiation in astrophysics according to references in [1,2]. One of the first papers devoted to k-distribution methods and available in English language was, to our knowledge, proposed by Arking and Grossman [3] in 1972. Extensive theoretical works, specifically dedicated to this approach over narrow spectral bands, were conducted during the 90s, with a reference work due to Lacis and Oinas [4] for atmospheric studies, and several specific developments for applications at high temperatures [5].

The principle of k-distribution models is relatively straightforward. Indeed, the approach is founded on the fact that if one wants to estimate the gas radiative properties averaged over a band, the exact knowledge of the spectral absorption coefficient is not necessary: only information about the fraction of wavenumbers inside the band such that the absorption coefficient takes specific values is required. This quantity is usually called the k-distribution. It is defined as [1]

$$f_b^{\Delta\nu}(k) = \left(\int_{\Delta\nu} I_{b,\nu}(T_P)d\nu\right)^{-1}\left(\int_{\nu\in\Delta\nu \text{ such that } \kappa_\nu = k} I_{b,\nu}(T_P)d\nu\right) \tag{1}$$

in which index "b" indicates that the distribution is weighted by the Planck function $I_{b,\nu}(T_P)$ at temperature T_P. The choice of T_P is dependent on the problem treated (temperature at the boundaries or inside the medium). This issue is out of the scope of the present work. The transmission function of an homogeneous gaseous path in the medium, of length L with absorbing species partial pressure xP, averaged over $\Delta\nu$ is, in terms of the k-distribution, obtained as

$$\overline{\tau}_b^{\Delta\nu}(xPL) = \int_0^{+\infty} \exp(-xPL\times k) f_b^{\Delta\nu}(k)dk \tag{2}$$

Eq. (2) shows that the transmission function can be expressed as the Laplace transform of the k-distribution. The problem that we have to solve, as our objective is to estimate this distribution, is to calculate an inverse Laplace transform. Many mathematical techniques have been proposed to solve this problem. A compendium of the existing ones can be found in Ref. [6].

Commonly, the cumulative distribution $g_b^{\Delta\nu}(k)$ defined as

$$g_b^{\Delta\nu}(k) = \int_0^k f_b^{\Delta\nu}(k')dk' = \left(\int_{\Delta\nu} I_{b,\nu}(T_P)d\nu\right)^{-1} \times\left(\int_{\nu\in\Delta\nu \text{ such that } \kappa_\nu \le k} I_{b,\nu}(T_P)d\nu\right) \tag{3}$$

is introduced. This function is smoother than $f_b^{\Delta\nu}(k)$ and grows monotonically (which implies that its reciprocal exists). Using this new function, we can rewrite Eq. (2) as

$$\begin{aligned}\overline{\tau}_b^{\Delta\nu}(xPL) &= \int_0^{+\infty} \exp(-xPL\times k)dg_b^{\Delta\nu}(k)\\ &= \int_0^1 \exp(-xPL\times k(g_b^{\Delta\nu}))dg_b^{\Delta\nu}\end{aligned} \tag{4}$$

The integrals given by Eq. (4) can be estimated using numerical quadratures. Indeed, as $g_b^{\Delta\nu}(k)$ is invertible, we can write Eq. (4) in the following form:

$$\overline{\tau}_b^{\Delta\nu}(xPL) \approx \sum_{i=1}^{N} \omega_i \exp[-xPL\times k(g_i)] \tag{5}$$

where ω_i and g_i are the weights and abscissas of the quadrature. The new absorption coefficients involved in Eq. (5) are obtained as solutions of the set of implicit equations:

$$g_b^{\Delta\nu}[k(g_i)] = g_i \Leftrightarrow k(g_i) = \underbrace{(g_b^{\Delta\nu})^{-1}}_{\text{inverse function of } g_b^{\Delta\nu}}(g_i) \tag{6}$$

Generally, the use of quadratures with small orders N (typically from 10 to 20) is enough to provide highly