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A database for the SLMB modeling of the full spectrum radiative properties of CO_2

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ABSTRACT

Development and application of a database for the Spectral-Line Moment-Based (SLMB) modeling of the full spectrum radiative properties of mixtures of carbon dioxide and nitrogen is presented. The critical issue of the definition of a reference thermophysical condition is addressed together with the suggestion of a coherent and precise methodology to derive parameters of the model for any other configuration. The database is built accordingly from the CDSD-1000 high temperature spectroscopic databank for gas and blackbody-weighting temperatures in the range [300; 2700 K]. Accuracy of both the modeling and the database is assessed through comparisons with LBL results in terms of full spectrum *k*-distributions and emission functions. Results obtained from the application of FSK correlations and the Leckner's formula are also provided for extended analyses.

1. Introduction

Radiative transfer in molecular gases is an important heat exchange phenomenon in many high temperature systems such as engines, boilers, furnaces. The most reliable model for the radiative properties of gases is the line-by-line (LBL) model that, due to large computational requirements, cannot be applied for practical simulations involving complex 3D geometries and coupled heat transfer mechanisms. In these cases, approximate models are required. A comprehensive description of them can be found in Refs. [1,2].

Recently, the spectral-line moment-based (SLMB) model was proposed for the approximate evaluation of the radiative properties of gases [3]. It allows using any band width for the spectral averaging of gas properties, by application of the *k*-moment method [4] to reordered absorption coefficient spectra. On wide bands and for full spectrum modeling, the approach was demonstrated [3] to provide simple and accurate mathematical formulas: (1) for the blackbody-weighted transmission function (BTF) of uniform gaseous columns and (2) for the cumulative distribution function of the absorption coefficient. This work introduces a database for the SLMB modeling of the full spectrum radiative properties of mixtures of carbon dioxide and nitrogen for temperatures of gases and of the weighting Planck functions in the range [300; 2700 K]. It should be noticed that application of the model to non-homogeneous non-isothermal media, although out of the scope of the present paper, requires at least that spectral intervals over which blackbody-weighted moments are averaged together with path integration on the nonuniform gas columns, are strictly the same in any of the thermophysical conditions. Use of corresponding formulas provided in Ref. [5] would be appropriate provided the absorption coefficient is assumed scaled. Even if the present work is dedicated to uniform (homogeneous isothermal) gaseous media, this issue is anticipated and addressed by introducing a

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Nomenclature

l	column length (cm)
P	pressure (atm)
T	temperature (K)
x	molar fraction of radiating molecular specie

Greek symbols

ε	emissivity
ϕ	composition variable
v	wavenumber (cm^{-1})
σ	Stefan–Boltzmann constant ($=5.670\times10^{-8}$ W/m^2K^4)
τ	transmissivity

Subscripts

b	blackbody and blackbody-weighted
P	Planck weighting
g	gas

Superscripts

ref	reference

reference thermophysical condition to provide a fixed discretization of the spectral space to be used in any other condition.

The paper is organized as follows: the full spectrum SLMB model, mathematically formulated according to a reference thermophysical condition, is presented in Section 2. Parameterization associated with the building of a database and resulting theoretical formulas is given and applied to line-by-line data in Section 3. Parameters are then employed for the approximate calculation of radiative properties of carbon dioxide and nitrogen mixtures in the results and discussion section. Comparisons against several models from the literature demonstrate the quality of both the full spectrum SLMB modeling and the database.

2. Formulation of the full spectrum SLMB modeling with a reference thermophysical condition

This part relies heavily on previously published results. The interested reader may refer to Refs. [3,4] for comprehensive information about the SLMB modeling details and assumptions.

As specific difference with formerly released material about the model, we introduce a thermophysical condition, called "reference", given by the state vector $\underline{\phi}^{ref}$ whose components are the absorbing and emitting gas molar fraction x, the total gas pressure P and its temperature T_g. In this "reference" condition, the pressure-based spectral absorption coefficient of the gas $\kappa_v(\underline{\phi}^{ref})$, takes values that are comprised between a minimum, $k_{\min}(\underline{\phi}^{ref})$, and a maximum, $k_{\max}(\underline{\phi}^{ref})$. The interval $[k_{\min}(\underline{\phi}^{ref});k_{\max}(\underline{\phi}^{ref})]$ can be divided into N smaller intervals of $\kappa_v(\underline{\phi}^{ref})$ values, $[\tilde{k}_{i-1}(\underline{\phi}^{ref});\tilde{k}_i(\underline{\phi}^{ref})]$, $i=1,N$, so that $\cup_{i=1,N}[\tilde{k}_{i-1}(\underline{\phi}^{ref});\tilde{k}_i(\underline{\phi}^{ref})]=[k_{\min}(\underline{\phi}^{ref});k_{\max}(\underline{\phi}^{ref})]$ where $\tilde{k}_0(\underline{\phi}^{ref})=k_{\min}(\underline{\phi}^{ref})$ and $\tilde{k}_N(\underline{\phi}^{ref})=k_{\max}(\underline{\phi}^{ref})$. From this discretization of $[k_{\min}(\underline{\phi}^{ref});k_{\max}(\underline{\phi}^{ref})]$, it is possible to derive another one for the full spectrum $\mathbb{R}^+=[0;+\infty[$ into N+1 bands $\Delta v(i,\underline{\phi}^{ref})$, $i=0,\ldots,N$ such that for each wavenumber $v\in\Delta v(i,\underline{\phi}^{ref})$, we have $\kappa_v(\underline{\phi}^{ref})\in[\tilde{k}_{i-1}(\underline{\phi}^{ref});\tilde{k}_i(\underline{\phi}^{ref})]$, and $\kappa_v(\underline{\phi}^{ref})=0$ (transparency regions of the gas absorption spectrum) if $v\in\Delta v(0,\underline{\phi}^{ref})$.

The reference thermophysical condition does not have the same meaning as the usually encountered one, and should not be confused with it. In fact, the "reference" condition is generally introduced to correlate absorption spectra associated with different thermophysical conditions, which requires solving systems of implicit equations (see Ref. [1] for examples and justifications). In the present work, it essentially provides a way to define a discretization of the wavenumber space, which is set identical for any thermophysical condition. Such a predetermined reference spectral grid cannot be avoided to be able to calculate moments over spectral bands of the path-integrated absorption coefficient, which are required for BTFs evaluations in nonuniform media [5].

If we now consider a gas in a thermophysical state different from the reference one ($\underline{\phi}\neq\underline{\phi}^{ref}$), the full spectrum transmission function of a uniform column (of length l) of the gas weighted by the Planck distribution of blackbody intensity at a temperature T_P, defined by

$$\tau(l,T_P,\underline{\phi})\frac{\sigma T_P^4}{\pi}=\int_0^{+\infty}e^{-xPlk_v(\underline{\phi})}I_{b,v}(T_P)\,dv=\sum_{i=0}^{N}\int_{\Delta v(i,\underline{\phi}^{ref})}e^{-xPlk_v(\underline{\phi})}I_{b,v}(T_P)\,dv \quad (1)$$

can be approximated, on the basis of the previously defined spectral discretization, as

$$\tau(l,T_P,\underline{\phi})=a_0(T_P,\underline{\phi}^{ref})+\sum_{i=1}^{N}a_i(T_P,\underline{\phi}^{ref})\bar{\tau}_{b,v}^{\Delta v(i,\underline{\phi}^{ref})}(l,T_P,\underline{\phi}) \quad (2)$$

where we have introduced the following coefficients:

$$a_i(T_P,\underline{\phi}^{ref})=a[T_P,\tilde{k}_{i-1}(\underline{\phi}^{ref}),\tilde{k}_i(\underline{\phi}^{ref})]=\frac{\pi}{\sigma T_P^4}\int_{\Delta v(i,\underline{\phi}^{ref})}I_{b,v}(T_P)\,dv \quad (3)$$