Pergamon

Int. J. Heat Mass Transfer. Vol. 40, No. 4, pp. 987–991, 1997

0017–9310/97 $17.00+0.00

PII: S0017–9310(96)00129–9

TECHNICAL NOTE

High temperature gas radiative property parameters of statistical narrow-band model for H_2O, CO_2 and CO, and correlated-K model for H_2O and CO_2

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(*Received* 13 *December* 1994 *and in final form* 2 *April* 1996)

1. INTRODUCTION

The aim of this technical note is to present some gaseous radiative property data which have been obtained at EM2C laboratory and which are available on a floppy disk. These data, i.e. the parameters of statistical narrow-band (SNB) and correlated-K (CK) models, are useful for accurate calculation of radiative transfer in gases at high temperature. They may also serve as a basis for benchmark comparisons between various methods for the resolution of radiative transfer problems in gases.

The parameters have been obtained theoretically. In a first step, high temperature approximate spectroscopic databases have been generated for H_2O [1] and CO_2 [2]. They include all the lines of HITRAN 92 [3], those of Flaud *et al.* [4] for H_2O near 2.7 μm, and generated lines which significantly contribute to absorption and emission at temperatures up to 2500 K. Details related to comparison with experiments and to the conditions of validity of these databases are given in refs. [1, 2]. In a second step, the model parameters described here have been obtained from the previous spectroscopic databases by using line-by-line (LBL) calculations. In the case of CO, SNB parameters have been calculated from the spectroscopic data of refs. [5, 6].

2. STATISTICAL NARROW-BAND MODEL PARAMETERS

It has been shown [7] that the most accurate statistical model for the species considered here is the random model with the S^{-1}-exponential-tailed distribution of line intensities due to Malkmus [8]. When using this model in the conditions of Lorentz line shapes, the transmissivity averaged over a $\Delta\nu$ wide spectral interval of a homogeneous and isothermal column of length l (in cm), total pressure p (in atm), and molar fraction x in the considered absorbing gas, is

$$\bar{\tau}^{\Delta\nu} = \exp\left[-2\frac{\bar{\gamma}}{\bar{\delta}}\left(\sqrt{1+xplk\frac{\bar{\delta}}{\bar{\gamma}}}-1\right)\right]. \quad (1)$$

In this expression k (in $\mathrm{cm}^{-1}\ \mathrm{atm}^{-1}$), $1/\bar{\delta}$ (in cm) and γ (in cm^{-1}) are the model parameters. The parameter γ is a typical collisional half-width of the lines of the absorbing gas. The chosen expressions of γ (in cm^{-1}), resulting from a bibliographical survey, are

$$\gamma_{CO_2} = \frac{p}{p_S}\left(\frac{T_S}{T}\right)^{0.7}[0.07x_{CO_2}+0.058(1-x_{CO_2}-x_{H_2O})+0.1x_{H_2O}]$$

$$\gamma_{H_2O} = \frac{p}{p_S}\left\{0.462x_{H_2O}\left(\frac{T_S}{T}\right)+\left(\frac{T_S}{T}\right)^{0.5}\times[0.079(1-x_{CO_2}-x_{O_2})+0.106x_{CO_2}+0.036x_{O_2}]\right\}$$

$$\gamma_{CO} = \frac{p}{p_S}\left\{0.075x_{CO_2}\left(\frac{T_S}{T}\right)^{0.6}+0.12x_{H_2O}\left(\frac{T_S}{T}\right)^{0.82}+0.06\left(\frac{T_S}{T}\right)^{0.7}(1-x_{CO_2}-x_{H_2O})\right\} \quad (2)$$

with p_S and T_S equal to 1 atm and 296 K, respectively. For each spectral range, the remaining parameters k and $1/\bar{\delta}$ (related to CO_2, H_2O and CO) depend in a first approximation only on temperature T. They are tabulated for a set of spectral intervals, 25 cm^{-1} wide and characterized by a significant absorption. The considered temperatures and spectral ranges are 300–2900 K and 150–9300 cm^{-1}, respectively.

In practice, the procedure used to calculate the parameters k and $1/\bar{\delta}$ consists of line-by-line (LBL) computing of the transmissivities for various optical depths and extracting the parameters from a least-square fit of the transmissivity curve. For given mixture composition, temperature and spectral range, the parameter k is adjusted in optically thin conditions and $1/\bar{\delta}$ is then obtained by using a nonlinear least-square fitting in which column lengths are chosen such that the transmissivity averaged over $\Delta\nu$ takes the values 0.02, and 0.05–0.95 with an increment of 0.05. This procedure based on the adjustment of the curves of growth has been preferred to the use of the parameter definitions (see for instance ref. [7]) since it reduces the errors inherent to the assumptions made in SNB models as illustrated in Fig. 1.

SNB parameters have been generated with a constant 25 cm^{-1} spectral resolution. It has been shown in ref. [9] that this width is sufficiently narrow to assume a constant Planck function inside each band for a given temperature in the range 300–2500 K. This resolution may be easily downgraded using an adjustment procedure similar to that described above applied to averaged transmissivities calculated from the parameters with $\Delta\nu = 25\ \mathrm{cm}^{-1}$.

For nonisothermal and nonhomogeneous columns, the simple Curtis–Godson approximation [10] is often convenient for heat transfer applications [7]. In the case of a mixture of gaseous species absorbing in the same spectral range, the transmissivity averaged over $\Delta\nu$ of a mixture col-

umn is approximated to a good accuracy as the product of the averaged transmissivities of the different absorbing species. Correlation effects between absorption spectra of different species are negligible. The extension of the SNB model to the Voigt line régime has been undertaken in some studies. A bibliographical survey may be found in ref. [11], where the results of such an approach are compared with those of LBL and CK calculations.

3. CK MODEL PARAMETERS

The CK model parameters related to absorption by CO_2 or H_2O have been here only generated for applications at atmospheric pressure in the temperature range 300–2500 K. The transmissivity averaged over $\Delta\nu$ of a nonisothermal and nonhomogeneous gas column, dicretized into N isothermal and homogeneous elements m, of length l_m (in cm), is obtained by using a seven-point quadrature (the same for all the $\Delta\nu$ intervals) [9, 12]:

$$\bar{\tau}^{\Delta\nu} = \sum_{j=1}^{7} \omega_j \exp\left(-\sum_{m=1}^{N} k_{mj} l_m\right). \tag{3}$$

The weights ω_j associated with the different quadrature points j are, by increasing j, 0.045, 0.245, 0.32, 0.245, 0.0561111111, 0.051248583, 0.037640306. The accuracy of this quadrature has been discussed in ref. [12]. For each element m, the k_{mj} are pseudo-absorption coefficients given by

$$k_{mj} = x p_S [TQ(T)]^{-1} k^*_{mj} \tag{4}$$

where $Q(T)$ is the partition function of the absorbing molecule, adjusted by Gamache *et al.* (private communication) [13] for CO_2 and H_2O. The quantities k^*_{mj} (in $cm^{-1}\ atm^{-1}\ K$) are the parameters of the CK model. In the case of CO_2, they practically do not depend on x_{CO_2} and are only tabulated vs T. In the case of H_2O they are also tabulated vs x_{H_2O}. These parameters have been obtained for the set of 16 temperature values, i.e. 300, 375, 425, 500, 600, 700, 800, 900, 1100, 1300, 1500, 1700, 1900, 2100, 2300, 2500 K and the set of five x_{H_2O} values, i.e. 10^{-2}, 10^{-1}, 0.4, 0.66, 1. A linear interpolation both for T and x_{H_2O} is generally convenient. The CK parameters have been generated with a variable width $\Delta\nu$ of spectral bands in such a manner that the relative variations of the spectral equilibrium intensity inside a band remain less than four percent for the whole considered temperature range.

More details related to the quality of the CK approach and to the implementation of the CK method, particularly in the case of mixtures of gases absorbing in the same spectral region, are given in refs. [9, 12]. Neither CK nor SNB models are convenient for long-range sensing applications related to absorption of radiation emitted by a hot gaseous column by a long atmospheric cold column. In this case, accurate results are obtained by using the ckfg approach [11, 12, 14].

4. EXAMPLES OF RESULTS

Typical comparisons between transmissivities calculated using SNB, CK and LBL approaches are given here for homogeneous and isothermal columns in order to illustrate the accuracy of the parameters generated in this study. High resolution LBL results have been convolved with a rectangular $\Delta\nu$ wide window to enable relevant comparisons with approximate model results. The absolute differences between the transmittivities issued from SNB or CK models and those from the LBL approach are also plotted. Figures 2 and 3 are related to the SNB parameters for H_2O and CO_2, respectively. Figures 4 and 5 are related to CK parameters. The temperature and molar fraction conditions of these figures do not belong to the set of conditions used to generate model parameters. Simple linear interpolations have been used. For the uniform considered conditions, a good agreement is observed for all the spectrum, both for SNB and CK methods. It is worth noticing that for uniform conditions, the approximations used in the CK approach are related to

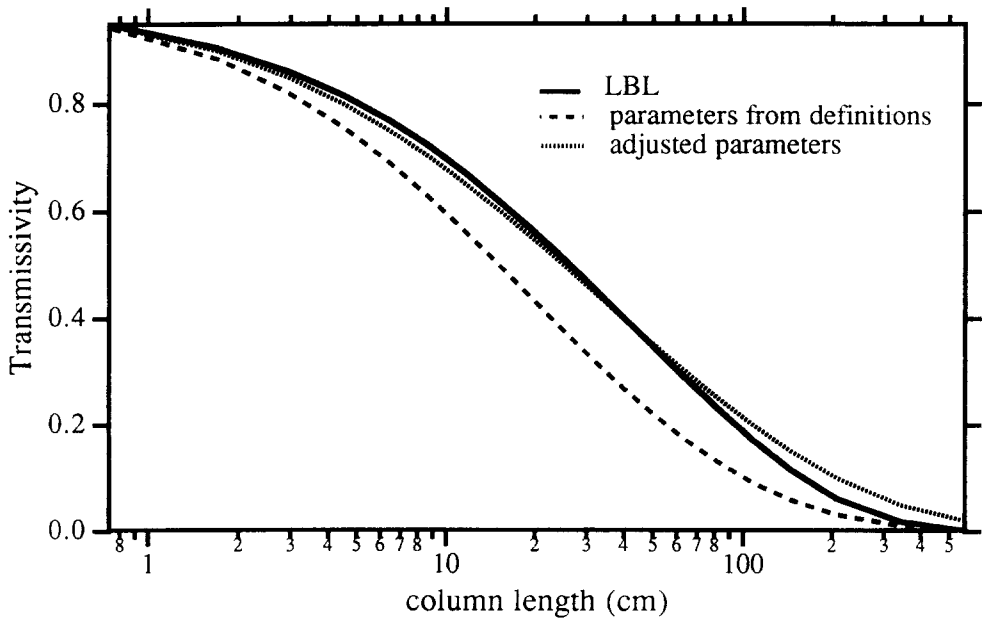

Fig. 1. Curves of growth of the transmissivity averaged over a spectral range, 25 cm^{-1} wide, centered at 675 cm^{-1}, vs the column length. SNB curves are obtained using both adjusted parameters and parameters calculated from their definitions; $T = 240$ K, $p = 1$ atm, $x_{CO_2} = 0.01$, $x_{N_2} = 0.99$.

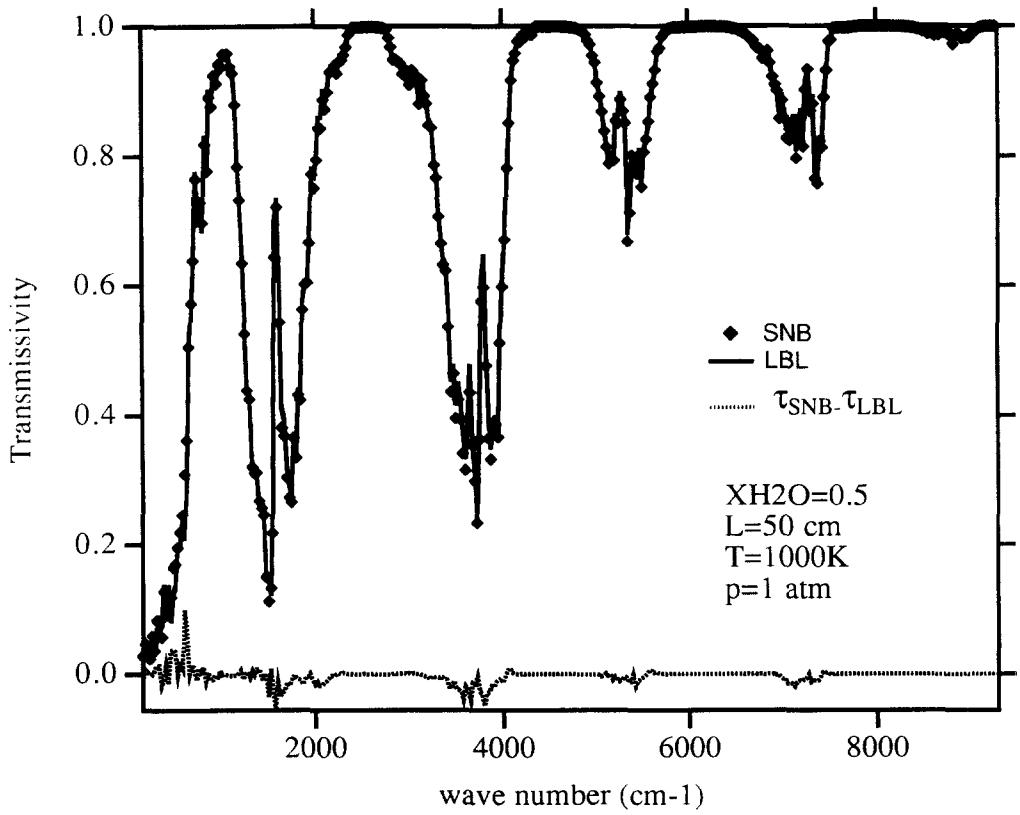

Fig. 2. Transmissivity of an isothermal and homogeneous column of a H_2O–N_2 mixture; spectral resolution equal to 25 cm^{-1}.

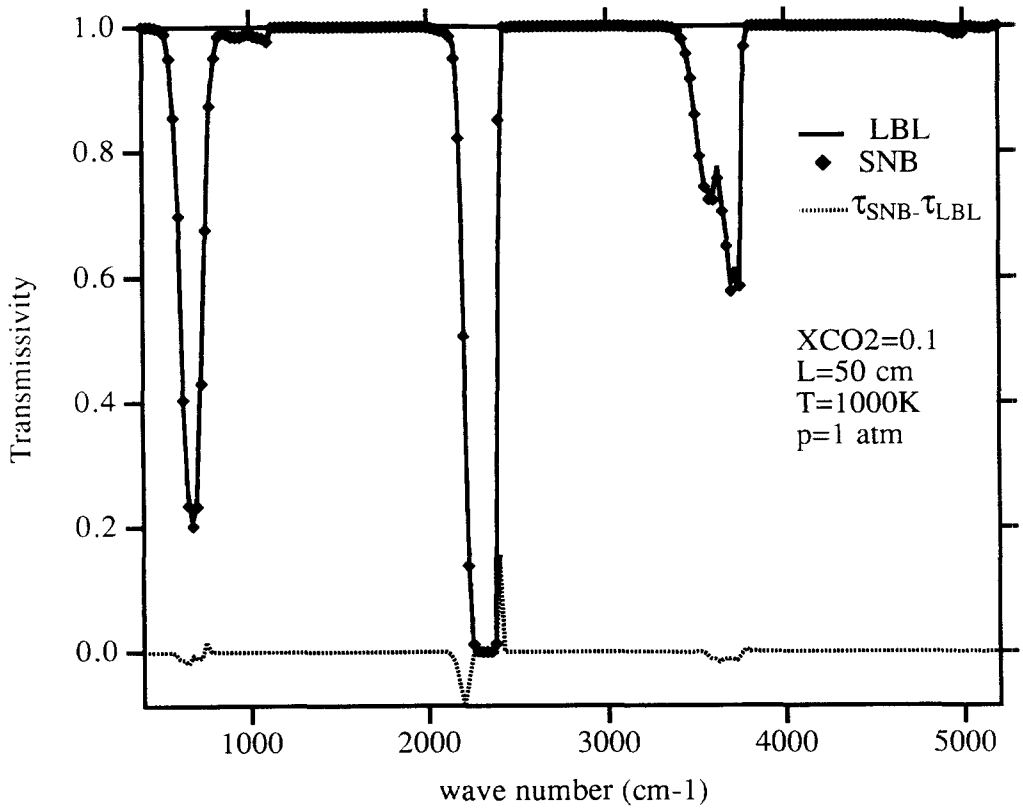

Fig. 3. Transmissivity of an isothermal and homogeneous column of a CO_2–N_2 mixture; spectral resolution equal to 25 cm^{-1}.

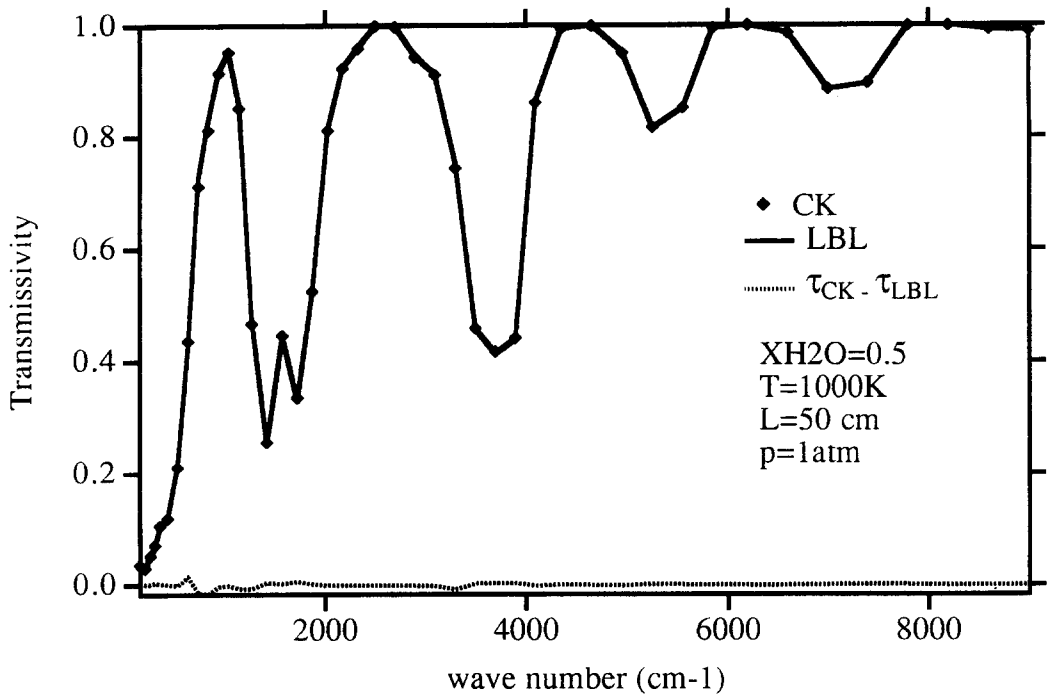

Fig. 4. Transmissivity of an isothermal and homogeneous column of a H_2O–N_2 mixture, variable spectral resolution (the same as for CK parameters).

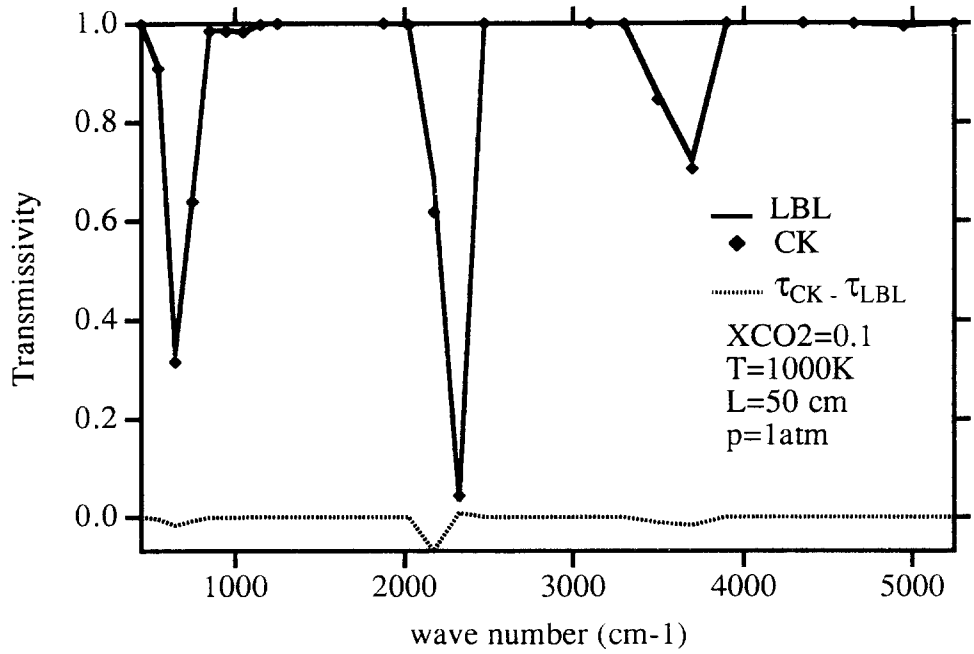

Fig. 5. Transmissivity of an isothermal and homogeneous column of a CO_2–N_2 mixture, variable spectral resolution (the same as for CK parameters).

the integration quadrature and to the temperature and molar fraction interpolations. Results from the CK approach seem then to be slightly more accurate than those from the SNB model. The treatment of nonuniform columns requires of course further approximations which reduce the accuracy of the models. These approximations have been studied in refs. [7, 10, 12] for SNB models and in refs. [9, 11, 12] for the CK model.

Acknowledgements—The authors acknowledge the contributions of Stéphane Langlois, Laurent Pierrot, Philippe Rivière, Laurence Rosenmann and Dragos Scutaru, particularly for generation of the spectroscopic databases. This study has been supported in part by the 'Fonds de la Recherche Technologique' of the French 'Ministère de la Recherche et de la Technologie'.

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