

# Engineering correlations for full spectrum $k$ -distribution of H<sub>2</sub>O from the HITEMP spectroscopic databank

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## Introduction

Radiative transfer in gases is significant in many applications like combustion systems or modeling atmospheric processes. Line-by-line calculations using spectral databases yield the highest accuracy possible, but are computationally very expensive. Hence, one needs to resort to more efficient and less computationally intensive methods, which—while less accurate than the line-by-line calculations—are considerably faster and yet sufficiently accurate for most engineering applications.

The cumulative full-spectrum  $k$ -distribution  $g(T_p, T_g, p, x; k)$ , or rather its inverse  $k(T_p, T_g, p, x; g)$  [1] is used by today's sophisticated spectral solution methods, like the Spectral-Line-Based Weighted-Sum-of-Gray-Gases (SLW) [2–6], the Absorption-Distribution-Function (ADF) [7, 8], and the Full-Spectrum  $k$ -Distribution (FSK) [9–11]. While  $k$ -distribution methods are very accurate, and offer tremendous cpu savings over line-by-line calculations, their assembly from high-resolution databases (like HITRAN [12] and HITEMP [13]) can prove rather tedious, making them out of reach for most simple engineering calculations. To allow efficient determination of full-spectrum  $k$ -distributions Denison and Webb [14–16] proposed simple correlations for H<sub>2</sub>O and CO<sub>2</sub>. However, their correlations were based on the outdated HITRAN92 [12] database, combined with some early extrapolation of their own for higher temperatures. This note provides a replacement of the correlation for water vapor based on the new and more accurate HITEMP database [13] considered reliable for temperatures up to at least 1000 K.

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## Mathematical Formulation

The  $k$ -distributions are obtained by reordering the spectrally varying absorption coefficient into a monotonically increasing function. This has been described in detail in the original papers by Modest and Zhang [1, 9, 10]. Mathematically, such full-spectrum  $k$ -distributions are defined as

$$f(T_p, T_g, p, x; k) = \frac{1}{I_b} \int_0^\infty I_{b\eta}(T_p) \delta(k - \kappa_\eta) d\eta, \quad (1)$$

where the Planck-function temperature  $T_p$  dependence comes through the black-body intensity  $I_{b\eta}$ ; the state of the gas appears through the absorption coefficient  $\kappa_\eta(T_g, p, x; \eta)$ , which is a function of gas temperature  $T_g$ , absolute pressure  $p$ , mole-fraction  $x$  and wavenumber  $\eta$ .

For RTE solutions the cumulative full-spectrum  $k$ -distribution is used, defined by

$$g(T_p, T_g, p, x; k) = \int_0^k f(T_p, T_g, p, x; k) dk = \frac{1}{I_b} \int_0^\infty I_{b\eta}(T_p) H(k - \kappa_\eta) d\eta, \quad (2)$$

where  $H(k - \kappa_\eta)$  is the Heaviside unit step function. Physically,  $g$  is the Planck-function-weighted fraction of the spectrum over which the absorption coefficient  $\kappa_\eta < k$ . Following Denison and Webb [14] we propose the following correlations,

$$g(T_p, T_g, p = 1\text{bar}, x = 0; k) = \frac{1}{2} \tanh[P(T_p, T_g, p = 1\text{bar}, x = 0; k)] + \frac{1}{2}, \quad (3a)$$

with  $P$  given by

$$P(T_p, T_g, p = 1\text{bar}, x = 0; k) = \sum_{l=0}^3 \sum_{m=0}^3 \sum_{n=0}^3 a_{lmn} \left[ \frac{T_g}{T_{ref}} \right]^n \left[ \frac{T_p}{T_{ref}} \right]^m \left[ \log_{10} \left( \frac{k}{k_{ref}} \right) \right]^l \quad (3b)$$

where  $T_{ref}=1000$  K,  $k_{ref}=1 \text{ cm}^{-1}\text{bar}^{-1}$  are reference values for temperature and pressure-based absorption coefficients, and the  $a_{lmn}$  are parameters to be found from a least-mean-square-error fit. As indicated, equation (3) is valid for air-broadening only (mole-fraction of  $\text{H}_2\text{O}$ ,  $x = 0$ ) and, since water vapor is a strong self-broadener, equation (3) needs to be modified to account for the different broadening in the presence of substantial amounts of water-vapor ( $x > 0$ ). While this can be done in a number of ways, we note that for a fixed value of the cumulative  $k$ -distribution,  $g$  (and thus for a fixed  $P$ ), the corresponding absorption coefficient  $k$  is a function of  $x$  (as well as  $T_p$  and  $T_g$ ). Therefore, if for a certain value of  $k$  and  $x$  we can find the value of  $k_0 = k(x = 0)$  corresponding to the same  $g$ -value, we can use equation (3) directly. The relationship between  $k$ ,  $x$  and  $k_0$  (with both  $k$  and  $k_0$  evaluated at the same  $g$ ) is shown in Fig. 1 for several different conditions. It is seen from Fig. 1 that, for large values of  $k$  (i.e., those most important in heat transfer calculations), there is essentially no dependence on Planck function temperature  $T_p$ . Through numerical experimentation it was found that the following series (independent of  $T_p$ ) adequately represents the relationships between  $x$ ,  $k(x)$  and  $k_0$  (evaluated at identical  $g$ ):

$$\log_{10} \left( \frac{k_0}{k_{ref}} \right) = \log_{10} \left( \frac{k}{k_{ref}} \right) + \sum_{l=0}^2 \sum_{m=0}^2 \sum_{n=0}^1 b_{lmn} \left[ \log_{10} \left( \frac{k}{k_{ref}} \right) \right]^n [x]^{m+1} \left[ \frac{T_g}{T_{ref}} \right]^l, \quad (4)$$

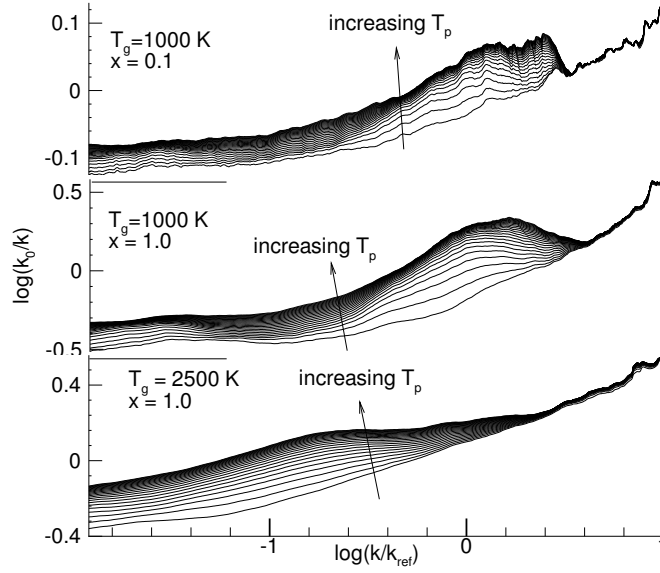


Figure 1: Variation of  $k(x)$  vs.  $k_0$  at identical cumulative  $k$ -distribution value  $g$ .

with the coefficients  $b_{lmn}$  obtained by a least-square fit over all databased values of  $k$  (23 temperatures each for  $T_p$  and  $T_g$  between 300 K and 2500 K, 6 mole-fractions  $x$  between 0 and 1.0, and 2000 values for  $g$ ). Note that the form of equation (4) has been chosen to be explicit in  $k_0$  [but implicit in  $k(x)$ ]. This allows for direct substitution of equation (4) into equation (3): If absorption coefficient  $k$  and mole-fraction  $x$  are freely chosen, equation (4) provides the corresponding  $k_0(k, x)$  (for the same  $g$ ), and

$$g(T_p, T_g, p = 1\text{bar}, x; k) = \frac{1}{2} \tanh[P(T_p, T_g, p = 1\text{bar}, x; k)] + \frac{1}{2}, \quad (5a)$$

with  $P$  given by

$$P(T_p, T_g, p = 1\text{bar}, x; k) = \sum_{l=0}^3 \sum_{m=0}^3 \sum_{n=0}^3 a_{lmn} \left[ \frac{T_g}{T_{ref}} \right]^n \left[ \frac{T_p}{T_{ref}} \right]^m \left[ \log_{10} \left( \frac{k_0(T_g, k, x)}{k_{ref}} \right) \right]^l. \quad (5b)$$

With the coefficients  $b_{lmn}$  in equation (4) already determined, the coefficients  $a_{lmn}$  were determined in a similar least-square fit using the same databased values. The correlation coefficients  $a_{lmn}$  and  $b_{lmn}$  are listed in Tables 1 and 2 respectively, and some representative  $k$ -distributions built from the correlation, plotted together with exact ones, are shown in Figures 2 and 3. Shown are  $k$ -distributions for two gas temperatures, 500K and 1000K, four different values of Planck-function temperature for each gas temperature; in Fig. 2 a vanishingly small amount of  $\text{H}_2\text{O}$  is considered ( $x=0$ ), while Fig. 3 is for pure water vapor ( $x=1$ ). From the plots it can be seen that the correlation approximates the  $k$ -distributions more closely at higher  $k$  values than at lower ones. This is because more weight has been given to higher  $k$  values (due to their importance in heat transfer calculations) during the fitting process. The importance of this will become more apparent when the accuracy of the correlations is demonstrated by solving some heat transfer problems.

Table 1:  
Correlation coefficients  $a_{lmn}$  appearing in equation (5) ( $T_{ref}=1000\text{K}$ ,  $k_{ref}=1\text{cm}^{-1}\text{bar}^{-1}$ ).

|           | $l$ | $m \setminus n$ | 0           | 1           | 2            | 3            |
|-----------|-----|-----------------|-------------|-------------|--------------|--------------|
| $d_{lmn}$ | 0   | 0               | 1.172739    | -0.792337   | 0.45678      | -6.7356E-02  |
|           |     | 1               | 0.88261     | 3.3022      | -2.048       | 0.394137     |
|           |     | 2               | -0.28465    | 1.6339      | 1.09924      | -0.20874     |
|           |     | 3               | 5.2641E-02  | 0.26822     | -0.18706     | 3.5073E-02   |
|           | 1   | 0               | 0.27995     | 0.527055    | -0.43156     | 0.13503      |
|           |     | 1               | 1.31104     | -1.3535E-02 | 2.39465E-02  | -3.7574E-02  |
|           |     | 2               | -0.61658    | -8.1576E-02 | 0.15935      | -2.2954E-02  |
|           |     | 3               | 0.10234     | 1.70129E-02 | -3.84058E-02 | 6.51758E-03  |
|           | 2   | 0               | 8.6277E-02  | 0.34948     | -0.20189     | 5.5391E-02   |
|           |     | 1               | 0.31365     | -1.06025    | 0.857        | -0.17833     |
|           |     | 2               | -0.136779   | 0.5768      | -0.48058     | 9.1345E-02   |
|           |     | 3               | 2.007E-02   | -9.727E-02  | 8.1344E-02   | -1.14502E-02 |
| 3         | 0   | 5.5203E-02      | -9.0309E-02 | 0.22803     | -5.04129E-02 |              |
|           | 1   | -2.64678E-02    | -6.3565E-02 | -0.13107    | 3.717E-02    |              |
|           | 2   | 1.333E-02       | 6.7414E-02  | 2.5817E-02  | -1.325E-02   |              |
|           | 3   | -2.5024E-03     | -1.3749E-02 | -1.4234E-03 | 1.9916E-03   |              |

Table 2:  
Correlation coefficients  $b_{lmn}$  appearing in equation (4) ( $T_{ref}=1000\text{K}$ ,  $k_{ref}=1\text{cm}^{-1}\text{bar}^{-1}$ ).

|           | $l$ | $m \setminus n$ | 0            | 1            |
|-----------|-----|-----------------|--------------|--------------|
| $b_{lmn}$ | 0   | 0               | -0.89871     | 0.539        |
|           |     | 1               | 1.0116       | -0.58957     |
|           |     | 2               | -0.48279     | 0.2747       |
| 1         | 0   | 0               | 1.0985       | -5.829E-02   |
|           |     | 1               | -1.0454      | 0.11542      |
|           |     | 2               | 0.4717       | -5.623E-02   |
| 2         | 0   | 0               | -0.22529     | -6.06033E-03 |
|           |     | 1               | 0.18432      | -1.6727E-02  |
|           |     | 2               | -7.69132E-02 | 1.035E-02    |

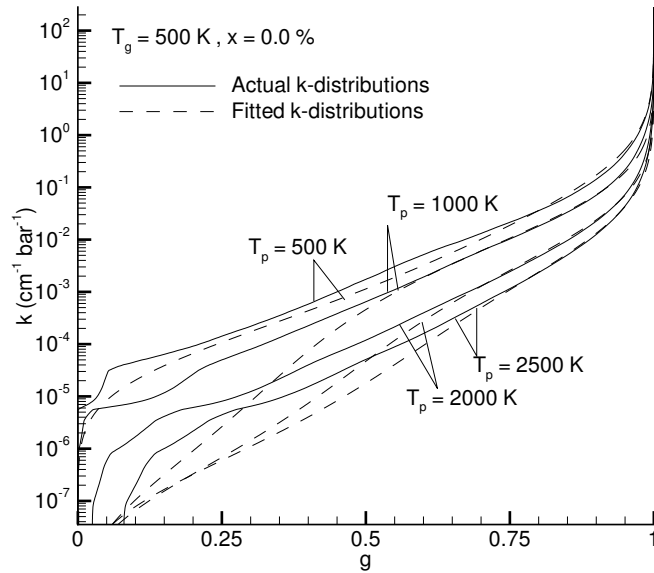


Figure 2: Actual and Fitted full-spectrum  $k$ -distribution functions for  $\text{H}_2\text{O}$  calculated at a fixed gas temperature of 500K and  $x=0$ , for different Planck function temperatures.

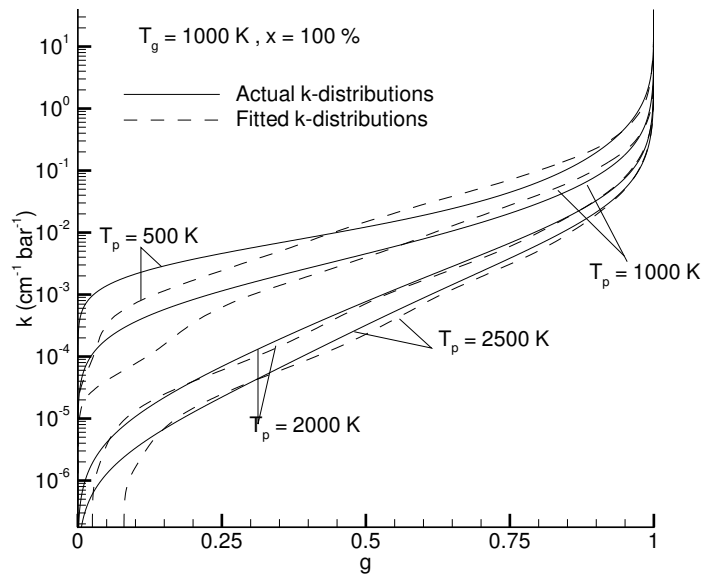


Figure 3: Actual and approximate full-spectrum  $k$ -distribution functions for  $\text{H}_2\text{O}$  calculated at a fixed gas temperature of 1000K and  $x=1.0$ , for different Planck function temperatures.

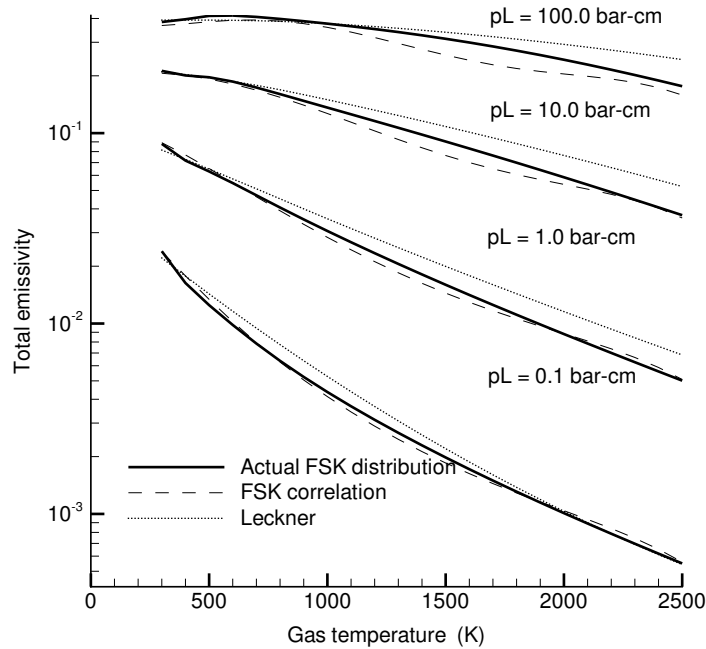


Figure 4: Total emissivities for different pressure path lengths from Leckner’s correlation, direct calculations from HITEMP and from the present correlation.

As a first test of the correlations their resulting cumulative  $k$ -distributions are used to calculate the total emissivity of isothermal  $\text{H}_2\text{O}-\text{N}_2$  mixtures. Figure 4 shows total emissivities obtained directly from the HITEMP database (using LBL or, equivalently, FSK calculations), from the present correlation and from Leckner’s correlation [17], which is based on (somewhat dated) experimental data. As can be seen, the maximum error between emissivities calculated using the  $k$ -distributions and those from the correlation never exceeds about 20%, while the maximum discrepancy between Leckner’s formula and those from the present correlation never exceeds about 35%. Above 1000K, HITEMP results are consistently smaller than those from Leckner’s correlation indicative of missing “hot lines” in HITEMP.

Next, the Planck-mean absorption coefficients, plotted in Fig. 5 for all the 23 temperatures, shows a maximum error of around 5% except near 300K, i.e., a temperature with little importance in combustion applications.

Two simple one-dimensional heat transfer problems for  $\text{H}_2\text{O}-\text{N}_2$  mixtures confined between two infinite parallel black walls are presented to further test the accuracy of the correlation as compared to “exact” (LBL or FSK) results obtained from the HITEMP databank. While in the first problem both the walls are black and cold, in the second, one of them is hot and the other cold. In the first problem, the mixture temperature is varied from 300K to 2500K, while both bounding walls are cold. This kind of arrangement tests the accuracy of the correlation for emission-dominated applications. The flux exiting at the walls is plotted in Fig. 6 against the gas temperature for three different pressure path lengths. The maximum error between the

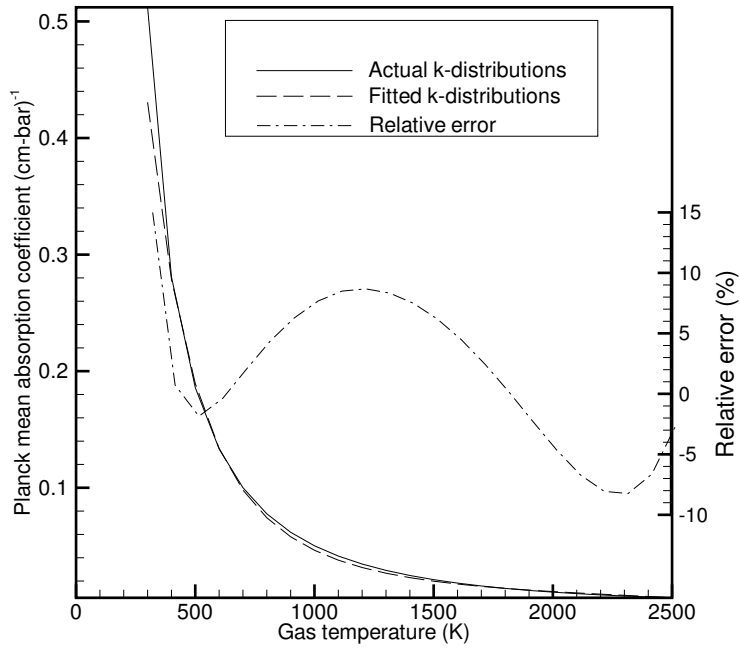


Figure 5: Planck mean absorption coefficients calculated using exact and approximate full-spectrum  $k$ -distributions for  $H_2O$ .

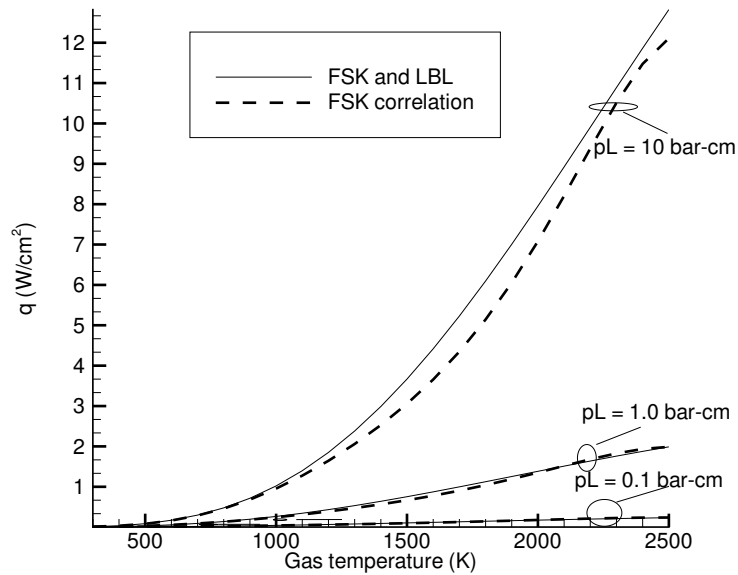


Figure 6: Radiative flux leaving a hot, isothermal, 90%  $N_2$ -10%  $H_2O$  mixture bounded by cold walls for varying gas temperatures and pressure path lengths.

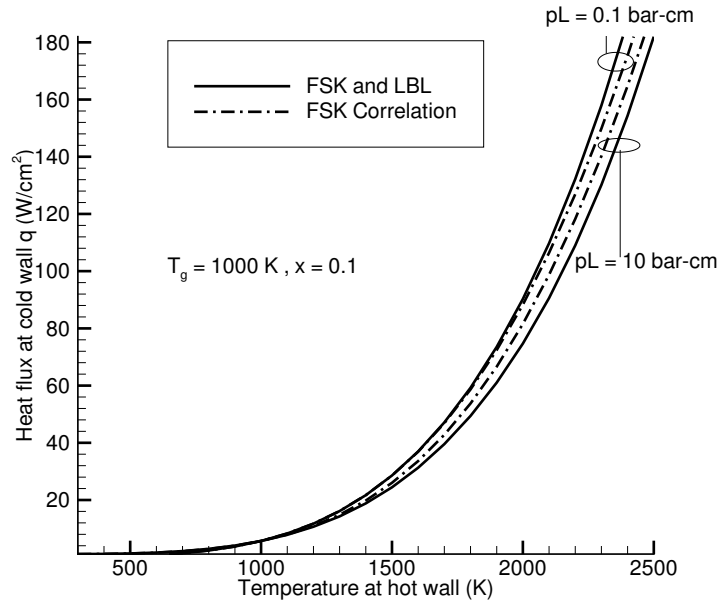


Figure 7: Radiative flux leaving from cold end of an isothermal, 90% N<sub>2</sub>-10% H<sub>2</sub>O mixture at 1000K between a hot and a cold wall for varying hot wall temperatures.

correlation and LBL calculations is about 8%.

In the second problem, to test the accuracy of the correlation for transmission-dominated situations, a hot gas slab at 1000K bounded by one hot wall and one cold wall is considered. The hot wall temperature is varied between 300K and 2500K and the flux exiting at the cold wall is plotted vs. the hot wall temperature in Fig. 7. The maximum error between the correlation and the LBL calculations is around 5%.

## Conclusion

A simple correlation of N<sub>2</sub>-H<sub>2</sub>O mixtures was developed for full-spectrum *k*-distributions based on the HITEMP database. The correlation is tested through various simple one-dimensional problems and found to achieve reasonable accuracy as compared to full-spectrum *k*-distributions obtained directly from the database.

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