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A Full-Spectrum *k*-Distribution Table for Radiative Transfer in Nonhomogeneous Gaseous Media

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In order to treat radiation in nongray media accurately as well as efficiently, several models have been proposed based on the idea of reordering the absorption coefficient across the entire spectrum, including the spectral-line-based weighted-sum-of-gray-gases (SLW) model [1], the absorption distribution function (ADF) [2] and the full-spectrum *k*-distribution (FSK) method [3]. The first two, developed before the FSK, are step-wise constant approximations of the FSK. The FSK has become the most promising method for radiative heat transfer calculations in nongray media. A single *k*-value in FSK corresponds to many wavenumbers with the same absorption coefficient, which reduces the number of required RTE evaluations from over one million to around ten. FSK results tend to be very accurate, usually being within a few percent of “exact” LBL calculations. The drawback of all three methods is that FSKs are very cumbersome to calculate. For each state the methods require the assembly of three different *k*-distributions or, for a CFD domain with several hundred thousand cells, on the order of one million FSKs. Modest et al. [3, 4] have described a narrowband database, from which FSKs can be assembled efficiently. However, creation of a single FSK still requires between 0.0549 s to 0.469 s [5] (depending on mixing model used for gas mixtures). Clearly, if one million FSKs are needed per time step/iteration this becomes computationally prohibitive. This has prompted the development of simple correlation formulas of limited accuracy, which, in addition, are limited to single species as well as single pressure [5].

To avoid runtime assembly of *k*-distributions and mixing, an FSK look-up table is generated for gas mixtures within a certain range of thermodynamic states of three species (CO_2, H_2O and CO), as given in Table 1. To decrease the nonlinear effects due to both mixing and self-broadening, a range of mole fractions between 0 and 0.25 is considered for inclusion in the FSK look-up table.

Table 1. Pre-calculated gas states and reference temperatures of FSK look-up table

Parameters	Range	Values	Number of points
Species	CO_2, H_2O and CO		3
Pressure (total)	0.1~0.5 bar	Every 0.1 bar	34
	0.7 bar	0.7 bar	
	1.0~14.0 bar	Every 1.0 bar	
	15.0~80 bar	Every 5 bar	
Gas temperature	300~3000 K	Every 100 K	28
Reference temperature	300~3000 K	Every 100 K	28
Mole fraction of CO_2	0.0~0.04	Every 0.01	7
	0.05~0.25	[0.05, 0.25]	
Mole fraction of H_2O	0.0~0.04	Every 0.01	10
	0.05~0.25	Every 0.05	
Mole fraction of CO	0.0~0.25	[0.0, 0.01, 0.05, 0.1, 0.25]	5

As required for a mixture, the *k*-distributions are based on the linear absorption coefficient, which is calculated from HITEMP-2010 [6]. For every thermodynamic state, both *k*-values and *a*-values at 32 Gauss-Chebyshev quadrature points are tabulated as outlined in [4].

FSKs for arbitrary mixture conditions are obtained by multiple linear interpolations among databased values (pressure, temperature, reference temperature and three concentrations). A memory management approach called dynamic loading is employed to guarantee the lowest memory cost without affecting the runtime efficiency when using the FSK look-up table.

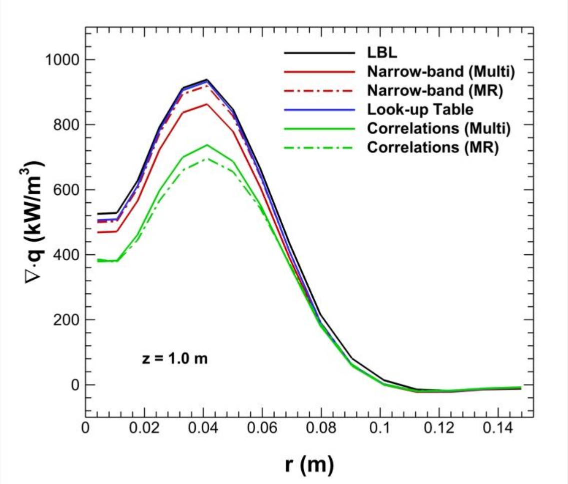

Figure 1. Comparison of the radiative heat source $\nabla \cdot q$ by different spectral models

Table 2
Comparison of CPU times for calculations of the Sandia D flame case using different databases

Database	Mixing model	CPU (s)
Narrow-band	Multiplication	1513.57
	MRmixing	8422.88
Correlations	Multiplication	1.76
	MRmixing	13.34
Look-up table	–	1.56

Figure 1 shows a comparison of the radiative heat source $\nabla \cdot q$ calculated by the LBL database, the narrow-band database [4], the correlations [5] and the new FSK look-up table at one fixed axial positions of a scaled Sandia D flame [7] employing a P_1 RTE solver. Table 2 shows CPU times using different databases. The results show that FSK look-up tables can provide a computationally cheap alternative without much sacrifice in accuracy.

References

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