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LINE-BY-LINE RANDOM-NUMBER DATABASE FOR PHOTON MONTE CARLO SIMULATIONS OF RADIATION IN COMBUSTION SYSTEM

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Gas molecules in a combustion medium continuously emit energy in the form of photons into random directions at distinct wavenumbers, which are determined by the energy difference between the two quantized energy levels of an emitting molecule before and after emission. Photons may be absorbed or scattered by other molecules during transmission. Photon Monte Carlo (PMC) methods directly simulate such processes by releasing representative photons bundles (rays) into random directions, which are traced until they are absorbed at certain points in the medium or escape from the domain. The PMC method can deal with complicated problems, such as radiation from highly nongray combustion gases, with relative ease. Due to the rapid increase in computational power, conducting line-by-line (LBL) calculations, the most accurate radiative heat transfer simulation, has become possible. However, for nongray analysis the wavenumber carried by photon bundles must be determined in a statistically meaningful way. Line-by-line spectral models were developed with a random number-wavenumber relation database, specifically applied to the PMC method. The Line-by-line spectral model resolves all individual spectral lines and is the most accurate spectral model, and may be combined with PMC to serve as benchmark for other radiative transfer equation (RTE) solvers and spectral models. Statistically meaningful wavenumbers for the emitting photons are found from a database, which tabulates wavenumber–random number relations for each species. In order to cover most conditions found in industrial practices, a database tabulating these relations for CO_2, H_2O, CO, CH_4, C_2H_4 and soot is constructed to determine emission wavenumbers and absorption coefficients for mixtures at temperatures up to 3000 K and total pressures up to 80 bar.

The spectral emission from a participating gaseous medium is the Planck function weighted by the spectral absorption coefficient, i.e., $\kappa_\eta I_{b\eta}$, which determines the probability of photons emitted in a differential wavenumber interval dη. Spectral absorption coefficients for CO_2, H_2O and CO are generated from HITEMP 2010 (Rothman et al., 2010), which is limited to only five species (CO_2, H_2O, CO, NO and OH), but contains data for hot lines, which become active at high temperature. For CH_4 and C_2H_4, the spectral absorption coefficients are generated from HITRAN 2012 (Rothman et al., 2013). The absorption coefficients of soot particles are determined using the small particle limit of Rayleigh scattering as described in (Modest, 2013). The PMC–LBL spectral database is then constructed based on the generated spectral absorption coefficients. Since fractional $(0, \eta)$ emissions for individual species, $R_{\eta,i}$, are different, a database tabulating both random number-wavenumber $(R_{\eta,i}-\eta)$ and absorption coefficient-wavenumber $(\kappa_{P\eta,i} - \eta)$ relations of each species will be utilized to determine emitting species and emission wavenumber for a mixture (Ren and Modest, 2013). Table 1 summarizes the thermodynamic states stored in the current database. Due to weak self-broadening

for CO_2, CO, CH_4 and C_2H_4, only a single mole fraction, say 0.0, is required for these species. However, two mole fractions, 0.0 and 0.25, are required for H_2O because of the strong self-broadening. The random-number relation for soot is pressure independent and absorption coefficient is directly proportional to the volume fraction. Therefore, the relation at 28 temperatures and a normalized volume fraction of "1" are tabulated for soot in the database.

Table 1: Thermodynamic states of PMC-LBL random-number relation database

Parameters	Range and values
	0.1–1.1 bar, every 0.1 bar
P_{total}	2–14 bar , every 1 bar
	15–80 bar , every 5 bar
T	300–3000 K , every 100 K
x_{CO_2}	0
x_{H_2O}	0, 0.25
x_{CO}	0
x_{CH_4}	0
$x_{C_2H_2}$	0
f_{vSoot}	"1"

The accuracy of the database is tested by reconstructing absorption coefficient spectra from the tabulated database. One-dimensional test cases are used to validate the database against analytical LBL solutions. The database is available from the corresponding author's website upon request at *http://eng.ucmerced.edu/people/mmodest*

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