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New correlations for the weighted-sum-of-gray-gases model in oxy-fuel conditions based on HITEMP 2010 database

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ABSTRACT

Oxy-fuel combustion is one of the promising options for carbon dioxide capture in future coal power plants. Radiative properties of combustion gases and heat transfer characteristics inside oxy-fuel furnaces are different from those found in air-fired furnace. Nowadays, few publications provide appropriate radiation property correlations for oxy-fuel conditions. The available correlations are based on previous versions of HITRAN database, which is not accurate for prediction of spectral intensities at high temperature in combustion applications or above 1000 K. This paper considers the determination and evaluation of new correlations for the weighted-sum-of-gray-gases model to predict the radiative transfer in gases under oxy-fuel conditions. The new correlations are fitted from emittance charts calculated from the up-to-date HITEMP 2010 database for molar ratios of water vapor to carbon dioxide between 0.125 and 4, temperature range of 400–2500 K, and pressure path-length varying from 0.001 to 60 bar m. The new correlations are validated by comparing the radiative source term with line-by-line calculations from HITEMP 2010 database for a one-dimensional slab system. The radiative transfer equation is solved with the discrete ordinate method.

1. Introduction

According to the new Copenhagen protocol [1], Global CO_2 emission from power generation is rising due to an increasing world demand for electricity. In order to reduce CO_2 emission, oxy-fuel combustion is considered as one of the promising technologies for carbon dioxide capture and storage (CCS) to mitigate climate change. However, oxy-fuel plants are still pilot-scaled designs [2], so combustion in oxy-fuel conditions are at the moment investigated for a scale-up plant. Computational fluid dynamics (CFD) has been an efficient tool for oxy-fuel combustion researches [3–14] to provide predictions of temperature, heat transfer, and chemical species from combustion process inside furnaces. However, several sub-models in CFD require revision to account oxy-fuel environments, especially radiation modeling, which is by far different from air-fired conditions [15].

In oxy-fuel combustion, fuel is burned in a mixture of gases composed of oxygen, carbon dioxide and water vapor and flue gas after the combustion process is recycled and mixed with oxidant at burner to reduce the intense high temperature oxy-fuel flame close to the burner region [16]. Radiation properties of combustion gases in oxy-fuel combustion are considerably different from those found in air-fired conditions due to the higher amount of carbon dioxide and water. Thus, some of the still widely employed radiation correlations, such as those provided in [17], are no longer applicable. To provide a good prediction of oxy-fuel combustion, new data and correlations are needed. Recently, there have been some attempts to model radiation properties of gases under oxy-fuel conditions. For example, Johansson et al. [18] proposed weighted-sum-of-gray-gases (WSGG) correlations with the use of four gray gases from fitting of emittance data that was calculated by statistical narrow band (SNB) model with EM2C database [19,20]. The study accounted for molar ratios (MR) of H_2O to CO_2 from 0.125 to 2, and pressure path-lengths between 0.01 and 60 bar m in the temperature range of 500–2500 K. However, EM2C database is based on the HITRAN 1992 database combining with H_2O line near 2700 cm^{-1} and additional spectral hot lines. Therefore those WSGG correlations probably lack accuracy in combustion conditions, in which hot lines are important above 1000 K [21]. Yin et al. [22] proposed new parameters for WSGG model with four gray gases derived from fitting emittance data calculated by exponential wide band (EWB) model [23] at atmospheric pressure, with temperatures between 500 and 3000 K, and path-lengths from 0.001 to 60 m. Predictions of radiative source term applying these new coefficients for a 0.8 MW oxy-natural gas furnace and 609 MW tangential fired utility boiler were compared with the predictions

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Nomenclature

a_l	quadrature weights for the solution of the RTE with DOM
A_v	Avogadro constant, molecules/mole
$b_{i,j}$	temperature dependent polynomial coefficients for emittance in the general formulation
c	speed of light in vacuum, m/s
$c_{i,j}$	temperature dependent polynomial coefficients for emittance in the normalized formulation
d	degeneracy factor
d_{ind}	state-independent degeneracy factor
E	state energy of the transition, cm^{-1}
f_k	line shape function of k^{th} transition line
h	Planck constant, J s
I	total radiation intensity, $W/(m^2\,sr)$
I_η	spectral radiation intensity, $W/(m^2\,sr)$
I_b	total blackbody radiation intensity, $W/(m^2\,sr)$
$I_{b,\eta}$	spectral blackbody radiation intensity, $W/(m^2\,sr)$
k_B	Boltzmann constant, J/K
L	distance between one dimensional parallel infinite plates or path-length, m
L_p	path length related to partial pressure p of a specific gas, m
n	coefficient of temperature dependence of the air-broadened half-width
n_r	refractive index
$\hat{n}$	normal vector outward a surface element
N_a	number of particles in the gas, molecules
N_c	number of polynomial coefficients for the weighting factors
N_g	total number of gray gases
N_p	total number of path-lengths for procedure of fitting correlations
N_t	total number of temperatures for procedure of fitting correlations
N_{mesh}	number of computational cells
N_{mol}	number density of the absorbing molecules, molecules/cm^3
N_w	number of ordinates and quadrature weights for DOM
P	total pressure of gases, bar
P_a	sum of partial pressure of absorbing gases, bar
q	radiative heat flux, kW/m^2
q_w	radiative heat flux at wall, kW/m^2
$\dot{q}$	radiative source term, kW/m^3
Q	total internal partition sum (TIPS)
Q_r	rotational partition functions
Q_v	vibrational partition functions
r	position vector for RTE
R	universal gas constant, $cm^3\,atm\,mol^{-1}\,K^{-1}$
$\hat{s}$	direction vector for RTE
s'	the incoming direction vector for RTE
S_k	spectral line intensity for k^{th} transition line, $cm^{-1}/(molecule\,cm^{-2})$
T	gas temperature, K
V_a	volume of the absorbing gases, cm^3
Var	variance of the deviation of the total emittance from the LBL integration of HITEMP 2010 database
w_i	weighting factor of gray gas i
x	length coordinate, m
Y	molar fraction of gas

Abbreviations

CCS	carbon capture and storage
CFD	computational fluid dynamics
DOM	discrete ordinate method
EWB	exponential wide band
HITRAN	high-resolution transmission molecular absorption database
HITEMP	high-temperature spectroscopic absorption database
LBL	line-by-line
LM	Levenberg–Marquardt algorithm
MR	molar ratio of H_2O to CO_2
RTE	radiative transfer equation
SNB	statistical narrow band
WSGG	weighted-sum-of-gray-gases

Greek symbols

γ_k	pressure broadened line half-width, 1/cm
γ_{air}	air-broadened half-width at half maximum, 1/(cm atm)
γ_{self}	self-broadened half-width, 1/(cm atm)
ε	total emittance
η	wavenumber, cm^{-1}
κ	absorption coefficient, 1/(bar m)
μ_l	ordinates weights for the solution of RTE with DOM
σ	Stefan–Boltzmann constant, $W/(m^2\,K^4)$
Ω'	solid angle for the solution of RTE with DOM

Subscripts

a	absorbing gas
b	blackbody value
i	index of gray gases
j	index of temperature dependent polynomial order of weighting factor
k	index of transition lines
l	index of ordinates and quadrature weights for DOM model
m	index of numerical nodes
p	index of path-lengths
r	rotational state
t	index of temperature
v	vibrational state
w	wall surface

calculated with correlations proposed by Smith et al. [17] for air-fired conditions. Rehfeldt et al. [24] determined new parameters for the WSGG model using four gray gases based on the fitting of emittance data computed from EWB model in the temperature range of 600–2400 K, and molar ratio of H_2O to CO_2 ranging from 0.056 to 2.167, in which the remaining 5% of gas was non-radiating species (N_2 or O_2). Wall radiative heat fluxes calculated from the correlations were compared with EWB model for a rectangular furnace using a CFD tool. However, the study lacked all details of the determined parameters. Krishnamoorthy [25] developed new WSGG model with five gray gases based on least square fit of total emittance correlations that are available in Perry's Chemical Engineers Handbook [26] for the molar ratio H_2O/CO_2 of 0.5, 1.0, 2.0 and 3.0, and at temperatures of 1000, 1500 and 2000 K. No correlation was presented in that work. Radiative source terms calculated using the correlations were compared with results from SNB model in a three dimensional enclosure having a non-uniform gas temperature profile in air-fired conditions in a mixture of 5% CO_2, 15% H_2O and 80% N_2. Khare [27] fitted correlations for WSGG model with total emittances calculated from EWB model. However, no details of the correlations were published. Although the parameters of the WSGG models can be easily implemented for predictions of