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A comprehensive evaluation of different radiation models in a gas turbine combustor under conditions of oxy-fuel combustion with dry recycle

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ABSTRACT

The oxy-fuel combustion is a promising CO₂ capture technology from combustion systems. This process is characterized by much higher CO₂ concentrations in the combustion system compared to that of the conventional air-fuel combustion. To accurately predict the enhanced thermal radiation in oxy-fuel combustion, it is essential to take into account the non-gray nature of gas radiation. In this study, radiation heat transfer in a 3D model gas turbine combustor under two test cases at 20 atm total pressure was calculated by various non-gray gas radiation models, including the statistical narrow-band (SNB) model, the statistical narrow-band correlated-k (SNBCK) model, the wide-band correlated-k (WBCK) model, the full spectrum correlated-k (FSCK) model, and several weighted sum of gray gases (WSGG) models. Calculations of SNB, SNBCK, and FSCK were conducted using the updated EM2C SNB model parameters. Results of the SNB model are considered as the benchmark solution to evaluate the accuracy of the other models considered. Results of SNBCK and FSCK are in good agreement with the benchmark solution. The WBCK model is less accurate than SNBCK or FSCK. Considering the three formulations of the WBCK model, the multiple gases formulation is the best choice regarding the accuracy and computational cost. The WSGG model with the parameters of Bordbar et al. (2014) [20] is the most accurate of the three investigated WSGG models. Use of the gray WSGG formulation leads to significant deviations from the benchmark data and should not be applied to predict radiation heat transfer in oxy-fuel combustion systems. A best practice to incorporate the state-of-the-art gas radiation models for high accuracy of radiation heat transfer calculations at minimal increase in computational cost in CFD simulation of oxy-fuel combustion systems for pressure path lengths up to about 10 bar m is suggested.

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1. Introduction

To meet the challenges of global climate change, carbon capture and storage (CCS) technologies are one promising and

effective possibility to reduce carbon dioxide (CO₂) emissions to the atmosphere. Herein, oxy-fuel combustion offers the feasible opportunity to capture CO₂ from combustion systems. The major characteristic of oxy-fuel technology is that the oxidizer consists of pure oxygen and recycled flue gas [1]. Thus, the flue gas stream contains mainly CO₂ and water vapor (H₂O) with much higher CO₂ concentrations in comparison to conventional air based combustion systems. As these molecules show strong absorption and emission characteristics in

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Nomenclature*Roman letters*

a	weight of gray gas
A	surface of enclosure [m ²]
b_{ij}	emissivity gas temperature polynomial coefficients for air-firing
$C1_{ij}, C2_{ij}, C3_{ij}$	coefficients for c_{ij} of WSGG model from Johansson et al.
c_{ij}	emissivity gas temperature polynomial coefficients for oxy-fuel
$C_{ij,k}$	coefficients for c_{ij} of WSGG model from Bordbar et al.
$d_{i,k}$	coefficients for molar ratio dependent absorption coefficient of WSGG model from Bordbar et al.
F	blackbody fraction
f_b	burnout factor
f_m	mixing factor
f_r	radial factor
I	radiative intensity [W m ⁻² sr ⁻¹]
k	band in WBCK model
\bar{k}_ν	mean line intensity to line spacing ratio [m ⁻¹ bar ⁻¹]
$K1_i, K2_i$	coefficients for molar ratio dependent absorption coefficient of WSGG model from Johansson et al. [m ⁻¹ bar ⁻¹]
l	index over all values along a line
L	path length [m]
L_{domain}	mean path length based on dimensions of the whole enclosure [m]
L_x, L_y, L_z	dimensions of enclosure [m]
m	index of absorbing gas in WBCK MGF model
MR	molar ratio of H ₂ O to CO ₂
N_g	number of gray gases
N_m	number of absorbing gases
p	(partial) pressure [bar]
r	radial distance from centerline [m]
s	direction vector for RTE
T	temperature [K]
V	volume of enclosure [m ³]
X	molar fraction of the species [kmol/kmol]
x, y, z	coordinates of enclosure [m]

Greek letters

$\bar{\beta}_\nu$	average line-width to spacing ratio
$\bar{\gamma}_\nu$	average line Lorentz half-width [cm ⁻¹]
$\bar{\delta}_\nu$	mean line spacing [cm ⁻¹]
Δ_f	relative error of wall heat fluxes [%]
Δ_s	relative error of radiative source terms [%]
$\Delta\nu_i$	reordered wavenumber region in WBCK model [cm ⁻¹]

ϵ_{tot}	total emissivity of WSGG model
η	wavenumber [cm ⁻¹]
κ	absorption coefficient [m ⁻¹ , m ⁻¹ bar ⁻¹]
κ_j	basic absorption coefficient in WBCK model [m ⁻¹ bar ⁻¹]
$\kappa_{j-1/2}, \kappa_{j+1/2}$	limiting absorption coefficients in WBCK model [m ⁻¹ bar ⁻¹]
$\nu(\kappa)$	reordered wavenumber of band k in WBCK model [cm ⁻¹]
σ	Stefan–Boltzmann constant [W m ⁻² K ⁻⁴]
$\bar{\tau}_\nu$	narrow-band averaged gas transmissivity
ϕ	physical quantity

Subscripts

abs	absorbing gas
b	blackbody
c	state at centerline
CO_2	physical quantity of carbon dioxide
d	state of the diluent
e	completely mixed state at exit
f	state of the FOM
f,b	burnt state of FOM
f,i	initial state of FOM
H_2O	physical quantity of water vapor
i	i th gray gas
$mean$	mean value of considered quantity
ref	reference state
tot	total physical quantity
w	state at wall

Abbreviations

ADFFG	absorption distribution function model with fictitious gases
CFD	computational fluid dynamics
CW	cumulative wavenumber
EWB	exponential wide-band
FOM	fuel/oxidizer mixture
FS	full spectrum
FSCK	full spectrum correlated-k
GGF	gray gases formulation
LBL	line by line
MGF	multiple gases formulation
NB	narrow-band
RTE	radiative transfer equation
SLMB	spectral line moment based
SLW	spectral line based WSGG
SNB	statistical narrow-band
SNBCK	statistical narrow-band correlated-k
SPF	spectral formulation
WBCK	wide-band correlated-k
WSGG	weighted sum of gray gases

the infrared spectrum, they greatly alter the thermal radiation transfer in such combustion systems. Since thermal radiation is the main heat transfer mode in combustion systems, it is critical to accurately predict radiation heat transfer.

The absorption coefficient of a real gas is a strongly erratic function of wavelength. To describe this characteristic, radiation models with different spectral resolutions have been developed. Line by line (LBL) calculations [2]

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