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# Influence of gray particle assumption on the predictive accuracy of gas property approximations

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## ABSTRACT

In this study, influence of gray particle assumption on the predictive accuracy of gas property models is investigated for conditions typically encountered in industrial coal-fired furnaces. The aim is (i) to identify how the share of gas radiation is influenced by the presence of particles and particle properties and (ii) to determine the effect of gray particle assumption on the predictive accuracy of gas property approximations. For that purpose, predictive accuracy of a simple gas property model is benchmarked against that of Spectral Line-Based Weighted Sum of Grey Gases Model (SLW) in the presence of gray/non-gray particles with different ash compositions, particle loads and boundary conditions. Input data required for the radiation code and its validation are provided from two combustion tests previously carried out in a 300 kWt Atmospheric Bubbling Fluidized Bed Combustor (ABFBC) test rig burning low calorific value Turkish lignite with high volatile matter/fixed carbon (VM/FC) ratio in its own ash. Comparisons reveal that gray particle assumption leads to over-estimation of particle radiation, which leads to under-estimation of gas radiation share in total radiative heat exchange. This under-estimation is found to be reflected on the predictive accuracy of gas property models, that is, a simple gas property model can be found to be “accurate” if particles are assumed to be gray although that is not the case. Furthermore, share of particle radiation in total radiative heat exchange is demonstrated to be strongly dependent on the spectral nature of particle properties. The results show that accurate gas property models such as SLW are needed to represent the spectral behavior of combustion gases even at high particle loads.

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## 1. Introduction

Modelling of radiative heat transfer in combusting systems is of considerable importance and necessitates not only accurate but also computationally efficient radiative property estimation methods for both combustion gases and particles. Nevertheless, spectral resolution of gas and particle properties included in the solution of radiative transfer equation (RTE) is reflected on the computational cost of the radiation model as it directly determines the number of intensity equations to be solved. For gas radiation, a wide variety of gas spectral radiative property models with different degrees of complexity and accuracy are available in the literature [1]. For multidimensional problems, global gas property models are usually preferred as they offer a solution for the high CPU requirement of detailed spectral models. One of the most commonly used global models is the spectral line-based weighted sum of gray gases (SLW) model, which expresses the gray gas weights in terms

of an absorption-line blackbody distribution function [2–4] derived from the high resolution databases [5]. SLW has been validated against reference solutions on a wide variety of problems including absorbing-emitting and scattering media and shown to be the best choice with regard to computational time and accuracy [2–4,6–8]. This is why SLW has been implemented into CFD software packages such as Fluent or OpenFoam [9–11]. Furthermore, global SLW model has been recently applied in a banded form to incorporate non-gray strongly absorbing, emitting and scattering particles in the solution of spectral RTE [12].

Spectral properties of particles demonstrate a less complex behavior contrary to those of gas radiation. In fact, spectral dependency of particle properties is often neglected in the majority of relevant literature and it is common to use a gray approach by deploying representative complex index of refraction values for different particles such as coal, char and ash [13]. Nevertheless, it has recently been shown that spectral particle radiation is of significant importance for accurate calculation of radiative heat transfer in combusting systems even at low particle loads [14] and that negligence of the spectral behavior of either combustion gases or particles can lead to significant errors in both heat flux and source term predictions [14–16].

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## Nomenclature

$a$	gray gas weight (-)
$c$	speed of light (m/s)
$\tilde{C}_{\text{abs}}$	supplemental absorption cross section
$E_b$	blackbody emissive power ( $\text{W m}^{-2}$ )
$F$	conventional blackbody fractional function (-)
$g$	asymmetry factor (-)
$g_c$	k-distribution function for $\text{CO}_2$
$g_w$	k-distribution function for $\text{H}_2\text{O}$
$I$	radiative intensity ( $\text{W m}^{-2} \text{sr}^{-1}$ )
$I_b$	blackbody intensity ( $\text{W m}^{-2} \text{sr}^{-1}$ )
$k_t$	time constant with dimension $(\text{m/s})^{-1}$
$L_m$	mean beam length (m)
$N$	molar density ( $\text{mol/m}^3$ )
NB	number of spectral points within the $j$ th band
$r$	position vector (-)
$P$	pressure (Pa)
$T$	temperature (K)
$w$	quadrature weight (-)

### Superscripts

$m$	ordinate index
$m'$	incoming ordinate
$l$	index for a discrete direction
$l'$	incoming discrete direction

### Subscripts

$b$	blackbody
$g$	gas
$i$	quadrature point
$j$	spectral wide band number
$k$	gray gas number index for $\text{H}_2\text{O}$
$l$	gray gas number index for $\text{CO}_2$
$l$	index for a discrete direction
$l'$	incoming discrete direction
$m$	ordinate index
$m'$	incoming ordinate
$p$	particle
$tr$	transport approximation
$w$	wall

### Greek

$\lambda$	wavelength ( $\mu\text{m}$ )
$\nu$	wavenumber ( $\text{cm}^{-1}$ )
$\gamma$	angular differencing coefficient (-)
$\varepsilon$	emissivity (-)
$\Phi$	Scattering phase function
$\eta$	direction cosine (-)
$\theta$	scattering angle (rad)
$\kappa$	absorption coefficient ( $\text{m}^{-1}$ )
$\mu$	direction cosine (-)
$\xi$	direction cosine (-)
$\sigma$	scattering coefficient ( $\text{m}^{-1}$ )
$\tau$	transmissivity
$\Omega$	direction of radiation intensity (-)

Studies involving both participating combustion gases and absorbing-emitting-scattering particles, on the other hand, state that total radiative heat transfer within the combustor is dominated by the particle radiation [8,17–26]. Accordingly, improvement achieved in the accuracy of heat flux / source term predictions by deploying CPU intensive accurate gas property models such as SLW, SNB, SNBCK is found to be marginal compared to that of even gray gas approximation in the presence of particles [8,17–20]. In

other words, RTE is needed to be solved for only several times in the presence particles, which is a very important advantage especially if RTE is coupled with a CFD solver. However, majority of these assessment studies [17–23] ignore the spectral dependency of the particle cloud properties, which has been recently shown to be of significant importance [14–16]. Therefore, accuracy of simpler gas property models in the presence of particles and/or dominant role of particle radiation in total radiation becomes questionable as they have been discussed only within the frame of gray particle assumption. To the author's best knowledge, no numerical study comparing the accuracy of simple gas property models in the presence of gray and non-gray particles is available in the literature.

Therefore, objective of this paper is to assess the predictive accuracy of a simple gas property model by benchmarking its predictions against those of an accurate gas property model in the presence of gray and non-gray particles in order to investigate the influence of gray particle assumption on gas and particle radiation shares in solid fuel fired combustions systems. For that purpose, accuracy of three simple gas property models, namely gray gas, gray wide band (GWB) and gray narrow band approximations (GNB), are tested by benchmarking their predictions against those of SLW. Investigation is performed through mathematical modeling by using the experimental data on two coal combustion tests previously performed in 300 kWt ABFBC test rig, for which complete experimental data required for the model and its validation are available in the literature [27].

## 2. Description of the methods

### 2.1. Test case description

Input data required for the radiation model and its validation are provided from two coal combustion tests previously carried out in a 300 kWt Atmospheric Bubbling Fluidized Bed Combustor (ABFBC) test rig burning low calorific value Turkish lignite in its own ash [27]. The main body of the ABFBC test rig is the modular combustor formed by five modules of internal cross-section of 0.45 m x 0.45 m and 1 m height. The combustor is equipped with baghouse filter and a cyclone, which can recycle collected particles back to the combustor (with recycle case). Inner walls of the modules are lined with alumina-based refractory bricks and insulated. The first and fifth modules from the bottom refer to bed and cooler, respectively, and the ones in between are the freeboard modules, where the radiative heat transfer is modeled. Two cooling surfaces exist in the modular combustor, one in the bed with 0.35  $\text{m}^2$  cooling surface and the other in the cooler providing 4.3  $\text{m}^2$  of cooling surface. A schematic representation of the ABFBC test rig is presented in Fig. 1(a).

Process values such as flow rates and temperatures of each stream, gas composition, and temperature along the combustor are logged to a PC by means of a data acquisition and control system (Bailey INFI 90). Radiative heat fluxes incident on the refractory side-walls of the freeboard were measured by water cooled radiometer with Medtherm 48P-20-22 K heat flux transducer during the steady state operation of the test rig. Measurements were carried out for two combustion tests utilizing low calorific value and high ash content Turkish lignite, namely Beypazari lignite, one without (Test 1) and the other with recycle of particles collected in the cyclone (Test 2). Table 1 lists the operating conditions for these two combustion tests relevant to radiative heat transfer calculations. It should be noted here that major difference between these two combustion tests is one order magnitude increase in particle load due to the recycling of collected particles back to the combustor.

In order to further investigate the applicability of the outcomes of this study, hot refractory-lined walls of the pilot scale test rig

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