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# Application of the WSGG model for the calculation of gas–soot radiation in a turbulent non-premixed methane–air flame inside a cylindrical combustion chamber

Felipe Roman Centeno [a,*], Rogério Brittes [a], Francis H.R. França [a], Cristiano Vitorino da Silva [b]

[a] Department of Mechanical Engineering, Federal University of Rio Grande do Sul, Rua Sarmento Leite, 425, 90050-170 Porto Alegre, RS, Brazil
[b] Department of Engineering and Computer Sciences, Regional Integrated University of Alto Uruguai and Missions, Av. Sete de Setembro, 1621, 99700-000 Erechim, RS, Brazil

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ABSTRACT

This paper presents a study of the effect of soot on the radiative heat transfer in a turbulent, non-premixed methane–air flame inside a combustion chamber. In this problem, an important aspect to be considered is the steep variation of the radiative properties of the medium, which is treated with the weighted-sum-of-gray-gases (WSGG) model based on the superposition of correlations recently obtained for water vapor, carbon dioxide mixtures and soot. The discrete ordinates method (DOM) is employed for the angular integration of the radiative transfer equation (RTE), taking into account turbulence–radiation interactions (TRI). Calculations indicate that the global contribution of soot to the radiative heat transfer in the chamber was of 8%, which is compatible with methane flames. However, in the region with the highest concentration of soot, it was observed a local increase of 30% in the radiative volumetric source in the medium, and of 25% in the radiative heat flux on the wall. In the second part of the paper, the WSGG model is compared with the line-by-line (LBL) integration using the final temperature and concentrations fields obtained from the global flame calculation, leading to average and maximum normalized errors of 1.2% and 4.8%, respectively, and requiring only 1/7000 of the computation effort of the LBL integration. This result indicates that the WSGG model, in spite of its relative simplicity, can provide accurate results for the spectral integration of the radiative properties of gas–soot mixtures in combustion processes.



## 1. Introduction

The numerical simulation of combustion processes involves the coupled solution of complex phenomena, such as turbulent fluid flow, chemical kinetics of gaseous species and soot, and combined convection–radiation heat transfer. Due to the formation of participating gases at high temperature, thermal radiation is generally the dominant mechanism, and, in particular, soot can play an important role in the radiative exchanges even in relatively small concentrations. Therefore, an accurate description of gas–soot combined radiation is of great importance in the simulation of combustion.

High-resolution transition lines of several participating gases, such as $H_2O$ and $CO_2$, can be generated by means of spectral database such as HITRAN, built at a reference temperature of 296 K for atmospheric applications, and HITEMP, for high temperature applications. In its latest update, HITEMP2010 [1] was released as a major improvement to previous versions, expanding the number of transition lines for $H_2O$ and $CO_2$, and being valid for temperatures up to 4000 K. However, the highly complex dependence of the absorption coefficient with the thermodynamic state and the wavenumber, which is typically characterized by hundreds of thousands or millions of transition lines, still imposes a major challenge for accurate, efficient calculation of thermal radiation in participating gases, especially in coupled phenomena problems. The absorption coefficient of soot presents a much simpler linear dependence with the wavenumber, but modeling the combined gas–soot radiation can become even more difficult due to their different spectral behaviors.

The line-by-line (LBL) integration of the radiative transfer equation (RTE) over the spectrum is excessively expensive for most global calculations, so the development of accurate, efficient gas models continues to be an intense research field. Extensive discussion of gas models can be found in major textbooks in the field [2,3]. Among the available models, the weighted-sum-of-gray-gases (WSGG) [4] makes perhaps the best compromise between accuracy and computation demand, especially in global simulation

* Corresponding author. Fax: +55 51 3308 3222.
*E-mail address:* frcenteno@mecanica.ufrgs.br (F.R. Centeno).

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of combustion processes in which the RTE is solved together with the fluid flow, chemical kinetics and heat transfer. In the WSGG model, the spectrum is represented by a few portions having constant pressure absorption coefficients. The weighting coefficients account for the contribution of each gray gas, and can be interpreted as the fraction of the blackbody energy in the spectrum portions corresponding to each absorption coefficient. In practice, those coefficients are obtained from fitting total emittance data, such as those presented in [5–8]. Although the WSGG model has often been regarded as a crude approximation to the real spectrum, recent studies have demonstrated that the model can provide accurate results for highly non-homogeneous, non-isothermal gas mixtures [7–10].

The literature presents a number of combustion simulations considering gas/soot chemistry and radiation in fires and diffusion flames using global or detailed chemistry [11–23]. In this set of works, it can be found comparisons of the results obtained with different gas models (gray gas, WSGG, SNBCK, SLW, narrow band) and/or validation against experimental data. Overall, those studies were mainly focused on the influence of soot on the flame structure, or on studying the influence of radiation on soot formation, flame structure, flame height, temperature/species fields, but none of them analyzed the relative importance of soot to total radiation, exception is made for the investigation in [24], in which the authors studied the role of thermal radiation in ethylene–methane flames. In the present work, it is considered a turbulent non-premixed methane–air flame in a cylindrical combustion chamber, as the case described in [25], for which there are spatial measurements for the main gas species concentrations and for the temperature field. The spectral integration of the RTE is carried out by means of the WSGG model, using correlations for $H_2O$ and $CO_2$ obtained in [7] based on HITEMP2010 database, while for soot they are taken from [8]. The calculations take into account a turbulence–radiation interactions (TRI) model developed for RANS simulations [13]. In this way, the present paper makes an advance in a previous study [26], which investigated the same combustion chamber but neglected soot kinetics and radiation.

Although the numerical simulation is compared with the experimental data provided in [25], it is not a simple task to estimate the errors arising from modeling each different phenomenon, that is, the turbulent fluid flow, kinetics, thermal radiation, etc. In this study, the error in the computation of the radiation heat transfer using the WSGG is estimated by comparisons with the LBL integration of the spectrum of $H_2O$–$CO_2$ mixture and soot. Due to its highly demanding computational effort, the LBL integration is carried out using the final temperature and species concentrations fields obtained from the converged solution obtained from the global combustion calculation using the WSGG model. In this way, the error of the application of the WSGG model can be directly estimated from this comparison. To the authors' best knowledge, there are no previous reports of gas model evaluation against LBL solution for mixtures of gases and soot in a typical combustion simulation. In this manner, the present study aims at improving the understanding of soot radiation in a typical air-methane combustion chamber, and at evaluating the accuracy of the WSGG model when applied to a mixture of soot, $CO_2$ and $H_2O$ in a realistic combustion scenario.

## 2. Problem statement

The physical system under study consists of the natural gas combustion chamber described in [25], which presents several challenges for radiation modeling, since it involves turbulence–radiation effects and a highly non-isothermal, non-homogeneous participating medium. Several experimental data for temperature and species concentrations profiles along axial and radial coordinates were presented in [25], in addition to the results provided in other investigations [26–29], making it a good test case for the methodology that is presented in the current study. The cylindrical chamber has length and diameter of 1.7 m and 0.5 m, respectively, as shown in Fig. 1. Natural gas is injected into the chamber by a duct aligned with the chamber centerline, leading to a non-swirling flame. The burner provides the necessary amount of air and natural gas as required by the process, and it is treated as a boundary condition. A fuel excess of 5% (equivalence ratio of 1.05) is prescribed. For a fuel mass flow rate of 0.01453 kg/s at a temperature of 313.15 K, this requires an air mass flow rate of 0.1988 kg/s, at a temperature of 323.15 K. The fuel enters the chamber through a cylindrical duct having 0.06 m diameter, while air enters the chamber through a centered annular duct having a spacing of 0.02 m. For such mass flow rates, the fuel and air velocities are 7.23 and 36.29 m/s, respectively. With a Reynolds number at the entrance of approximately $1.8 \times 10^4$, the flow is fully turbulent. The inlet air is composed of oxygen (23% in mass fraction), nitrogen (76%) and water vapor (1%), while the fuel is composed of 90% of methane and 10% of nitrogen. The burner power is about 600 kW. The combustion chamber operational pressure is $p = 101{,}325$ Pa. Buoyancy effects are neglected due to the high velocities that are provided by the burner (the Richardson number, $Ri$, for the present combustion chamber is about $1.0 \times 10^{-2}$, which is less than the critical value of $10^{-1}$, so the flow is dominated by forced convection). Fig. 1 depicts additional thermal boundary conditions: symmetry in the centerline, and prescribed temperature on the walls of 393.15 K. Moreover, impermeability and no-slip conditions were assumed on the walls. In the symmetry line, it was assumed that both radial velocity and velocity gradient were null. The same procedure was adopted for the turbulent kinetic energy and its dissipation rate, enthalpy, and chemical species concentrations in the symmetry line. In the outlet, null diffusive fluxes were assumed for all variables, the axial velocity component was corrected by a factor to satisfy mass conservation, and the radial velocity was imposed to be null. The chamber walls, and its inlet and outlet ducts were modeled as black surfaces. While the temperature of inlet duct was prescribed as equal to the fuel and the oxidant temperatures, the temperature at the outlet duct was equal to the outlet flow bulk temperature.

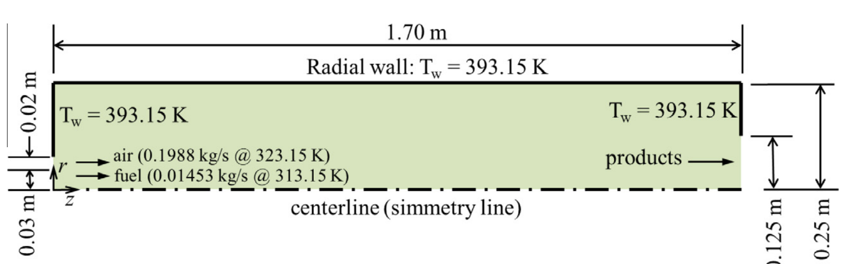


**Fig. 1.** Combustion chamber geometry.