International Journal of Thermal Sciences 87 (2015) 68–84

Contents lists available at ScienceDirect

International Journal of Thermal Sciences

journal homepage: www.elsevier.com/locate/ijts

Detailed radiation modeling of a partial-oxidation flame

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ARTICLE INFO

Article history:
Received 14 March 2014
Received in revised form
29 July 2014
Accepted 29 July 2014
Available online 7 September 2014

Keywords:
Radiation modeling
Partial oxidation
SLW
WSGG
MDA
DOM

ABSTRACT

A numerical study of a laminar methane partial oxidation flame (POX-flame) is presented to investigate different radiation modeling approaches. A laminar reference flame for large-scale gasification, which was previously investigated both experimentally and numerically by Stelzner et al. [1], is particularly suitable for such a study because of the distinct temperatures and radiating species concentrations. A second study of a well-known methane–air flame [2] is also included. The fully resolved and coupled solution of the reactive flows was achieved with an OpenFOAM® based solver using detailed approaches for diffusion and chemistry. Different combinations for solving the radiative transfer equation (RTE) and the evaluation of the radiative properties were implemented and investigated. The discrete ordinate method (DOM), the modified differential approximation (MDA), the P1 model and the optically thin model (OTM) were used for the solution of the RTE, whereas the spectral line-based weighted sum of gray gases model (SLW), the weighted sum of gray gases model (WSGG) and gray absorption (RADCAL) was used for the evaluation of the radiative properties.

In both flame setups gaseous radiation was found to be important and needs to be considered. In the POX-flame radiative absorption has a significant impact on the radiative source terms and significant non-gray gas effects were found. Simple radiation modeling approaches, typical for combustion regimes, namely the OTM with RADCAL, were not able to capture these effects. More sophisticated radiation models were required. The MDA with both the SLW and the WSGG provided reasonable results at still acceptable computational costs. In contrast, in the methane–air flame, the simple radiation models achieved a reasonable agreement with the temperature measurements.

Finally, particular combinations of RTE solution methods and property models are recommended for the different flame setups based on the differences in the temperature and the radiating species concentrations in the different flame regions.

1. Introduction

Partial oxidation has become an established process for the production of hydrogen and carbon monoxide rich syngas for chemical and energetic use. The feedstock, fossil or renewable hydrocarbons, is usually converted at a high global equivalence ratio of $\Phi = 2–3$, with pure oxygen and additional water vapor as moderator. This leads to a flame-like oxidation zone and an endothermic post-flame conversion zone with slow reforming reactions. In order to investigate the interaction of chemistry and fluid mechanics under these conditions, which significantly differ from air-combustion, a laminar reference flame was developed by Stelzner et al. [1]. This flame aims to reproduce the conditions occurring in large-scale gasification processes. The flame was previously investigated experimentally and numerically [3–5]. In these investigations, complex physical and thermo-chemical phenomena were found to be important such as strong differential diffusion, thermal diffusion and slow reforming reactions [3,4]. Furthermore, it was found that gaseous radiation has a significant effect on the flame structure [4]. Thus, simple radiation modeling assuming an optically thin gas and a fully gray medium failed to predict flame temperatures correctly [4]. However, the same numerical and modeling setup was shown to be suitable for a geometrically similar laminar methane–air flame [2,6,7].

A large variety of radiation modeling procedures are available, significantly differing in their complexity and thus their

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http://dx.doi.org/10.1016/j.ijthermalsci.2014.07.022
1290-0729/

computational effort. However, most flame simulations, especially for air combustion, apply very simple radiation modeling procedures, e.g. Refs. [8,9] due to the low computational effort and a reasonable agreement with the experimental data. Furthermore, investigations of radiation modeling in flames were performed previously, where also effects of CO_2 dilution and high temperatures in oxy-fuel combustion were investigated, see e.g. Refs. [10,11]. Here, the importance of accurate radiation modeling could be shown. However, most of these investigations applied 1D simulations or rather simple chemical approaches. In contrast, the computational requirement significantly increases in a 2D/3D laminar flame with detailed chemistry. However, simulations considering detailed radiation modeling are available for laminar flames with air combustion, see e.g. Refs. [12–15] and also turbulent reactive flows, e.g. Refs. [16–19]. A very recent study focused on the experimental and numerical evaluation of soot and radiation characteristics of an oxygen-enhanced laminar ethylene flame applying the SNBCK [20]. In this study, however, no modeling aspects were discussed. The current study thus focuses on the evaluation of radiation modeling approaches in 2D laminar oxy-fuel flames with high temperatures and CO_2 dilution employing complex chemistry.

Radiation modeling is split into two aspects. First, the spectral radiative properties of the gas mixture must be determined. Here, it is important to figure out, what are the radiating chemical species. Further, the fundamental high temperature spectroscopic data for these molecules contribute to the radiative properties in the models. Second, these properties are used to solve the radiative transfer equation (RTE).

For the property calculations, so-called property models are used. A variety of models differing in model complexity, accuracy and computational requirements are available. The most accurate models are the line-by-line (LBL) calculations [21] and the statistical narrow band model (SNB) [22], which are not applicable in large-scale problems with locally varying temperature and species concentrations due to complex chemistry [16]. The statistical narrow band correlated-k model (SNBCK) [23–25] applies a cumulative absorption distribution function methodology (k-distribution) to provide absorption coefficients for the considered bands. This achieves compatibility with the RTE modeling approaches applied in CFD but at a high computational cost. A simpler, popular (less computationally expensive) model are global non-gray absorption coefficients with a weighted sum of gray gases (WSGG) [26]. The spectral line-based weighted sum of gray gases model (SLW), an extension of the WSGG model, employs an absorption line blackbody distribution function (ALBDF) based on a k-distribution methodology for the spectral discretization of the absorption coefficient. In a very similar manner, the full spectrum correlated-k model (FSCK) [27] extends the k-distribution methodology of the SNBCK directly to the whole spectrum resulting in a global model. On the other hand the simplest property models are global gray models, which assume a spectrally constant absorption coefficient, i.e. a totally gray gas, for a given medium. Such models are very computationally efficient but may also introduce a serious error due to the crude assumption for the usually very selective gaseous absorbers and emitters.

Furthermore, several solution methods for the radiative transfer are available. These methods are based on various assumptions resulting in different complexity, accuracy and computational cost. Benchmark solution methods with very high accuracy are the zonal method [26] solving balance equations for the discretized enclosure as well as the statistical Monte Carlo method (MCM). Widely used for CFD applications despite the high computational requirements is the discrete ordinates method (DOM), where the RTE is solved for a set of discrete rays spanning a full sphere around their origin. The P1 approximation employs spherical harmonics to transform the integro-differential problem of solving the radiative transfer into a simple partial differential equation [28]. This method has gained significant popularity due to its simple and economic nature and the good results obtained in optically dense regimes [29]. However, shortcomings of the P1 approximation have been discovered in (partially) optically thin media where radiative intensity varies strongly with direction [30]. One option to overcome these limitations is the modified differential approximation (MDA) proposed by Olfe [31] and extended by Modest [32]. The radiation phenomenon is split into a gas-emitted part modeled with the P1 approach and into a wall-emitted part modeled with ray tracing approaches. Finally, the optically thin method (OTM) is the simplest way of describing the radiative transfer. Absorption by the medium is neglected and therefore the radiative source term can be calculated with a simple algebraic equation.

Hence, numerous possibilities to model radiation at various levels of accuracy and efficiency are available. Further details on the state of the art are given in Appendix A. In the present study, several radiation modeling strategies considering accuracy and/or computational efficiency are tested in fully coupled numerical simulations of a laminar partial oxidation flame and a laminar methane–air flame using an in-house solver, based on OpenFOAM®. Specifically we look at DOM, MDA, P1 and OTM with SLW, WSGG, RADCAL and a chosen constant absorption coefficient, respectively. The chosen combinations of solution methods and property models are evaluated with respect to their performance in the investigated cases.

The governing equations are presented in Sec. 2 with a detailed description of the employed radiation modeling approaches in Sec. 2.2 including a validation in simple, well-established test cases in Sec. 2.3. Further, the numerical setups of the investigated laminar flames are briefly described in Sec. 2.4. Subsequently, the results of the simulations are illustrated in Sec. 3 considering predicted mean absorption coefficients, radiative source terms and temperatures. This leads to a first recommendation concerning the applicability of the discussed radiation models. Finally, a conclusion is given in Sec. 4. Additionally, more detailed results of radiation modeling aspects are shown in Appendix B–E.

2. Mathematical description

The mathematical models and numerical solver for this laminar reactive flow regime are briefly outlined in Sec. 2.1, details are given in Refs. [3,7] with respect to the general transport equations and the diffusion modeling. Further, the radiation modeling is described in detail in Sec. 2.2 and is validated in Sec. 2.3. Finally, the numerical setups for the partial oxidation flame and the methane–air flame are presented in Sec. 2.4.

2.1. Governing equations

The governing transport equations for the density ρ, the velocity $\boldsymbol{u}$, the total enthalpy h and species mass fractions Y_i are

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}) = 0, \tag{1}$$

$$\frac{\partial}{\partial t}(\rho\boldsymbol{u}) + \nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla\cdot\boldsymbol{\tau} + \rho\boldsymbol{g}, \tag{2}$$

$$\frac{\partial}{\partial t}(\rho h) + \nabla\cdot(\rho\boldsymbol{u}h) = -\nabla\cdot\sum_{i=1}^{I} h_i\boldsymbol{j}_i + \nabla\cdot(\lambda\nabla T) - \nabla\cdot\boldsymbol{q}_R, \tag{3}$$