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Evaluation of radiation modeling approaches for non-premixed flamelets considering a laminar methane air flame

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ABSTRACT

The scope of this investigation is to evaluate different radiation modeling approaches for both Lagrangian and Eulerian flamelet models by comparing them to fully resolved simulation data of a non-premixed flame. The numerical investigations are performed for a well established laminar methane diffusion flame [1]. The available experimental data is used to validate the CFD results, which clearly show that radiation must be considered in this flame to accurately describe the flame structure.

Based on the validated CFD results the main focus is to analyze the applicability of radiation modeling approaches within the flamelet framework for unity Lewis number and differential diffusion. An unsteady Lagrangian flamelet model with direct integration of the radiation source term as well as an enthalpy defect formulation for steady and unsteady flamelet calculations are considered. Several model variants are introduced and discussed and the corresponding time scales for mixing, radiation and chemistry are analyzed. Based on the Lagrangian flamelet time and the enthalpy defect, both postprocessed from the CFD solution, flamelet calculations are carried out and detailed comparisons to the CFD simulation results are performed for the temperature and several species along the axis and in several radial slices. The results are finally used to evaluate the different approaches concerning their applicability and accuracy for use in coupled CFD-flamelet simulations.

1. Introduction

Stricter regulations for emissions and efficiency have led to considerable improvements of combustion systems in the past and this trend is likely to continue in the foreseeable future. Both computational modeling and experimental investigations are driving in the development process. In computational modeling, a large challenge is to capture the chemistry-turbulence interaction. One of the popular modeling frameworks is the laminar flamelet concept [2]. In addition, radiation was found to have a significant influence on flame structure, species profiles and pollutant emissions [3,4]. Hence it is crucial to capture this phenomena appropriately.

In order to understand and improve the existing flamelet models the flamelet results can be compared with detailed numerical simulations, e.g. a laminar flame provides the opportunity to solve the full transport equations including realistic chemistry for smaller fuels with reasonable computational effort and no additional models such as for the turbulent viscosity are required.

For this purpose, the selected test case is a confined co-flow axisymmetric non-premixed methane/air laminar flame. The burner characteristics were originally defined by McEnally and Pfefferle [5]. Experimental data for several flame configurations are taken from Bennett et al. [1] with a completely non-premixed configuration. This well-known flame has been numerically investigated in several publications [1,6–9]. Claramunt et al. [7] observed that radiation effects cannot be neglected in the energy equation for this flame. Gaseous thermal radiation in this laminar diffusion methane flame reduces the local temperatures significantly. Hence, the chosen flame setup provides the opportunity to study radiation modeling within the flamelet approach.

Several radiation modeling approaches are reported in the literature [10–12] to account for enthalpy losses within numerical investigations. There are also several different approaches for radiation modeling within the flamelet concept, see e.g. [6,13–16]. The difficulty here is an accurate modeling when using pretabulated flamelet solutions. None of these models has been rigorously tested for a laminar flame. The present study investigates the applicability of those different implementations and derived variants of flamelet radiation models using constant and varying enthalpy defects as well as the radiation source term within the flamelet approach. Hence, this first investigation within the flamelet serves as an analysis which flamelet approach has the highest potential for a CFD coupling. Further investigations concerning a coupling to the CFD code can be based on these findings. The relative radiative heat loss of the considered flame in the temperature

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field is about 15% [1] and thus radiation is investigated in the optically thin radiation limit.

Additionally, differential diffusion effects with or without radiation cannot be described very well using the flamelet concept for this flame in particular [6,9]. On the other hand, assuming a unity Lewis number for all species results in a very good agreement for the flamelet and the CFD results [6,8,9], but leads to considerably different results compared to the experimental data [7,8]. Hence, the effect of differential diffusion is also considered throughout the investigation.

A description of the mathematical formulation of the transport equations is given in Section 2.1. The flamelet framework employed here is described in Section 2.2 inlcuding radiation modeling and the different models that are investigated are listed separately. The CFD solver is validated against experimental data and a flame structure analysis is performed in Section 3. Finally, the results and discussion concerning Lagrangian flamelets and radiation modeling are presented in Section 4.

2. Mathematical model formulation

In the following the mathematical model for both the CFD calculation and the flamelet analysis is presented.

2.1. Detailed CFD calculation

Detailed CFD calculation include the governing transport equations with the radiation source term, the discription of the molecular diffusion, thermodynamic and transport properties as well as the numerical solution method.

2.1.1. Governing transport equations

The governing equations for the density ρ, the velocity vector $\mathbf{v}$, the total enthalpy h (see Eq. (6)) and the species mass fraction Y_i are given below.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{1}$$

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

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \mathbf{v} h) = -\nabla \cdot \mathbf{q} - \dot{Q}_R \tag{3}$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \mathbf{v} Y_i) = -\nabla \cdot \mathbf{j}_i + R_i, \qquad i \in \{1, \ldots, N-1\} \tag{4}$$

Here p is the pressure and $\boldsymbol{\tau}$ the laminar momentum flux, $\boldsymbol{g}$ the gravity, $\mathbf{q}$ the laminar energy flux, R_i the chemical source term and $\mathbf{j}_i$ the laminar diffusive mass flux (see Eq. (10)). The total enthalpy h is defined by

$$h(T) = \int_{T_0}^{T} \sum_{i=1}^{N} Y_i c_{p,i}(T')dT' + \sum_{i=1}^{N} Y_i h_{0,i} \tag{6}$$

where $h_{0,i}$ denote the standard formation energy of the species i at the reference temperature T_0. For the laminar flame simulation the energy equation was simplified by neglecting viscous dissipation and the substantial derivative of the pressure within the small Mach number limit. The pressure was assumed to be constant and equal to the static pressure. Further, the reversible exchange of mechanical energy into internal energy is extremely low for this kind of open flame [2]. The radiative source term $\dot{Q}_R$ was calculated with an optically thin radiation model

$$\dot{Q}_R = 4\sigma p \sum_{i=1}^{N} X_i a_i (T^4 - T_{back}^4) \tag{7}$$

based on the Planck mean absorption coefficient a_i of species i as can be found in [17]. Further, σ is the Stefan–Boltzmann constant, T the local temperature, T_{back} = 298 K the background temperature and X_i the mole fraction. The radiative species considered are H_2O, CO_2 and CO. The optically thin radiation model was applied by many groups with success, e.g. [18,19] and self-absorption was found to be negligible, e.g. in the CH_4-air flame studied in [17]. On the other hand, shortcomings of this model were found, e.g. for CO_2 dilution and low-strain flames even in CH_4-air flames in [20–22] and the influence of self-absorption was found to be evident but e.g. smaller than the kinetic mechanism in [23]. However, for the considered non-premixed CH_4-air flame a relative radiative heat loss of about 15% as found in [1] justifies the assumption of optically thin radiation and a comparison with the experimental data showed reasonable agreement, see Section 3.

2.1.2. Molecular diffusion flux modeling

For a detailed molecular diffusion flux modeling taking into account Stokes' law for Newtonian fluids within Eq. (2), the laminar momentum flux $\boldsymbol{\tau}$ reads:

$$\boldsymbol{\tau} = \mu(\nabla \mathbf{v} + \nabla \mathbf{v}^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{v})\mathbf{I} \tag{8}$$

Here, μ is the molecular mixture viscosity and the symbol $\mathbf{I}$ represents the identity matrix. The laminar energy flux $\mathbf{q}$, solved to fulfill Eq. (3), is described by:

$$\mathbf{q} = \underbrace{\sum_{i=1}^{N} h_i \mathbf{j}_i}_{\text{Inter-diffusion}} \underbrace{-\lambda \nabla T}_{\text{Fourier's law}} \tag{9}$$

Inter-diffusion represents the redistribution of internal energy due to species diffusion with the specific enthalpies of each species h_i. In addition, Fourier's law describes the diffusive flux of energy due to heat conduction, where λ is the mixture heat conductivity. Further, Dufour and Soret effects have been neglected so far, which becomes a reasonable simplification for this flame as seen in [7]. The laminar diffusive flux $\mathbf{j}_i$ in Eqs. (4) and (9) was expressed in the form of a diffusion velocity relative to the mass average velocity. This describes the transport of species i mathematically due to a mixture-averaged (MA) diffusion approach via:

$$\mathbf{j}_i = \rho(\mathbf{u}_{D,i} + \mathbf{u}_C)Y_i, \qquad i \in \{1, \ldots, N\} \tag{10}$$

The ordinary diffusion velocity $\mathbf{u}_{D,i}$ is expressed as the sum of two diffusion velocities [24]:

$$\mathbf{u}_{D,i} = -\frac{1}{Le_i}\frac{\lambda}{\rho c_p Y_i}\nabla Y_i - \frac{1}{Le_i}\frac{\lambda}{\rho c_p \overline{M}}\nabla \overline{M}, \qquad i \in \{1, \ldots, N\} \tag{11}$$

with $\overline{M}$ being the mean molecular weight of the mixture. A pseudo-Fickian diffusion coefficient $D_{m,i}$ of a species i into the mixture m was defined based on Bird et al. [25].

$$D_{m,i} = \frac{1 - Y_i}{\sum_{j \neq i}^{N} (X_j / \mathcal{D}_{ij})}, \qquad i \in \{1, \ldots, N\} \tag{12}$$

The first-order binary diffusion coefficient $\mathcal{D}_{ij}$, describing the diffusive transport from species i into species j, follows the Chapman-Enskog theory [26]. Based on this averaged diffusion coefficient, the Lewis number in Eqs. (11) and (14) is defined as:

$$Le_i = \frac{\lambda}{\rho c_p D_{m,i}}, \qquad i \in \{1, \ldots, N\} \tag{13}$$

The approach using MA diffusion coefficients usually does not fulfill the constraint that all diffusion fluxes add up to zero. Thus, to ensure mass and especially element conservation, a correction velocity (Eq. (14)) has to be evaluated following Coffee and Heimerl [27]: