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Modelling heat loss effects in high temperature oxy-fuel flames with an efficient and robust non-premixed flamelet approach

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ABSTRACT

The non-premixed steady flamelet model is extended by two simple, robust and effective heat loss modelling approaches. The heat release damping (HRD) approach decreases the chemical source term in the energy equation by a constant factor, while the artificial radiation (AR) approach introduces an augmented temperature dependent radiative source term. The models are tested in a simulation of the 0.78 MWth IFRF (International Flame Research Foundation) pilot scale, non-premixed, natural gas/oxygen flame. Both approaches are applied in steady laminar flamelet calculations with detailed chemistry, tabulating the thermo-chemical state as a function of mixture fraction and normalised heat loss. The turbulence-chemistry interaction is modelled using the β-PDF approach. An enthalpy transport equation is solved to keep track of the heat loss, while radiative heat transfer is calculated by the P-1 model. We observe that the major species, temperature, velocities and velocity fluctuations show a good agreement with the available experimental data. The heat loss modelling yields a significant improvement over the adiabatic model. Interestingly, both heat loss models (HRD and AR) show negligible differences in the simulations of the turbulent flame and permit to apply the steady laminar flamelet model to oxy-fuel processes in a simple, robust and user friendly manner.

1. Introduction

High temperature combustion processes using pure oxygen (oxy-fuel) are attractive for their low NO_x emission and the modelling of such flames on technically relevant scales has gained much attention recently. Global reaction mechanisms, which have been developed for air flames, are not capable of predicting the thermophysical state of oxy-fuel flames, since the released local reaction energy is much higher and not diluted by nitrogen components. More detailed and computationally expensive combustion mechanisms like GRI 3.0 [1] for methane/oxygen flames must therefore be chosen, or specifically reduced for the particular conditions. Furthermore, as a result of the very high flame temperatures due to the lack of diluting gases, the effect of radiative heat transfer in pure oxy-fuel flames becomes more significant than in air flames and must be included in the combustion model [2]. The strong impact of heat losses on gas composition in oxy-fuel flames has been shown by Brink et al. [3] and Bruessing et al. [4]. They simulated an oxy-fuel flame using an equilibrium approach and a global scheme for the chemical kinetics in combination with the eddy dissipation concept and the discrete transfer radiation model and showed that radiative heat losses are crucial for oxy-fuel processes, as equilibrium states drastically change with enthalpy. However, expensive and complicated calculations with detailed chemistry and species transport are a big obstacle for industry, while such a high degree of detail is not needed for most industrial applications.

Another difficulty is that in non-premixed turbulent flames, combustion takes place in the mixing layer on small scales. To overcome this problem, a number of models have been developed and successfully applied. These models include the conditional moment closure [5], the linear eddy model [6], the eddy dissipation concept [7], the transported probability density function method [8] and the steady laminar flamelet model (SLFM) [9–13]. To predict the flame conditions for igniting and quenching states, Pitsch made use of the unsteady flamelet equations [14], where Lagrangian time histories were required to predict the flamelet states. In order to take account of ignition and quenching states with less computational effort, the SLFM model for non-premixed flames was extended by a flamelet progress variable (FPV) – a linear combination of reaction products [15,16]. These basic tabulated chemistry models separate the CFD simulation from the chemical calculation and deliver a sufficient accuracy for most applications. Especially the flamelet approach allows the reduction of computational effort by tabulation of the thermochemical state as a function

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of only few variables, like the mixture fraction and the scalar dissipation rate, while the flamelet tables are generated by solving the one dimensional flamelet equations. Because the flamelet model was developed for processes in which heat losses are less important, enthalpy losses are often neglected. Non-adiabatic, non-premixed flamelets for air flames were modelled by Bray and Peters [17] and Hossain et al. [18], using an enthalpy defect approach. The heat loss was enforced by lowering the inlet temperatures of the flamelets, which limits the amount of heat loss that can be considered. Chen et al. [19] introduced a radiative sink term to the steady laminar flamelet equation and realized thereby another heat loss model, which was later extended by Rogg and is applied in this work. Ihme and Pitsch [20] introduced a comparable approach by applying a radiation source term to a transient flamelet in order to capture different levels of heat losses for constructing a flamelet library, which was applied to LES.

In the context of premixed combustion, heat loss effects in flamelet generated manifolds were studied by Fiorina et al. [21], Ketelheun et al. [22], van Oijen et al. [23], Proch and Kempf [24], Tay-Wo-Chong et al. [25] and others, but for combustion with air only. Nevertheless, the approach suggested by Proch is the basis for one of the two approaches tested in the present paper. The amount of heat loss in high-temperature oxy-fuel processes differs clearly from that of air flames and was rarely simulated with flamelet approaches. The present paper extends the steady flamelet model by two different approaches which can account for very high heat losses. The approaches are introduced and validated against the OXYFLAM Burner case A [3]. Key targets for the development of both approaches were simplicity, robustness and hence applicability in industry, leading to models that can easily be used rather than just providing optimal results in a carefully controlled research environment.

2. The laminar non-premixed flamelet model

The laminar flamelet equations are formulated according to Peters [9,10]. They were obtained by coordinate transformation from physical space into mixture fraction space Z. Thus, in mixture fraction space, the flamelet is fully described by the temperature (1) and species transport (2) equations for a unity Lewis number:

$$\rho\frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2}+\sum_{k=1}^{K}\frac{h_k}{c_p}\dot{\omega}_k=0 \tag{1}$$

$$\rho\frac{\chi}{2}\frac{\partial^2 Y_k}{\partial Z^2}+\dot{\omega}_k=0 \tag{2}$$

The quantity χ represents the scalar dissipation rate, which is given by following term in three dimensional physical space:

$$\chi=2D\ |\nabla Z|^2 \tag{3}$$

The scalar dissipation in the mixture fraction space can be approximated by [26]:

$$\chi=\chi_{st}\frac{f(Z)}{f(Z_{st})} \tag{4}$$

The quantities χ_{st} and Z_{st} are used for parametrisation and are the scalar dissipation rate and the mixture fraction at stoichiometric conditions. The function $f(Z)$ gives the behaviour of χ in dependency of Z.

For the counter flow situation, Peters [9] gives the function as:

$$\chi(Z)=\frac{a}{\pi}e^{(-2[\mathrm{erfc}^{-1}(2Z)]^2)} \tag{5}$$

The term $\mathrm{erfc}^{-1}(x)$ represents the inverse of the complementary error function, where a represents the strain rate.

The flamelet equations can also be solved in physical space, with subsequent mapping to mixture fraction space, for example by solving reactive opposed jet configurations in physical space. This is described by Kee et al. [27], where the equations for continuity (6), radial momentum (7), energy (8) and species transport (9) of the opposed jet are given in one dimension.

$$\frac{d(\rho u)}{dz}+2\rho V=0 \tag{6}$$

$$\rho u\frac{dV}{dz}+\rho V^2=\frac{d}{dz}\left(\mu\frac{dV}{dz}\right)-\Lambda \tag{7}$$

with $\Lambda=1/\rho\ \partial p/\partial r=const.$ and $\rho V=\rho\ v/r=-dU(z)/dz$, the momentum equation is a function of the axial coordinate z only. With these assumptions, the temperature and compositions are given as:

$$\rho u c_p\frac{dT}{dz}=\frac{d}{dz}\left(\lambda\frac{dT}{dz}\right)-\sum_{k=1}^{K}\rho Y_k V_k c_{pk}\frac{dT}{dz}-\sum_{k=1}^{K}h_k M_k\dot{\omega}_k \tag{8}$$

$$\rho u\frac{dY_k}{dz}=-\frac{d}{dz}(\rho Y_k V_k)+M_k\dot{\omega}_k \tag{9}$$

Here, M_k represents the molecular weight, while $\dot{\omega}_k$ denotes the chemical source term and V_k the diffusion velocity of the species k.

3. Heat loss effects in laminar non-premixed flamelets

3.1. Generating the flamelet data

In this section, the two different approaches for the generation of the non-adiabatic flamelet databases will be discussed.

The heat release damping (HRD) approach, suggested by Proch et al. [24] for premixed flames, scales the chemical source term in the temperature equation by a constant factor. Thus, the heat loss itself is treated like an artificial damper, acting on the same time scale as the chemical heat release. This is based on the assumption that different origins of heat losses lead to similar flamelet libraries. Accordingly, the HDR approach is applied to the counterflow configuration by scaling the heat release term of the aforementioned temperature Eqs. (8) and (1), which become transformed to Eq. (10) in physical space and Eq. (11) in mixture fraction space:

$$\rho u c_p\frac{dT}{dz}=\frac{d}{dz}\left(\lambda\frac{dT}{dz}\right)-\sum_{k=1}^{K}\rho Y_k V_k c_{pk}\frac{dT}{dz}-(1-f_L)\sum_{k=1}^{K}h_k M_k\dot{\omega}_k \tag{10}$$

$$\rho\frac{\chi_{st}}{2}\frac{\partial^2 T}{\partial Z^2}+(1-f_L)\sum_{k=1}^{K}\frac{h_k}{c_p}M_k\dot{\omega}_k=0 \tag{11}$$

The scaling factor f_L ranges from 0 (adiabatic) to 1 (no heat release). The advantage of the scaling is that large heat losses can be realised very simply, without introducing non-linear terms. In fact, the system reacts more stably and converges faster due to the damping character of the heat loss term. The physical motivation for this modelling approach may seem questionable, but the results of the present paper show its capability. By comparing the results of a freely propagating flame and a burner stabilized flame using the same amount of heat loss, Fiorina et al. [21] demonstrated that generating heat losses by different procedures is applicable for (premixed) combustion. Proch et al. [24] applied the HRD approach for premixed flamelet generated manifolds (FGM) and came to the same conclusion.

The second heat loss approach is the artificial radiation (AR) approach. It introduces a radiative heat sink term to the temperature Eqs. (8) and (1) [19], in order to achieve the losses for the flamelet table generation. The factor ϵ is comparable to the factor f_L of the HRD approach, although it is not bounded by an upper limit. This means that ϵ can be set from 0 (adiabatic case) up to an arbitrary value, at which extinction occurs. For this model, the temperature equations in physical (12) and mixture fraction (13) space read:

$$\rho u c_p\frac{dT}{dz}=\frac{d}{dz}\left(\lambda\frac{dT}{dz}\right)-\sum_{k=1}^{K}\rho Y_k V_k c_{pk}\frac{dT}{dz}-\sum_{k=1}^{K}h_k M_k\dot{\omega}_k-\frac{dq_r}{dz} \tag{12}$$