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Transported scalar PDF calculations of a swirling bluff body flame ('SM1') with a reaction diffusion manifold

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ABSTRACT

The modeling of a reacting swirling flow behind a bluff-body burner (SM1) in the framework of RANS and transported scalar PDF is presented. The EMST mixing model is applied and the composition space is reduced to mixture fraction (Z) and a progress variable (CO_2 mass fraction, Y_{CO_2}) by means of a Reaction Diffusion Manifold (REDIM). With an ad hoc adjustment of the turbulent Schmidt number, the mean flow and mixing fields obtained are comparable to LES results from the literature. The REDIM reduction of the composition space to (Z, Y_{CO_2}) is discussed and its validity for the present swirling flame is first considered by an a priori comparison with experimental data. The (Z, Y_{CO_2}) – scatter plots from the transported PDF calculation show the capacity to reproduce the mixing between fresh air and hot products in the recirculation zone above the bluff-body. However, too little scatter is observed. The study of tracer trajectories helps to better understand the capacities and limitations of the modeling approach. Zones where mixing competes with reaction can be identified, and coincide with the highly rotating collar region where local extinction is expected to take place. However, in our modeling, the competition between mixing and reaction is not enough to lead to local extinction. An important modeling deficiency is claimed to be the use of a mean time scale in the EMST mixing model, which limits the possibilities to model high scalar dissipation rate events.

1. Introduction

Swirl-stabilized turbulent flames are important for many industrial applications, because the swirling motion creates recirculation zones which enhance mixing and stabilize the flame. This leads to better combustion efficiency and less pollutant formation. However, swirl flames are not yet fully understood. One of the complex phenomena concerns vortex breakdown leading to flow instability, i.e. a precessing vortex core and periodically expanding/shrinking recirculation zone. Several modeling approaches have been used to simulate these complex flows. The unsteady 3D effects are in principle better handled by LES than RANS, but LES calculations have a higher computational cost. Therefore, we consider it still useful to study hybrid RANS/PDF (probability density function) calculations, in particular for cases where there is no strong influence from a precessing vortex core.

Besides flow field complexity, local extinction is also important, as it leads to, e.g. incomplete combustion and therefore more pollutants. Physically, extinction in laminar non-premixed flames occurs due to local high gradients, resulting in excessive local heat (and mass) transfer, which cannot be sustained by local heat production from chemical reactions [1]. It is characterized by the local Damköhler number, defined as the inverse of the product of the chemical time scale and the scalar dissipation rate. In [2] Kolmogorov scale eddies are stated to be important in the extinction of turbulent non-premixed flames with a similar physical mechanism as for laminar flames. In [3], on the other hand, extinction is said to be caused by large-scale eddies through total flame stretching, and not through small-scale flame wrinkling. There are also other mechanisms for local extinction, e.g. radical pools being swept away by a vortex [4]. Apart from experiments, also DNS studies have been done to investigate local extinction of non-premixed flames. In [5], following Lagrangian particles in the flow, it is shown that local extinction is purely due to fluctuations of the scalar dissipation rate. In [6], where DNS with one-step global reaction is performed in order to study the influence of turbulent mixing on re-ignition, local extinction is again shown to be due to fluctuations of the scalar dissipation rate, causing excessive heat loss.

In transported PDF modeling, traditional mixing models use the mean integral turbulent time scale in order to determine the mixing time scale. Moreover, in a RANS framework, the flow and

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mixing fields in physical space are steady and not all fluctuations in scalar dissipation rate can be expected to be captured. The PSP model [7–10], which uses one-dimensional parametrized scalar profiles (PSPs) to model the unresolved scalar length-scales characterizing the scalar micro-mixing, can capture the fluctuations in scalar dissipation rate better, as it provides joint statistics of scalars and their scalar dissipation rate. In LES, resolved fluctuations in instantaneous flow and mixing fields result in resolved fluctuations of the scalar dissipation rate. In [11], where LES calculations with presumed PDF modeling and a flamelet generated manifold [12] are discussed, coherent structures of high scalar dissipation are seen to lead to flame stretching and local extinction.

In the present study, we investigate the swirling bluff body flame SM1 [13–17], which has been studied numerically in the past by several authors. Masri et al. [18] performed a joint velocity-scalar-frequency PDF calculation for a reacting case. James et al. [19] performed an LES/PDF calculation of two reacting cases (SM1 and SMA1) with satisfactory results. Unfortunately no detailed study of turbulence-chemistry interaction is reported. LES results of non-reacting and reacting cases have been presented with flamelet chemistry in [20–23] and with FGM chemistry in [24]. A comparable quality of flow and mixing field results is obtained here with axisymmetric steady RANS calculations with a non-linear k–ϵ model [25]. The obvious advantage of this approach is that transported (scalar) PDF simulations can be performed within reasonable computing time, in order to study turbulence-chemistry interaction.

For chemical reaction, a pre-calculated chemistry table is used. We adopt the Reaction Diffusion Manifold (REDIM) [26] approach, as it has already been used for calculations of non-swirling bluff-body flames [27,28]. In the latter, the combination of REDIM with EMST mixing model [29] led to reasonable results, but scatter in Y_{CO_2} space was clearly under-estimated. This was not attributed to the use of REDIM as reduced chemistry, but to the localness property of EMST leading to too little local extinction. In the present paper, we discuss results with similar model settings, but for a swirling flame. Moreover the trajectories in physical and composition space of computational particles are studied in detail. This proves to be useful in order to correlate positions in composition space and in physical space. It also permits to focus on the distinction between mixing and extinction, and to discuss the limitations of the modeling in a more precise manner—for instance to better formulate the limitation of EMST instead of generally referring to its 'localness in composition space'.

2. Test case description and modeling framework

2.1. Sydney swirling flame SM1

Figure 1 depicts the burner. The bluff body (50 mm diameter) contains the central fuel jet (3.6 mm diameter). Swirling air is provided through a 5 mm wide annulus surrounding the bluff-body. The swirl component is created by three tangential ports. The burner is placed inside a wind tunnel with square cross section. A wide range of testing conditions has been examined experimentally [13–17]. All cases are characterized by: the bulk axial velocity of the central jet (U_j), the bulk axial and tangential velocities of the swirling air annulus (U_s and W_s) and the bulk axial velocity of the co-flow of the wind tunnel (U_e).

We consider flame SM1 only, because for this flame the precessing vortex core is the weakest. This is important since we consider here a steady RANS modeling framework. In the experiments [17], velocity measurements were performed with CNG, while CH_4 was used for the composition measurements. No physical changes in the flow field are reported. We use CH_4 as fuel in the simulations. The stoichiometric mixture fraction is $Z_{st} = 0.054$. The flow parameters are summarized in Table 1 with the swirl number geometrically defined as $S_g = W_s/U_s$. The flow field of SM1 contains two recirculation zones: one close to (and caused by) the bluff body and one further downstream near the central axis (caused by vortex breakdown). The simulation results (Fig. 1, right) reproduce the qualitative experimental finding that the recirculation zones are separated by a region of high shear stress which coincides with a highly rotating collar. In [17], local extinction is believed to occur in this region of high shear stress between the two recirculation zones, while the hot, re-circulated combustion products from the second recirculation zone are believed to cause re-ignition.

2.2. Turbulence-chemistry interaction in RANS modeling framework

The non-linear k–ϵ turbulence model of [25] is used, as it takes into account the effect of streamline curvature and rotation on turbulence.

In order to deal with turbulence-chemistry interaction, a transported scalar PDF approach is used. In the transported scalar PDF approach, the transport equation is modeled and solved for the mass density function $\mathcal{F}_\phi(\boldsymbol{\psi}) = \rho(\boldsymbol{\psi}) f_\phi(\boldsymbol{\psi})$, with f_ϕ the joint scalar PDF [31], and with $\boldsymbol{\phi}$ the composition vector of independent scalars, (in this work) consisting of mixture fraction, Z, and CO_2 mass fraction, Y_{CO_2}:

$$\frac{\partial \mathcal{F}_\phi}{\partial t} + \frac{\partial \widetilde{U}_j \mathcal{F}_\phi}{\partial x_j} + \frac{\partial}{\partial \psi_\alpha}[S_\alpha(\boldsymbol{\psi})\mathcal{F}_\phi] = \underbrace{-\frac{\partial}{\partial x_j}\left[\left\langle u_j''|\boldsymbol{\psi}\right\rangle \mathcal{F}_\phi\right]}_{\text{gradient diffusion}} - \frac{\partial}{\partial \psi_\alpha}\left[\underbrace{\frac{1}{\rho(\boldsymbol{\psi})}\left\langle -\frac{\partial J_j^\alpha}{\partial x_j}|\boldsymbol{\psi}\right\rangle}_{\text{mixing model}} \mathcal{F}_\phi\right] \quad (1)$$

In this general equation, S_α is the reaction source term for scalar α and $\boldsymbol{J}^\alpha$ the molecular scalar flux.

A Lagrangian particle method is used to model and solve (1) [31]. The two terms on the right hand side need to be modeled. For the first term, the effect of conditional velocity fluctuations is modeled as a turbulent diffusion flux, by using a gradient diffusion model:

$$\frac{\partial}{\partial x_j}\left[\langle u_j''|\boldsymbol{\psi}\rangle \mathcal{F}_\phi\right] = -\frac{\partial}{\partial x_j}\left[\Gamma_T \frac{\partial(\mathcal{F}_\phi/\langle\rho\rangle)}{\partial x_j}\right], \quad (2)$$

where Γ_T is the turbulent diffusivity, modeled as $\Gamma_T = \mu_T/\mathrm{Sc}_T$, with μ_T the dynamic turbulent viscosity (from the model of [25]), and with the turbulent Schmidt number Sc_T chosen to be variable depending on $\widetilde{u}\widetilde{v}$ (see Appendix A). For the second term on the right hand side of Eq. (1), which represents the effect of molecular diffusion in the turbulent flow, we use the EMST mixing model [29] with $C_\phi = 2$.

2.3. Hybrid RANS/PDF approach

All calculations are steady axisymmetric and are performed with the same code PDFD [32], which has already successfully been applied to non-swirling Sydney bluff-body burner cases [27,28]. In transported PDF calculations, the equations are solved using a consistent hybrid finite-volume/particle method [32]. Mean velocity $\widetilde{U}$, turbulent kinetic energy k and turbulent dissipation rate ϵ are obtained by a standard finite-volume (FV) method based on a pressure correction algorithm. The transport equations for turbulent kinetic energy (k) and turbulent dissipation rate (ϵ) solved in the FV method provide the turbulent timescale, required in the mixing model. The mean density $\langle\rho\rangle$ in the FV method is obtained from the iteration averaged mean density in the particle method (averaged over 1000 particle time steps).