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Laminar near-wall combustion: Analysis of tabulated chemistry simulations by means of detailed kinetics

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ABSTRACT

Chemistry pre-tabulation is well suited to include information of detailed reaction kinetics at reasonable computational costs to allow for simulations of realistic devices. In order to evaluate its accuracy in the near wall region, a study with numerical simulations of flame–wall-interaction is performed in this work. A laminar side-wall-quenching scenario is considered to judge on the prediction of the global flame behavior as well as on local species formation of practical relevance. The configuration considered represents a subsection of a side-wall-quenching burner introduced recently with the purpose of numerical validation in mind. The measured temperature and carbon-monoxide concentration are used to identify deficiencies of the tabulated chemistry approach. Furthermore, detailed chemistry simulations are carried out to identify the root cause for those deficiencies. The corresponding analysis is based on the transformation of the species transport equation into the composition space where the physical significance of the scalar dissipation rates provides clear indications regarding the pre-tabulation assumptions. The evaluation of individual terms allows to quantify the interaction of flamelets in the near-wall region where diffusive fluxes cause a departure from the presumed manifold. Based on this analysis, improvements are then suggested. First, as a proof of concept, the direct tabulation of the thermo-chemical states obtained by the detailed chemistry simulation is applied to evaluate whether the reduction to controlling variables is in general possible in such a physical scenario. Second, as an alternative way of pre-tabulating, the reaction-diffusion-manifold (REDIM) approach is then adopted. By building the REDIM based on a gradient estimate from a computationally inexpensive transient one-dimensional flame–wall-interaction simulation it is possible to obtain realistic dissipation rates without a-priory knowledge. By this approximation a significant gain in prediction is achieved when compared to the original tabulation.

1. Introduction

In many technical combustion systems, the reaction zone approaches the enclosing walls rendering the flame–wall-interaction (FWI) an important area of research. In these devices, the flame can be in direct contact with a relatively cold wall, which can have an influence on the efficiency of the combustor as well as on the pollutant formation (Poinsot and Veynante, 2005). The phenomena become of increasing importance with e.g. downsizing concepts for internal combustion engines (ICE) (Dreizler and Böhm, 2015) or lean burn technologies within aero engines (Lazik et al., 2008).

Within scientific research as well as industrial developments, the numerical simulation represents a powerful tool of increasing importance. However, current capabilities enforce a trade-off regarding the accuracy, computational effort and the problem size considered. Besides the well-known turbulent closures required within computational fluid dynamics (CFD) of complex geometries, the chemistry treatment causes severe restrictions. At this, the application of a detailed reaction mechanism represents the most accurate one but is limited to simple domains since it requires to solve for all relevant species usually interacting in hundreds of elementary reactions. Accordingly, this approach has been exclusively applied to FWI in generic configurations to obtain a fundamental insight and understanding of the underlying processes. Numerous simulations covered the transient one-dimensional head-on-quenching (HOQ) scenario, which mimics the situation found in ICE where the flame approaches the wall with a parallel alignment. Valuable knowledge has been gained by investigating processes like unburnt hydrocarbon formation, heat fluxes, surface reactions, and the relevance of different transport phenomena depending on parameters like the fuel employed or the wall

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temperature (Ezekoye et al., 1992; Wichman and Bruneaux, 1995; Popp et al., 1996; Popp and Baum, 1997; Hasse et al., 2000). Likewise, similar studies have been carried out for the steady two-dimensional side-wall-quenching (SWQ) (Andrae et al., 2002; 2008). Utilizing significant computational resources, Gruber et al. (2010, 2012, 2015) investigated the FWI in a turbulent channel flow using direct numerical simulations (DNS) and a detailed hydrogen reaction mechanism. The studies provided insight into the flame-turbulence regimes in the near wall region and the mechanism of boundary layer flashback.

To enable the simulation of more complex geometries or even real devices, the chemistry has to be approximated in order to significantly lower the computational effort by reducing the number of variables computed and the spatial and temporal resolution requirements. A common approach is to use reduced mechanisms. They can be derived as a subset of the full mechanism by identifying the rate-determining reactions. Besides such mathematical reductions, often even just single step (or very few steps) are used to represent the chemistry. Due to the large loss of information, it is necessary to adjust their parameters to meet certain physical properties like the flame speed or its temperature. An alternative to reduced mechanisms is to use lookup tables. Such a lookup table contains all required thermo-chemical states parameterized based on only a few controlling variables that have to be solved for in the CFD. By pre-computing this chemistry database by means of the full reaction mechanism it enables to include valuable information of the underlying detailed chemistry into the CFD. However, obviously, with the type of detailed chemistry simulation conducted in advance, assumptions have to be made. If the actual physical situation differs from the pre-tabulation scenario, errors are introduced.

The most basic example of pre-tabulation is the parameterization onto the mixture fraction f for the prediction of non-premixed flames (see e.g. Burke and Schumann, 1928; Zel'dovich, 1949; Williams, 1985; Peters, 2000). If the strain rate in the real flow is different from the detailed chemistry simulation employed for the pre-tabulation, errors in the burnt gas temperature and species arise. This can be accounted for by introducing the strain by means of the scalar dissipation rate of the mixture fraction as an additional table dimension (Peters, 1984, 1986).

If premixing takes place the approach fundamentally fails due to its intrinsic *mixed is burnt* assumption and it is required to employ premixed flames for the pre-tabulation by employing a reaction progress variable $\mathscr{Y}$ (Gicquel et al., 2000; van Oijen and de Goey, 2000). This approach in turn can be extended for inhomogeneous systems by adding the mixture fraction as a second controlling variable (see e.g. Oijen, 2002; Ketelheun et al., 2009). However, again errors are introduced based on the dissipation rate of the latter. Accordingly, pre-tabulation can introduce errors as exemplified by the scalar dissipation rate or completely fail when the selected controlling variables cannot even approximate the physical situation as required by the *mixed is burnt* assumption. Hence, for an accurate prediction, the required a-priori knowledge and table dimensions can represent a significant challenge for its application. This is demonstrated by the multi-dimensional flamelet generated manifold approach of Nguyen et al. (2009) which requires a five-dimensional table for a physical situation that can be described by only two variables, i.e. besides the two variables the individual scalar dissipation rates as well as their cross scalar dissipation rate is required for the full description. Building and employing such a table is rather difficult and therefore generally less universal tables are utilized and certain errors are accepted.

In this work, we want to analyze chemistry tabulation approaches in the context of FWI. In contrast to the above-mentioned scenario where the alignment of concentration gradients determines the suitability and accuracy of the approach, within FWI the thermal boundary layer can cause a departure from the pre-computed states. For the analysis we consider a laminar methane-air SWQ configuration. The burner has been investigated experimentally by Jainski et al. (2017b) providing the near wall evolution of the temperature and CO concentration as a reference. The first simulations of this configuration have been carried out by Heinrich et al. (2017a) by means of a tabulation approach. They obtained satisfactory results regarding the flame shape and temperature distributions but significant errors considering the CO prediction. On the other hand, Ganter et al. (2017), who simulated only a sub-domain of the burner covering the near-wall region which allowed for the application of detailed chemistry, were able to match the measurements very closely. Accordingly, the simulation with pre-tabulation fails to predict species like CO due to the chemistry approximation, which we will detail in this work. We consider the most obvious choice of premixed tabulations based on a progress variable ($\mathscr{Y}$) and the enthalpy (h) to account for the heat losses. Specifically the objectives are:

- Conduct simulations using tabulation as well as detailed chemistry to show the root cause of the deficiencies. This is done by considering the processes in composition space where departures from the exact equation can be quantified by means of the scalar dissipation rates.
- Introduce an alternative approach that accounts for the enthalpy fluxes in the pre-tabulation process to improve the prediction quality for the FWI without increasing neither the tabulation nor the simulation effort noticeably.

In the following, Section 2 outlines the configuration considered followed by Section 3 providing information on the numerics including the detailed and tabulated chemistry. Section 4 then contains the results and the error analysis of the tabulation. Finally, in Section 5, improved tabulation techniques are suggested and evaluated. At the end a summary is given.

2. Configuration

The configuration that is analyzed in this work is sketched in Fig. 1. A stoichiometric methane-air mixture issues from the nozzle at ambient conditions ($p = 1$ atm, $T = 300$ K) and passes a rod ($\varnothing$ 1 mm) where a V-flame stabilizes. The nozzle flow Reynolds number is about 5000. The left flame branch approaches the wall at an angle of approximately 10° where the SWQ takes place. The wall temperature slightly varies along the water-cooled wall and is estimated to be between 300 and 350 K based on thermocouple measurements beneath the wall surface (Jainski et al., 2017a; 2017b). The burner has a thermal power of approximately 9.3 kW. As shown by Ganter et al. (2017), the relevant processes may be analyzed considering a reduced two-dimensional sub-domain (gray in Fig. 1) which enables the use of detailed chemistry simulations. The sub-domain, which covers about 80% of the considered flame branch, is magnified on the right of Fig. 1. Based on the experimental estimation, the wall is assumed to have a constant temperature of 300 K. Catalytic effects were not included since they are negligible at these wall temperatures (Popp and Baum, 1997). The reduction of the 3D experimental configuration implies the usage of a generic parabolic inflow velocity profile, which is visualized in Fig. 1 by white arrows on blue ground. The maximum velocity of the fresh mixture is 1.7 m/s. Since no rod is included in the 2D sub-domain, the flame is stabilized by injecting hot exhaust gas under equilibrium conditions ($T = 2202$ K) in a 0.5 mm wide section of the inlet as marked with red color in Fig. 1. The velocity of the hot gas was set to 3.81 m/s to compensate partially for the difference in density of the fresh and the burned inlet gases. Zero-gradients boundary conditions were applied at all outlets for velocity, enthalpy and species, which result in the freely developed velocity profiles given in Fig. 1.

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