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Numerical analysis of laminar methane–air side-wall-quenching

Sebastian Ganter[a,*], Arne Heinrich[a], Thorsten Meier[a], Guido Kuenne[a], Christopher Jainski[b], Martin C. Rißmann[b], Andreas Dreizler[b], Johannes Janicka[a]

[a] *Institute of Energy and Power Plant Technology, TU Darmstadt, Jovanka-Bontschits-Strasse 2, Darmstadt 64287, Germany*
[b] *Institute Reactive Flows and Diagnostics, TU Darmstadt, Jovanka-Bontschits-Strasse 2, Darmstadt 64287, Germany*

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ABSTRACT

Flame-wall-interaction (FWI) is investigated numerically using a premixed stoichiometric Side-Wall-Quenching configuration. Within the 2D fully resolving laminar simulation, detailed chemistry is used to study the stationary quenching of a methane–air (CH_4) flame at an isothermal inert wall of 300 K. The investigation is related to a recent experimental study that revealed that the carbon-monoxide distribution substantially differs in the near-wall region when compared to an undisturbed flame. Simulations are carried out using different reaction mechanisms (GRI and Smooke) as well as diffusion treatments (unity Lewis and mixture averaged transport) and the results are compared to the measured temperature and CO concentrations. Specifically regarding the latter, being an important pollutant, recent attempts based on tabulated chemistry failed in predicting its near-wall accumulation. Accordingly, within this work the detailed chemistry simulations are used to investigate the origin of CO near the wall. Therefore, a Lagrangian analysis is applied to quantify the contribution of chemical production and consumption as well as diffusion to understand the root mechanism of the high CO concentrations measured. The analysis revealed that the high CO concentrations near the wall results from a transport originating from CO produced at larger wall distances. In that region being not submitted to large heat losses, a high chemical activity and corresponding CO production is found. Accordingly, a diffusion process is initiated towards the wall where the chemical sources itself were actually found to be negative.

1. Introduction

The investigation of flame-wall-interaction (FWI) constitutes an important research field since in many technical combustors the reaction zone approaches the enclosing walls. In some applications flames are in direct contact with a relatively cold wall which can have an influence on the efficiency of the combustor and also on the formation of pollutants [1]. Downsizing concepts as found in IC engines which increase the surface to volume ratio may further amplify the importance of wall effects [2]. In order to optimize combustors, an understanding of the dominating phenomena in the close proximity of walls is essential. This work aims to contribute to a deeper insight in this research field.

Many publications concentrate on the prediction and measurement of quenching distances and wall heat fluxes. Popp and Baum [3] investigated the Head-On-Quenching (HOQ) of a methane flame using a one-dimensional detailed chemistry (DC) simulation. Ezekoye et al. [4] experimentally studied the HOQ of methane and propane flames using a constant volume chamber. Both works concluded that single step mechanisms and simplified chemical transport models can not predict the FWI correctly since low activation energy recombination reactions have a significant contribution during the quenching. Sidewall quenching (SWQ) was studied by Alshaalan and Rutland [5,6] within a three-dimensional direct numerical simulation (DNS) of a V-shaped flame in a turbulent Couette flow. They also used a single step reaction approach and therefore could not account for radical recombination effects near the wall. A turbulent three-dimensional DNS applying detailed chemistry has been carried out by Gruber et al. [7], who simulated an anchored V-shaped hydrogen flame within a channel flow. One of their major findings was that the flame speed does not drop to zero despite a vanishing reaction rate. Accordingly Gruber et al. [7] concluded an increasing importance of the diffusional contribution onto the flame speed at the wall. The role of the diffusion processes is also the central issue of this work. Chauvy et al. [8] performed detailed chemistry simulations in order to study the formation of unburnt hydrocarbon (HC). They considered the HOQ scenario as well as combustion in crevices and applied a skeletal mechanism mimicking iso-octane combustion. By contrast the current work focuses on the SWQ scenario and a methane–air flame.

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* Corresponding author.
E-mail address: ganter@ekt.tu-darmstadt.de (S. Ganter).

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This work continues the investigation of SWQ that was evaluated experimentally by Jainski et al. [9] using a premixed methane Side-Wall-Quenching burner. During his work extensive measurements regarding flow field, OH- and CO-distribution, and temperature were performed. Jainski et al. [9] observed an increased CO mass fraction at low temperatures near the wall when compared with a freely propagating flame. The measured data could not provide an adequate explanation for this behavior. First numerical simulations were carried out by Heinrich et al. [10], which covered the full SWQ burner configuration. Using the Flamelet Generated Manifold (FGM) chemistry reduction approach which allows for simulations of large computational domains they found that their simulation accomplishes to predict the major structures such as the distribution of CO_2 and temperature, but fails in predicting pollutants such as CO. Since the origin of the CO accumulation near the wall remained unclear the current work aims to explain the underlying phenomena. As a first preparing step it will be shown how the configuration which is basically three-dimensional can be approximated by a generic two-dimensional sub-domain in order to reduce the computational effort. The focus is then shifted to the thermo-chemical state during the quenching phenomenon in the vicinity of the cold wall, which requires a more detailed treatment of the chemical processes. Being a laminar configuration, the SWQ burner fulfills an essential condition for the reduction to the two-dimensional sub-domain since turbulence is an inherently three-dimensional phenomenon. Using this sub-domain enables the application of detailed kinetics in order to predict the chemical states in the quenching region near the wall. Furthermore, a Lagrangian description method is used to analyze the role of diffusion processes and chemical reactions for the CO distribution in the flame quenching region. Accordingly, the objectives of this work are:

- Assess the reliability of detailed chemistry simulations regarding the thermo-chemical states in a SWQ configuration using experimental data.
- Investigate the influence of the reaction mechanism and the diffusion treatment on the thermo-chemical state.
- Analyze the origin of the enhanced CO mass fraction in the close vicinity of the wall during quenching.

This work is organized as follows: In Section 2, the governing equations are introduced and the numerical methods are presented. The configuration is then described in Section 3, which also provides the justification to use a reduced simulation domain. In Section 4, the reliability of the simulation is assessed by a comparison with experimental results. Furthermore, an investigation of the occurring phenomena is performed in order to explain the measured data. The paper ends with a concluding section.

2. Numerical methods and modeling

All simulations are performed with the academic CFD code Fastest. The incompressible, variable density finite volume code uses a block-structured boundary fitted hexahedral mesh. The spatial interpolation of the velocity is based on the Taylor series expansion of Lehnhäuser and Schäfer [11] to maintain second order accuracy on non-regular cells. Boundedness of scalar quantities is assured by the total variation diminishing scheme suggested by Zhou et al. [12]. The code uses a cell centered variable arrangement on a non-staggered grid with selective interpolation of the mass fluxes as proposed by Rhie and Chow [13]. The time integration is done with an explicit three-stage Runge–Kutta scheme [14] combined with a pressure correction procedure to satisfy continuity. The SWQ configuration is simulated using tabulated as well as detailed chemistry. For the tabulated chemistry simulation the FGM approach is applied as detailed by van Oijen and de Goey [15] and Ketelheun et al. [16,17]. Beside the reaction progress variable the enthalpy is used to account for the enthalpy losses to the wall. The main results of this work are obtained from detailed chemistry simulations that were performed using different reaction mechanisms as well as diffusion treatments. Further description of the detailed chemistry implementation is provided below and can be found in [18,19].

2.1. Governing equations

The (laminar) flow is described by the conservation equation for mass and momentum neglecting volume forces:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i u_j\right) = \frac{\partial}{\partial x_i}\left(\rho \nu \frac{\partial u_j}{\partial x_i}\right) - \frac{\partial p}{\partial x_j} \tag{2}$$

where ρ, u_i, ν and p denote the density, velocity, kinematic viscosity and pressure, respectively. Detailed kinetics involves solving a transport equation for all species that are considered depending on the reaction mechanism applied:

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho\left(u_i + V_{k,i}\right)Y_k\right) = \dot{\omega}_k \tag{3}$$

where Y_k and $V_{k,\,i}$ are the mass fractions and the diffusion velocities, respectively. The transport equation for enthalpy h_s is solved in its sensible formulation:

$$\frac{\partial \rho h_\mathrm{s}}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i h_\mathrm{s}\right) = \frac{\partial}{\partial x_i}\left(\frac{\lambda}{c_\mathrm{p}}\frac{\partial h_\mathrm{s}}{\partial x_i}\right) + \dot{\omega}_\mathrm{T} \tag{4}$$

where the sensible enthalpy h_s and its source term $\dot{\omega}_\mathrm{T}$ can be formulated by the enthalpy h, the standard enthalpies of formation Δh^0_{fk} of all species, their mass fractions Y_k and their source terms $\dot{\omega}_k$ as:

$$h_\mathrm{s} = h - \sum_k \Delta h^0_\mathrm{fk} Y_k \tag{5}$$

$$\dot{\omega}_\mathrm{T} = -\sum_k \Delta h^0_\mathrm{fk} \dot{\omega}_k \tag{6}$$

2.2. Species, momentum and enthalpy transport properties

In the case of mixture averaged diffusion modeling (MixAvg) the diffusion velocities in Eq. (3) are replaced by

$$V_{k,i} = -\frac{\rho D_k}{W}\frac{\partial\left(Y_k W\right)}{\partial x_i} \tag{7}$$

[1] where W denote the average molar mass leading to

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i Y_k\right) = \frac{\partial}{\partial x_i}\left(\frac{\rho D_k}{W}\frac{\partial\left(Y_k W\right)}{\partial x_i}\right) + \dot{\omega}_k \tag{8}$$

The scalar diffusion coefficients D_k are approximated using binary diffusion coefficients D_{kj} and the mixing rule [20]

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k} \frac{X_j}{D_{kj}}} \tag{9}$$

where X_j denotes the mole fractions. The binary diffusion coefficients D_{kj} are derived from the kinetic theory of gases as done by Hirschfelder et al. [21]. The kinematic viscosity ν and the thermal conductivity λ that occur in Eqs. (2) and (4) are obtained from the viscosities and thermal conductivities of pure gases using the mixing rule for viscosities [22]:

$$\nu = \sum_{i=1}^{n} \frac{\nu_i}{1 + \frac{1}{X_i}\sum_{j=1,\, j\neq i}^{j=n} X_j \phi_{ij}} \quad \text{with} \quad \phi_{ij} = \frac{\left(1 + \left(\frac{\nu_i}{\nu_j}\right)^{\frac{1}{2}} \left(\frac{M_j}{M_i}\right)^{\frac{1}{4}}\right)^2}{(4/\sqrt{2})\sqrt{1 + (M_i/M_j)}} \tag{10}$$