Development of a Multi-Dimensional Flamelet Approach and its Validation with a Finite-Rate Chemistry Simulation

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Abstract

Tabulated chemistry combustion models are widely used together with the large eddy simulation (LES) approach for numerical studies of combustion systems where turbulence and chemistry occurs at the same time. In non-premixed and partially premixed combustion systems, the gas composition is usually described by a non-reactive scalar quantity, the mixture fraction [1], which is only valid for one-fuel and one-oxidizer systems.

In this study the premixed flamelet generated manifold approach combined with the artificial thickened flame method (PFGM/ATF) [2] is extended to account for multi-feed combustion systems. An artificial two-dimensional test case is designed with three different inlets, one oxidizer stream and two fuel streams. Oxygen (O_2) is selected as oxidizer and pure hydrogen (H_2) and a mixture of methane (CH_4) and oxygen are supplied through inlet 2 and 3 as fuel streams. The geometrical configuration and the boundary conditions of the test case are outlined in figure 1. The test case is tailored to fulfill the requirements of multi-feed burners as they are commonly used in nanoparticle synthesis reactors [3].

In the present study, two atomic mass fractions [4] are used to describe the composition of the mixture, the atomic mass fractions of carbon and hydrogen (Z_H and Z_C), respectively. One additional transport equation is solved for each of the two aforementioned control variables (Z_C and Z_H). The studies were performed with the LES in-house code PsiPhi [2,5], where the proposed combustion model is implemented. The progress of combustion is described with one additional transport equation for a combined progress variable, the sum of the species mass fractions Y_{H2O} and Y_{CO2}. To resolve the flame (which has a thickness of approximately 0.1 mm) on the numerical grid the progress variable is artificially thickened [6]. In the PFGM method the thermo-chemical quantities are determined a-priori with a detailed or skeletal reaction mechanism. In the present study the open source kinetics library Cantera [7] is used to solve a set of freely propagating 1-dimensional flames, using the reduced mechanism DRM22 [8] for methane combustion. The thermochemical quantities, such as density, viscosity and in particular the molecular diffusivity are stored in a look-up table as functions of the normalized control variables Z_{CN}, Z_{HN} and Y_{PN}. The normalization of the control variables is obtained from the minimum and maximum values of the corresponding quantity and has the advantage of an easy table access. The molecular diffusivity is determined assuming a unity Lewis number, as usual for turbulent flames. The model was verified by reference simulations performed with the open source code OpenFOAM [9] employing a finite rate chemistry model and using the same reaction scheme. However, the software was extended for access detailed transport properties of single species, in particular the diffusion coefficients and a unity Lewis number was enforced for algorithm validation. The thermochemical quantities in the reference simulation were determined on the fly for each time step, with the same models as used in the

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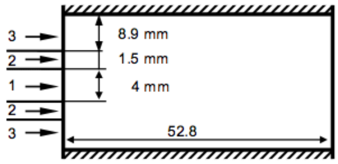
calculation of the flamelets.

The simulation results obtained with the new model are compared against the results from the validated finite rate chemistry model. As illustrated in figure 2 a good agreement could be achieved for the mean axial velocity component, the temperature, the major species (H_2, O_2 and H_2O) but also for the intermediate species, as shown for the mass fraction of OH. The obtained results suggest that the proposed model is suitable for the simulation of multi-feed combustion systems. However, further studies should be performed to validate the proposed combustion model with different case-setups.



Inlet	Y_{CH_4} [-]	Y_{H_2} [-]	Y_{O_2} [-]	U [m/s]	Re [-]	T [K]
1	0.4	0	0.6	5	558	453
2	0	1	0	5	34	453
3	0	0	1	5	1368	453

Figure 1 – Configuration and boundary conditions of the 2D test case

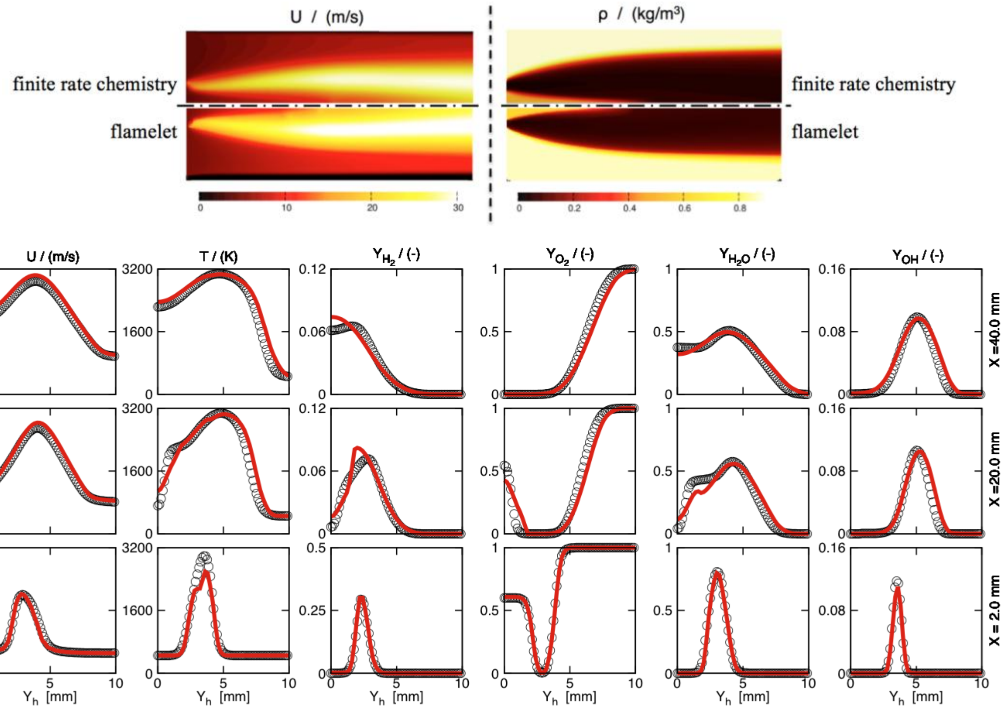


Figure 2 - Simulation results – top figure shows axial velocity field (left) and density (right). Bottom figure illustrates the radial line plots for the velocity, temperature, and mass fractions of H_2, O_2, H_2O and OH, for three different axial positions.

References

[1] Pitsch, H., An. Rev. of Fluid Mech. 38 (2006) 453-482.
[2] Rittler, A., Proch, F., Kempf, A. M., Comb. Flame 162 (2015) 1575-1598
[3] Kammler, H. K., Mädler, L., Pratsinis, S. E., Chem. Eng. Technol. 24 (2001) 583-596.
[4] Peters, N., Cambridge University Press (2000).
[5] Marincola, F. C., Ma, T., Kempf, A.M., Proc Comb. Inst. 34 (2013) 1307-1315
[6] Proch, F., Kempf, A., Comb. Flame 161 (2014) 2627-2646.
[7] Goodwin, D. G., http://code.google.com/p/cantera
[8] A. Kazakov and M. Frenklach, http://www.me.berkeley.edu/drm/
[9] Deng, L., Kempf, A. M., Wlokas, I., et al., Comb. Flame 162 (2015) 1737-1747.