

**Berlin Institute of Technology
(TU Berlin)**

Prof. Dr. Frank Behrendt
Fakultät III: Prozesswissenschaften,
Institut für Energietechnik

Chair Energy Process Engineering and
Conversion Technologies for
Renewable Energies (EVUR)
Fasanenstr. 89
10623 Berlin

Contact
info@flame-structure-2014.com
frank.behrendt@tu-berlin.de

Berlin Institute of Technology • Fasanenstr. 89 • 10623 Berlin

Institute for Combustion and
Gasdynamics - Fluid Dynamics,
University of Duisburg-Essen

Lei Deng
Carl-Benz Str. 199
47057 Duisburg

28. Mai 14

Confirmation of paper submission

Name: Lei Deng
Email: i.wlokas@uni-due.de
Co-author: Oleg P. Korobeinichev
2nd co-author: Andreas Kempf
3rd co-author: Irenaeus Wlokas
Title of Paper: Simulation of laminar flames with detailed
transport, chemistry and heat transfer in
complex geometries
Program: Laminar flames
Name of Institute: Institute for Combustion and Gasdynamics -
Fluid Dynamics, University of Duisburg-Essen

Titel

Simulation of laminar flames with detailed transport, chemistry and heat transfer in complex geometries

Authors

L. Deng, O.P. Korobeinichev, A. Kempf, I. Wlokas

Abstract

Accurate simulations of laminar flames require detailed modeling of the convective and diffusive transport, as well as of the reaction kinetics. Models based on the one-dimensional stream tube assumption are usually not able to reproduce the flow conditions in complex geometries. We present a finite volume based framework for the simulation of laminar flames in one, two and three dimensions. The suitability of this simulation approach and its validation are demonstrated for a H_2/O_2 diffusion flame and a premixed H_2/O_2 flame interacting with a probing nozzle. Our results show that the effect of the probing nozzle on the measured data cannot be neglected, which may suggest that detailed complementary simulations in two- or three-dimensions should be conducted with laminar flame experiments to quantify the bias introduced by the probing nozzle.

Introduction

Laminar flames are convenient for the investigation of the flame structure and detailed reaction kinetics but they require accurate modeling of the molecular transport phenomena of heat conduction, viscous stresses and mass diffusion. Thus simulations of laminar flames are usually conducted for simplified, one-dimensional, steady state problems [1,2] due to their moderate requirements for computational resources. Usually the experiments are conducted in a way that tries to achieve a one-dimensional flow. However, the measurement techniques are normally intrusive, violating many simplifying assumptions. With the computational power available now, the finite volume approach can be employed in one to three dimensions, but only few commercial simulation frameworks implement the models necessary for the detailed description of reacting flows [3]. A recent development, based partially on the open-source software OpenFOAM [4], was presented by Cuoci et al. [5]. However, two or three dimensional simulations of laminar, reacting flows are rarely performed as they require considerable computational times.

In this work we present a simulation framework for laminar, reacting flows with detailed transport, chemistry and heat transfer in two or three dimensions. The simulation results are evaluated by experimental data by Toro et al. [6] for a diffusion flame and by Knyazkov et al. [7] for a premixed flame.



www.flame-structure-2014.com

**Berlin Institute of Technology
(TU Berlin)**

Prof. Dr. Frank Behrendt
Fakultät III: Prozesswissenschaften,
Institut für Energietechnik

Chair Energy Process Engineering and
Conversion Technologies for
Renewable Energies (EVUR)
Fasanenstr. 89
10623 Berlin

Contact
info@flame-structure-2014.com
frank.behrendt@tu-berlin.de

Approach

The code basis for our implementation is the open-source finite volume framework OpenFOAM, which offers numerous flux discretization schemes. The low Mach number flow is described by the conservation of mass, species, momentum and energy. The pressure-velocity coupling is realized by a PISO scheme. An operator splitting technique is used for calculation of the finite rate chemistry source term. The heat conductivity and dynamic viscosity of the mixture are calculated according to the local composition and the temperature using the semi empiric formulas proposed by Wilke [8]. The heat conductivity and dynamic viscosity of the pure species are calculated from kinetic theory models for a wide range of temperatures prior to the simulations and are stored as polynomials that are evaluated at run time. The binary diffusion coefficients are calculated 'on-the-fly' from a kinetic theory model. The diffusion coefficients of individual species into the mixture are computed as mole fraction weighted average [9]. The thermodynamic properties of the mixture are computed as mass weighted average.

A very important aspect of flame simulations in complex geometries is an accurate treatment of the thermal boundary conditions. Cooled burner matrices, probing nozzles and burner chamber components strongly affect the flame and further violate the adiabatic assumption of the one-dimensional stream tube. Thus an accurate simulation requires a conjugate heat transfer model of heat transport in the solid parts. The heat conduction within solid parts opens an additional multi-scale issue: while the characteristic chemical time scale is in the magnitude of 10^{-9} s and the characteristic flow time is 10^{-3} s, the characteristic time of the heat conduction problem is in the magnitude of 10^2 s. This means that a solver will typically require many iteration steps before a steady state is reached. The cost for these simulations can however be reduced by lowering the heat capacity in the solid, which does not affect the steady state solution.

Two different laminar flames were simulated in order to evaluate the models: a diffusion flame [6] and a premixed H_2/O_2 flame [7]. In both

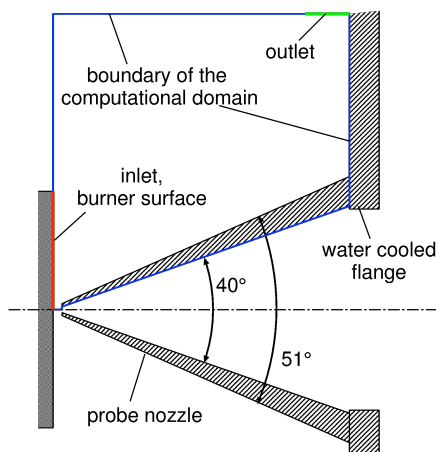


Figure 1 Experimental setup and computational domain for the premixed flame investigation.

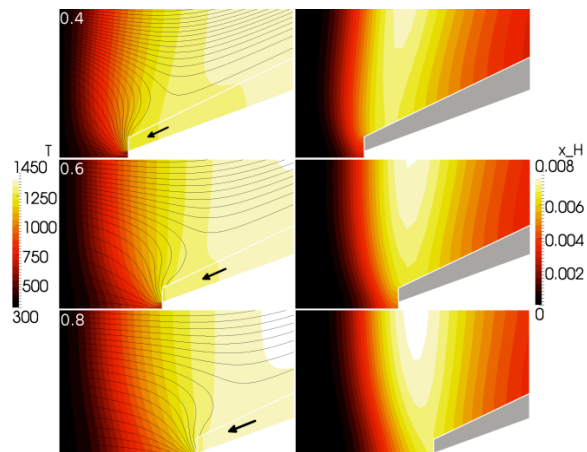


Figure 2 Temperature in Kelvin and streamlines (left column), and H radical mole fraction (right column) at probe positions of 0.4, 0.6 and 0.8 mm above the burner.

cases the detailed reaction mechanism proposed by Li et al. [10] was used. The hydrogen flame was found to be a good test case, as the presence of fast reactions and the high diffusion velocity of atomic hydrogen make the solution sensitive to the quality of the model implementation. The species concentrations and the temperature were measured by spontaneous Raman scattering and coherent anti-Stokes Raman scattering (CARS) techniques, which are non-intrusive and thus a good source for validation data. In their experiments, Toro et al. [6] investigated flames for three different fuel exit velocities, of which the case with 50 cm/s is presented in our work. The experimental setup of the premixed flame measurements is shown in Fig. 1, including the quartz nozzle used for the probing mass spectrometry. The nozzle causes a suction effect and extracts heat, which must be considered in the simulations. For most fuels, except hydrogen, the two or three dimensional simulation allows only the use of a reduced reaction kinetics mechanism. The temperature and velocity field obtained with the reduced mechanism are of reasonable accuracy, while the minor species concentrations may not be. However, more accurate species concentrations can be obtained in a post-processing step, where the flame along a streamline is simulated using detailed chemistry with a 1D solver, relying on the temperature field from 3D. In the present work we employed this two step approach for the premixed flame case in order to show the feasibility of this approach, which is necessary with more complex fuels.

Results and discussion

Hydrogen/oxygen diffusion flame

The simulation results are displayed in Fig. 3. The measurements were taken along the centerline and for the radial line at 3 mm above the burner. The simulations show a very good agreement with the experiment, suggesting a correct implementation of the transport models and the correctness of the reaction mechanism.



www.flame-structure-2014.com

**Berlin Institute of Technology
(TU Berlin)**

Prof. Dr. Frank Behrendt
Fakultät III: Prozesswissenschaften,
Institut für Energietechnik

Chair Energy Process Engineering and
Conversion Technologies for
Renewable Energies (EVUR)
Fasanenstr. 89
10623 Berlin

Contact
info@flame-structure-2014.com
frank.behrendt@tu-berlin.de

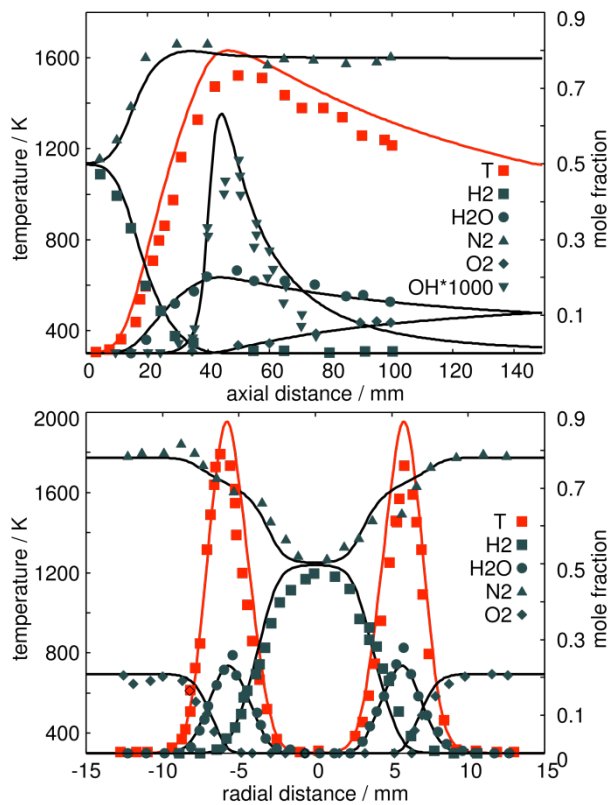
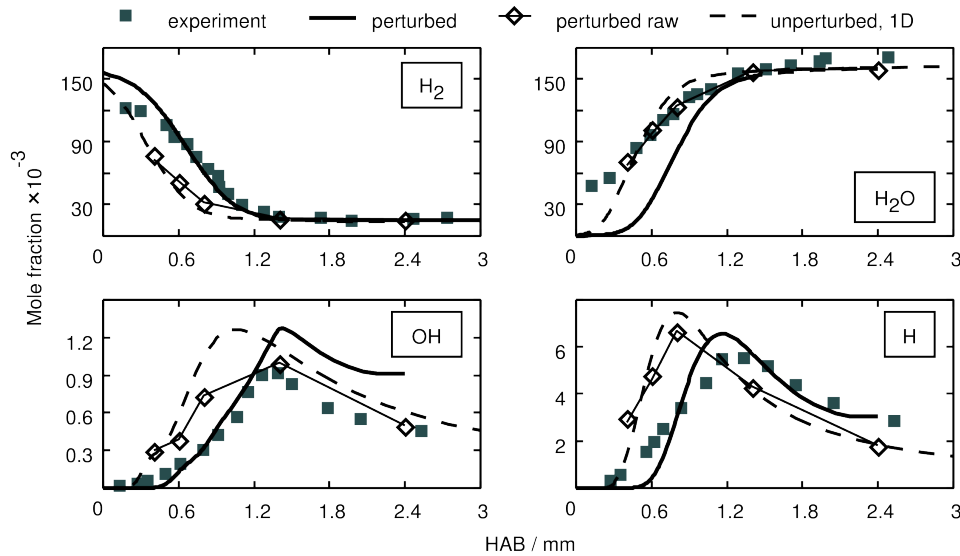


Figure 3 Simulation results for the diffusion flame. Left diagram shows the axial temperature and species mole fractions, right diagram shows the radial profiles at a height above burner of 3 mm.

Premixed hydrogen/oxygen flame

Figure 2 shows the streamlines and temperature distribution (left column) and the H radical mole fraction distribution (right column) calculated for different probe positions. Figure 4 shows the mole fractions of measured species and from simulation, obtained by the different simulation strategies. The simulation shows a good agreement with measurements, when the two step strategy is employed. The use of realistic temperature and velocity profiles could greatly improve the predictions over the one-dimensional simulation tool. The species concentrations in the orifice cross section from the two dimensional simulations shows a less accurate prediction, while the one-dimensional simulation of an unperturbed flame could not be confirmed by the measurements. The discrepancy between the raw, perturbed flame simulation result and the solution obtained by the two-step strategy is attributed to the slightly different formulation of the inlet-diffusion boundary conditions. A notable discrepancy was observed close to the burner for H₂ and H₂O in all simulations.



www.flame-structure-2014.com

Berlin Institute of Technology (TU Berlin)

Prof. Dr. Frank Behrendt
 Fakultät III: Prozesswissenschaften,
 Institut für Energietechnik

Chair Energy Process Engineering and
 Conversion Technologies for
 Renewable Energies (EVUR)
 Fasanenstr. 89
 10623 Berlin

Contact
 info@flame-structure-2014.com
 frank.behrendt@tu-berlin.de

Figure 4 Comparison of measurements [7] and the simulation of the perturbed and unperturbed flame.

Conclusions

The two and three dimensional simulations were found to show a very good agreement with the experimental data. For the investigation of the premixed flame, the modeling could be greatly improved in its prediction by using realistic temperature and velocity profiles through using a description in at least two dimensions. The computational effort for solving the flow in two- or three-dimensional geometries is much larger than for the steady state one-dimensional problems, making the approach little suited for parameter studies. However, we expect that such complex simulations will be used in the near future to consider the probe-induced disturbance in the optimization of kinetic mechanisms.

Acknowledgements

We would like to thank Dr. Denis A. Knyazkov for sharing the original experimental data.

References

- [1] R.J. Kee, F. Rupley, J.A. Miller, Chemkin II: A Fortran Chemical Kinetics Package for the Analysis of Gas-phase Chemical Kinetics, Sandia Report SAND89-8009 –Sandia National Laboratories, 1989.
- [2] D. Goodwin, "Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes", Caltech, Pasadena, 2009.
- [3] FLUENT 6 User's Guide, 2001. Volumes 1–4. Fluent Inc., Lebanon, December 2001.
- [4] OpenFOAM, www.openfoam.org, 2013.
- [5] A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi, A computational tool for the detailed kinetic modeling of laminar flames: Application

to C₂H₄/CH₄ coflow flames. Combust. Flame 160(5) (2013) 870-886.

[6] V.V. Toro, A.V. Mokhov, H.B. Levinsky, M.D. Smooke, Combined experimental and computational study of laminar, axisymmetric hydrogen–air diffusion flames. Proc. Combust. Inst. 30(1) (2005) 485-492.

[7] D.A. Knyazkov, O.P. Korobeinichev, A.G. Shmakov, I.V. Rybitskaya, T.A. Bolshova, A.A. Chernov, A.A. Konnov, Study of H₂/O₂/N₂ Flames Structure at Atmospheric Pressure by Molecular Beam Mass Spectrometry and Modeling, Proc. European Combust. Meeting, 2009.

[8] C.R. Wilke, A Viscosity Equation for Gas Mixtures, J. Chem. Phys. 18 (1950) 517

[9] R.B. Bird, W.E. Stewart, E.N. Lightfoot, Transport Phenomena, John Wiley and Sons, New York, 1960.

[10] J. Li, Z. Zhao, A. Kazakov, F.L. Dryer, An updated comprehensive kinetic model of hydrogen combustion. International Journal of Chemical Kinetics, 36(10) (2004) 566-575.



www.flame-structure-2014.com

**Berlin Institute of Technology
(TU Berlin)**

Prof. Dr. Frank Behrendt
Fakultät III: Prozesswissenschaften,
Institut für Energietechnik

Chair Energy Process Engineering and
Conversion Technologies for
Renewable Energies (EVUR)
Fasanenstr. 89
10623 Berlin

Contact
info@flame-structure-2014.com
frank.behrendt@tu-berlin.de