Application for the 19th ERCOFTAC da Vinci Competition

Title of PhD thesis: Modeling of near-wall flame dynamics in laminar and turbulent combustion
Name: Dr.-Ing. Matthias Steinhausen
E-Mail: steinhausen@stfs.tu-darmstadt.de
Affiliation: Technical University of Darmstadt, Department of Mechanical Engineering, Simulation of reactive Thermo-Fluid Systems, Otto-Berndt-Straße 2, 64287 Darmstadt, Germany

Name of supervisor: Prof. Dr.-Ing. Christian Hasse
Affiliation of supervisor: Technical University of Darmstadt, Department of Mechanical Engineering, Simulation of reactive Thermo-Fluid Systems, Otto-Berndt-Straße 2, 64287 Darmstadt, Germany

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Brief summary

To achieve a CO_2-neutral energy economy, combustion systems need to be updated to work efficiently and with low emissions using sustainable fuels from renewable sources. Designing these new combustion systems can greatly benefit from computer simulations. However, for the simulations to be effective, it is crucial to understand the complex interactions between the turbulent flow with walls and the combustion chemistry and incorporate them in the models employed. In technical combustion systems, like internal combustion engines or aero engines, combustion occurs inside an enclosed vessel. When the flame gets close to the walls of the vessel, the large temperature difference between the flame and the walls changes the combustion process. This can reduce the overall efficiency and increase the formation of unwanted pollutants. To address these issues, it is crucial to accurately simulate the interaction between the flame and the combustor walls. This allows for a knowledge-based optimization of new combustion systems. The nominee's thesis presents novel methods that accurately predict the complex interactions among turbulence, combustor walls, and combustion chemistry in computer simulations, enabling predictive designs of future combustion systems.

Scientific summary

For the transition to a CO_2-neutral energy economy, it is necessary to adapt technical combustion systems for low-emissions and highly efficient operation with alternative fuels from renewable sources. In the design of these novel combustors, numerical simulations have proven to be a powerful tool. However, the key to a simulation-aided design process is a comprehensive understanding of the fundamental physical processes and their integration into predictive combustion models. The interaction of flames with the turbulent boundary layer near combustor walls is one of these crucial physical phenomena. Flame-turbulence-wall interactions result in complex heat loss mechanisms that decrease the combustion efficiency and increase pollutant formation.
In the nominee's thesis, the modeling of laminar and turbulent flame-wall interactions is investigated in several generic configurations. The research begins with a comprehensive investigation of laminar flames under atmospheric conditions [P1], extending previous findings on fossil fuels to encompass alternative fuels. Subsequently, the effect of turbulence on the quenching flame is addressed [P2,P4,P5], providing detailed analysis and first-of-its-kind insights. It is important to note that since combustion in technical devices occurs under turbulent conditions, the consideration of turbulence is a crucial step during model development. A direct numerical simulation (DNS) of a premixed flame stabilized in a fully developed turbulent channel flow is performed and analyzed. Figure 1 (left) shows a snapshot of the investigated flame interacting with the turbulent channel flow and, finally, quenching in the turbulent boundary layer. The turbulence-chemistry interaction causes wrinkling of the flame and unsteady flame motion. The result is spatial and temporal fluctuations that, for example, lead to the distinctive flame tongue visible at the lower wall.
Using the detailed insights of the DNS, a flame-vortex interaction mechanism is revealed for the first time: In the vicinity of the wall, the interaction of the turbulent flow (vortices) with the flame tip results in the mixing of unburnt gases with cold exhaust gases. Figure 1 (right) shows a time series of a representative flame-vortex interaction event. The flame-vortex interaction affects the mixture

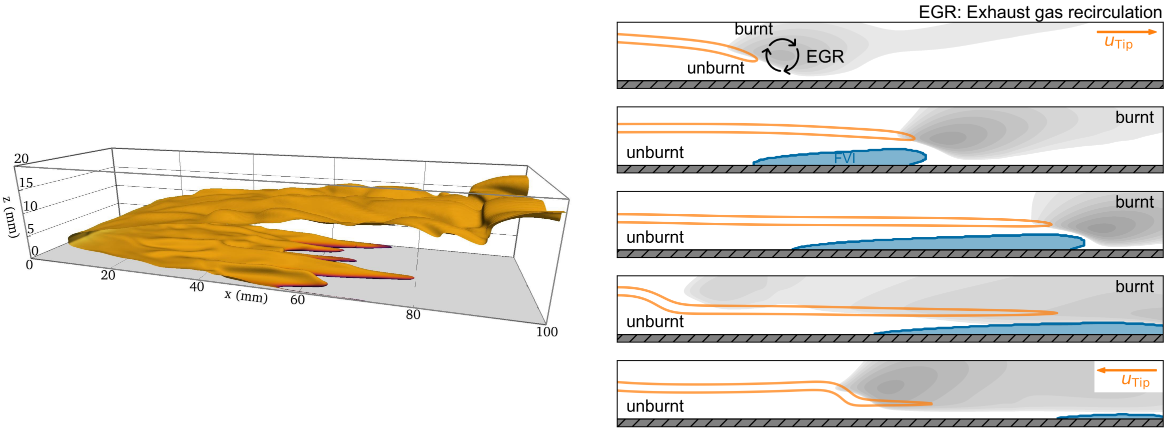

Figure 1: Left: Snapshot of the premixed V-flame stabilized in the turbulent channel flow. The channel walls are at $z = 0$ and $z = 20$ mm in the x-y plane. Right: Schematic illustration of a flame-vortex interaction event, depicted as a cut through the x-z plane. The flame front is depicted in orange, while the area of exhaust gas recirculation is colored in blue and the vortical structures in front of the flame are shown in grey. The time increases from top to bottom.

formation, flame reactivity, and pollutant formation and, therefore, needs to be considered in the combustion models employed, which had not been done in the literature so far. In his thesis, the nominee is the first to address two modeling challenges in turbulent flame-wall interactions:

- How can the effect of turbulence on the chemistry be captured in a reduced-order model? [P4,P5]
- How can the unresolved interactions of the turbulent flow, the combustor walls, and the flame, namely turbulence-chemistry interactions, be accounted for in Reynolds-Averaged Navier-Stokes (RANS) and Large-Eddy Simulations (LES)? [P2]

The nominee tackles these questions by developing two innovative modeling approaches: a reduced-order chemistry representation and a turbulence-chemistry interaction model based on the Conditional Quadrature Method of Moments (CQMOM). The CQMOM approach retains a quadrature approximation of the unknown probability density function (PDF) of the unresolved spatial and temporal fluctuations of the reactive scalars by transporting the distributions' moments. This way the turbulence-chemistry interaction can be accounted for in both RANS and LES. The derived modeling approaches demonstrate significant improvements over previous models reported in the literature. Figure 2 exemplary shows a comparison of the prediction capabilities of the improved reduced-order chemistry model and the most recent approach reported in the literature (standard model).

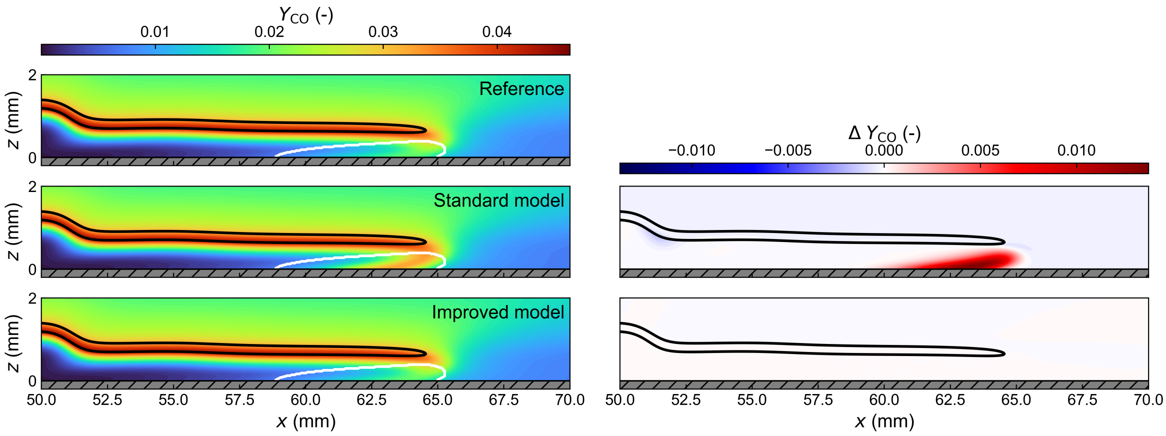

Figure 2: Comparison of the CO prediction accuracy of the most recent approach in the literature and the improved model derived. On the left, the CO mass fraction is shown, while the absolute prediction error is depicted on the right. The black isocontour displays the flame surface, while the white isocontour shows the area of flame-vortex interaction.

In the final step, the insights are transferred to more complex conditions encountered in technical

applications. Specifically, the effects of external mixture stratification [P3] relevant for effusion cooling applications and combustion under pressurized conditions are investigated.
In conclusion, the nominee's thesis significantly advances the modeling of flame-wall interactions, paving the way to simulate these phenomena in technical combustors. Figure 3 summarizes the configurations investigated, the related publications, and the respective modeling challenges. The impact of the nominee's work on engineering practice is underscored by a new research project initiated in collaboration with Rolls-Royce. This project aims to incorporate the derived modeling approaches into the company's simulation code, utilizing these insights to simulate future aero engines. In addition to his scientific work, the nominee significantly contributed to more sustainable software development at the institute leading to his current position as group leader for software development at the institute.

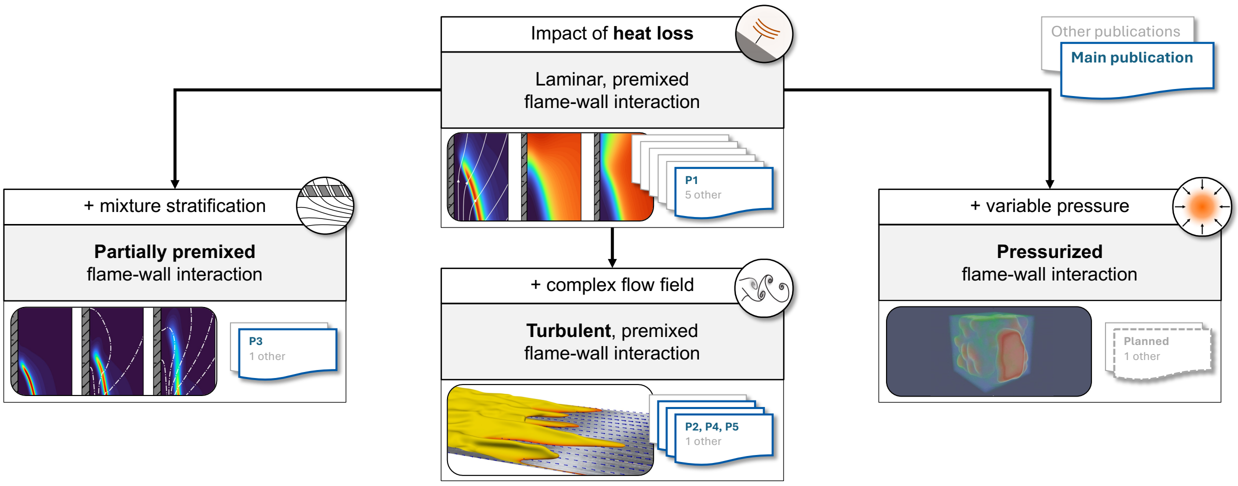

Figure 3: Overview of the configurations investigated in the nominee's thesis. The publications related to the configurations are indicated. In addition to the main publications listed below, the number of additional publications is indicated.

List of selected publications

The scientific findings from the nominee's doctoral thesis have been published in internationally recognized journals. The most important publications, in chronological order, are:

[P1] **M. Steinhausen**, Y. Luo, S. Popp, C. Strassacker, T. Zirwes, H. Kosaka, F. Zentgraf, U. Maas, A. Sadiki, A. Dreizler, and C. Hasse. "Numerical Investigation of Local Heat-Release Rates and Thermo-Chemical States in Side-Wall Quenching of Laminar Methane and Dimethyl Ether Flames". In: *Flow Turbul. Combust.* 106 (2021), 681–700. DOI: 10.1007/s10494-020-00146-w

[P2] **M. Steinhausen**, T. Zirwes, F. Ferraro, S. Popp, F. Zhang, H. Bockhorn, and C. Hasse. "Turbulent Flame-Wall Interaction of Premixed Flames Using Quadrature-based Moment Methods (QbMM) and Tabulated Chemistry: An a Priori Analysis". In: *Int. J. Heat Fluid Flow* 93 (2022), 108913. DOI: 10.1016/j.ijheatfluidflow.2021.108913

[P3] **M. Steinhausen**, F. Ferraro, M. Schneider, F. Zentgraf, M. Greifenstein, A. Dreizler, C. Hasse, and A. Scholtissek. "Effect of Flame Retardants on Side-Wall Quenching of Partially Premixed Laminar Flames". In: *Proc. Combust. Inst.* 39 (2023), 3745–3754. DOI: 10.1016/j.proci.2022.07.207

[P4] **M. Steinhausen**, T. Zirwes, F. Ferraro, A. Scholtissek, H. Bockhorn, and C. Hasse. "Flame-Vortex Interaction during Turbulent Side-Wall Quenching and Its Implications for Flamelet Manifolds". In: *Proc. Combust. Inst.* 39 (2023), 2149–2158. DOI: 10.1016/j.proci.2022.09.026

[P5] Y. Luo, **M. Steinhausen**, D. Kaddar, C. Hasse, and F. Ferraro. "Assessment of Flamelet Manifolds for Turbulent Flame-Wall Interactions in Large-Eddy Simulations". In: *Combust. Flame* 255 (2023), 112923. DOI: 10.1016/j.combustflame.2023.112923

In addition to these main publications, the nominee has collaborated with numerous national and international researchers, resulting in **eight other publications** (see his doctoral thesis or orcID).