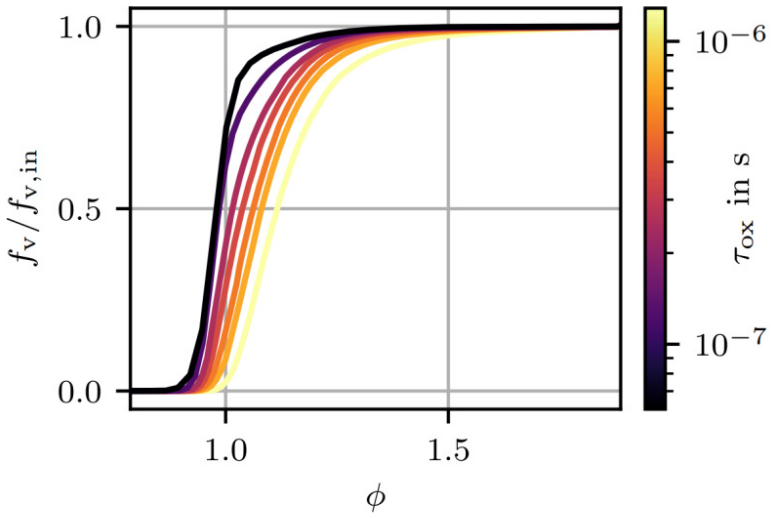
Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Reducing Pollutant Emissions in Sustainable Aero-Engine Combustors



Project Manager
Philipp Koob

Principal Investigator
Prof. Dr.-Ing. Christian Hasse

Project Term
2023 - 2024

Clusters
Lichtenberg II Cluster Darmstadt

Institute
Simulation of Reactive Thermo-Fluid Systems

University
Technische Universität Darmstadt

Introduction

Reducing pollutant emissions remains a key challenge in the development of nextgeneration aero-engines. In addition to experimental methods, computational fluid dynamics (CFD) has become an indispensable tool to minimize costs and development times. In industrial applications requiring numerous design variations, simplified soot models are generally used. These models, however, usually lack generality and are only valid for selected operating ranges and fuels. Therefore, accurate models valid over the whole application spectrum are desired. In this work, an existing soot model is used to study soot oxidation, relevant to reduce soot emissions, at engine-relevant conditions in a simplified configurations and then applied to a single sector model combustor operated at realistic temperatures and pressures to investigate the coupling between the mixture formation of the liquid fuel injection and the subsequent soot formation.

Methods

All studies performed during this project use a finite-volume method for the simulation of the reacting flow field. For the simplified configuration, a quasi-direct numerical simulation (DNS) approach is used to resolve all flow phenomena while the realistic combustor is simulated using large eddy simulations (LES). The gas-phase chemistry is modeled using direct chemistry for the quasi-DNS and a tabulated chemistry approach for the LES. Soot is modeled with the split-based extended

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quadrature method of moments (S-EQMOM).

Results

In the first six months of the project, soot oxidation was investigated in a simplified configuration. The mixing process of fresh air with burned products of a rich kerosene mixture containing soot is modeled in a 2D configuration similar to a laminar counterflow flame. All simulations are performed at an elevated pressure of 22 bar and 730K preheating temperature. Two parameters, the oxidation time scale and the soot particle size distribution, are varied to investigate their influence on soot formation. Results of this study show that soot is more prone to break through to the lean side with decreased oxidation time scales, leading to increased overall emissions. Additionally, larger particles are more prone to soot breakthrough due to slower oxidation. These observations led to the introduction of a breakthrough metric B, qualifying soot breakthrough depending on the oxidation time scale, the soot particle diameter and the soot models oxidation constant. The validity of the metric is verified by keeping the metric constant for varying mean particle diameters and oxidation time scales while keeping B constant. This is achieved by changing the oxidation constant accordingly. Results show that the curve of the soot volume fraction becomes identical for simulations with the same value for B. These findings were published in the Proceedings of the Combustion Institute. In the remaining time of the project, the interaction and coupling between liquid fuel spray injection found n aero-engines and soot formation are studied. Since modeling the fuel breakup inside the reactive LES results in significantly increased computational costs, it is usually not included and replaced by spray models. In this work, detailed simulations of the spray breakup are performed by the cooperation partner from the Karlsruhe Institute of Technology. The resulting spray droplet particle size distributions are used as boundary conditions for the reacting LES of the aero-engine model combustor. Different strategies are applied for the initialization of the spray droplets in the LES and their influence on soot formation is investigated. Simulation results are compared to experimental data provided by the German aerospace center (DLR) and show good agreement for the global flow characteristics and flame position. Comparing the soot emissions with the experimental data reveals the importance of the radial distribution of the fuel spray in the boundary condition for accurate soot predictions. By including this information, soot predictions are significantly improved and in line with the experimental results. Finally, a variation of the operating conditions shows that including the dependency of the spray on the operating point is again important to capture the correct trends of soot emissions over the full operating range. A publication of these results for the upcoming ASME Turbo Expo 2025 is currently in preparation.

Discussion

The first study underscores the importance of a precise description of the gas-phase mixing and the soot phase for accurate predictions of soot oxidation. It was shown, that the

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soot oxidation rate can be connected to a soot breakthrough metric depending on the oxidation time scale and the mean particle diameter. To improve the efficiency of future sustainable aero-engines, these results and methods have to be extended to configurations with increased complexity in the future. The second study revealed that accurate soot predictions are strongly dependent on the modeling of the mixture formation. Therefore, detailed knowledge of the liquid fuel spray breakup process is essential to capture soot formation over the large operation ranges of aircraft engines. In future works, the developed coupling between detailed spray breakup simulations (not performed within this project) and reactive LES of the model combustor has to be extended to the real aero-engine combustion chamber.

Figures

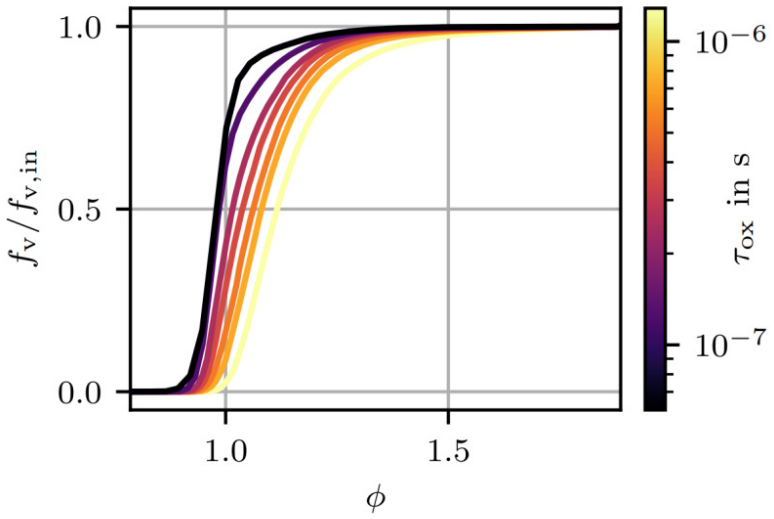

Figure 1: Soot volume fraction fv over the equivalence ration ϕ for varying mixing times τ_{ox}. f_V is normalized with the soot volume fraction at the inlet $f_{v,in.}$

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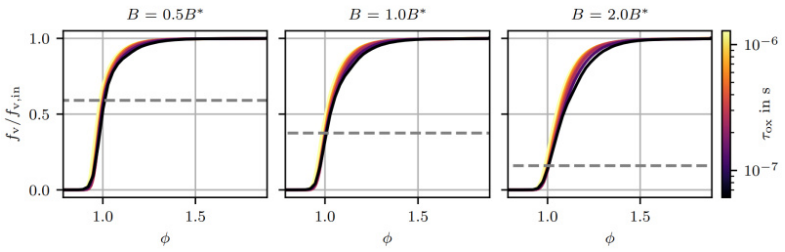

Figure 2: Soot volume fraction f_v over the equivalence ration ϕ for three different B and varying mixing times τ_{ox}. The gray dashed line represents the mean soot volume fraction at stoichiometric mixture conditions.

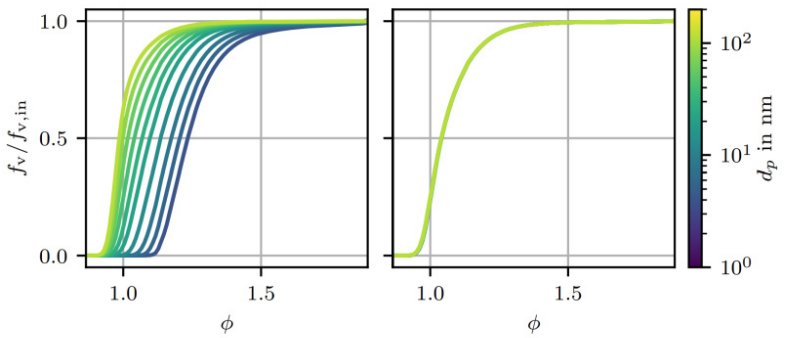

Figure 3: Soot volume fraction f_v over the equivalence ration ϕ for different mean particle diameters p_d with constant oxidation constant (left) and for a constant B (right).

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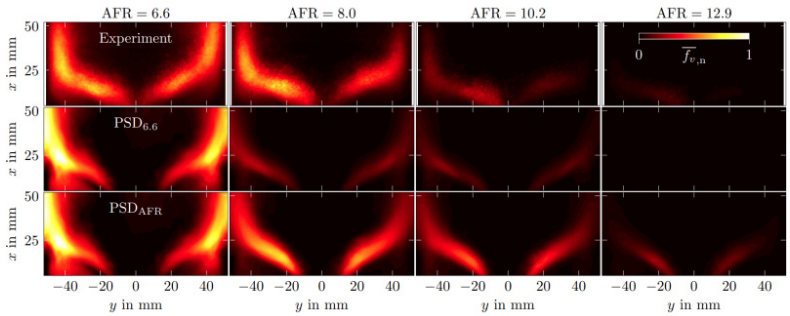

Figure 4: Mean normalized soot volume fraction in the primary zone of the combustor compared to the experimental data for different air-fuel ratios (AFRs). The first row represents the experimental data, the second row the CFD results whith the same spray PSD applied for all AFR while the bottom row shows the results when using the spray PSD corresponding to the specific AFR.

Publications

Koob, P.; Nicolai, H.; Schmitz, R.; Hasse, C.: "Analysis of potential soot breakthrough during oxidation at aero-engine relevant conditions", Proceedings of the Combustion Institute, Volume 40, Issues 1–4, 2024 https://doi.org/10.1016/j.proci.2024.105672

Philipp Koob: "Analysis of potential soot breakthrough during oxidation at aero-engine relevant conditions", Combustion Institutes 40th International Symposium, Milan, Italy, July 21-26, 2024

Last Update: 2025-01-11 16:25