Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Numerical Investigations on the Soot Formation of Oxymethylene Ether (OME) Flames

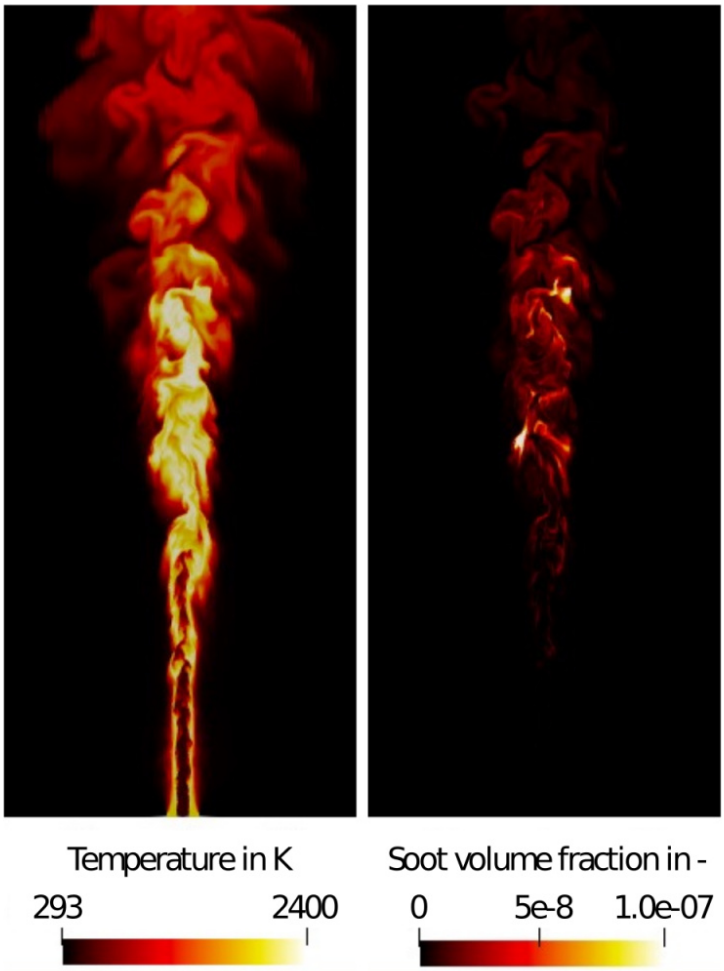


Figure1: Instantaneous temperature field (left) and soot volume fraction field (right) of a turbulent jet flame burning diesel surrogate fuel.

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Project Term
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Clusters
Lichtenberg II Cluster Darmstadt

Software
OpenFOAM

Additional Software
ULF

Institute
Simulation of Reactive Thermo-Fluid Systems

University
Technische Universität Darmstadt

JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN
TECHNISCHE UNIVERSITÄT DARMSTADT
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Introduction

Reducing pollutants is one of the main research interests for current and future combustion devices. Soot particles are unwanted byproducts generated from incomplete combustion of hydrocarbons. They exhibit carcinogenic effects on human health and a detrimental impact on climate change. The use of oxygenated, synthetic fuels can significantly reduce the emission of soot particles. Additionally, when synthetic fuels are produced using renewable energy, they could lower the overall impact of combustion devices on the global carbon balance. Promising candidates for use in self-ignition engines are oxymethylene ethers (OME) due to their properties which are similar to the ones of fossil diesel fuel. Synthetic fuels and especially OMEs are currently only available in small quantities due to limited production capacity and high production costs. A deep understanding of their effect on the underlying thermochemical processes during the combustion and pollutant formation is fundamental for designing future optimized and low-emission engines and the efficient application of such fuels. The investigation of OME fuel and its effect on sooting turbulent flames in a canonical laboratory configuration is, therefore, the aim of this research project.

Methods

Large eddy simulations (LES) were performed using the widely established toolbox OpenFOAM based on the cell-centered finite-volume method. The chemistry modeling was tabulated in a pre-processing step using 1-D diffusion flamelets resulting in a tabulated flamelet manifold. Two control variables for the mixture fraction and the progress of the combustion process were solved in the CFD simulation. It was combined with an additional transport equation for soot precursors, which reflects the slower time scales of these species and allows for coupling to the soot model. The soot formation was modeled using a univariate Split-based Extended Quadrature Method of Moments (S-EQMOM) considering the details of the soot evolution processes such as the inception, coagulation, and surface reactions of the soot particles. The number density function of the soot particles was approximated with two sub-number density functions by the S-EQMOM.

Results

The numerical study was performed on a piloted turbulent jet flame burning pre-vaporized fuel. A neat flame with a diesel fuel surrogate was used as a reference. The effect of OME_4 fuel on the chemistry, formation of soot precursor species, and finally on the individual soot formation processes was analyzed in a series of blended flames with diesel surrogate and OME_4. The results of the simulations were compared against experimental data provided by the institute of Reactive Flows and Diagnostics at TU Darmstadt for validation. The simulations with the detailed Method of Moments approach for the soot modeling allow a deeper insight into the soot formation processes under these turbulent conditions.

Discussion

Adding 50 % OME_4 fuel to the diesel flame (by volume) leads to significantly reduced soot particles in terms of soot volume fraction. The simulation data allows a detailed investigation of the cause-and-effect chain of processes in flames. In the OME_4 blended flames, the formation of soot precursor species is limited to richer conditions compared to the diesel surrogate reference flame, in which soot formation also occurs for slightly rich conditions. The formation of large polycyclic aromatic hydrocarbons is delayed in the OME flames. Soot particle formation can only take place in very rich pockets occurring very sparsely in the OME_4 flame under turbulent conditions. Additionally, the number density is reduced with OME_4 addition to the flame, and particles exhibit a smaller diameter. Subsequently, most of the soot particles get oxidized during their evolution in the flame. The future investigations will cover different operating conditions and additional OME mixtures to further inspect the effect of OME fuel in more detail.

Publications

Schmitz, R.; Ferraro, F. Numerical investigation of oxymethylene ether addition on soot formation, 6th International Sooting Flame (ISF) Workshop, Vancouver, Canada, Fri 22 July - Sat 23 July (2022)

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