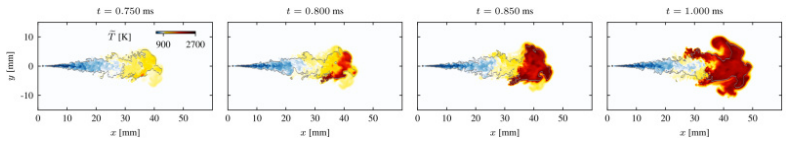
Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Mixture Formation and Combustion of Alcohols and Other Biogenic Fuels in Mixture-Controlled Combustion Processes



Introduction

This project aims to investigate various renewable fuels in 3D spray simulations (synthetic and biogenetic). For different fuels, locally identical fuel-air mass ratios result in the stationary phase, which can be specifically adjusted by the injection system. A fuel influence only comes into play during the transition from physical mixture formation to chemical combustion. Characteristics such as a (biofuel-typical) oxygen content leads to leaner mixtures. This allows focusing on chemical properties when selecting an alternative fuel. Problems of pollutant emission and finite resources can thus be addressed simultaneously and synergistically: By using renewable fuels with suitable chemical characteristics, the combustion process is specifically influenced to produce low emissions. In addition to the alcohol ethanol, HVO, OME_3,OME_4, OME_{mix}, 1-octanol and n-dodecane are to be investigated in this project. Based on this, the combustion process of alternative fuels in the injection chamber and finally also in the rapid compression machine will be analyzed and the application proximity will be successively maximized. The aim is to demonstrate the possibilities and limits of optimum combustion control using alternative fuels for one or a few operating point(s) in a real application.

Methods

The fuel injection process in modern diesel engines is a complex two phase problem. The cause effect chain (Injection-Evaporation-Mixing-Combustion) is strongly coupled and needs a variety of models to capture the physical and chemical modes of action. For the numerical discretization method, the finite volume method (FVM) is utilized. The physical domain is resolved by small discrete volumes that are called cells. The so-called Navier-Stokes- Equations are solved in order to obtain the flow field information in each of these cells. Additionally, equations for energy, chemical reactions and evaporation are solved. In contrast to the so-called Eulerian-Eulerian (e.g., Volume of Fluids (VOF)) simulation, which resolves both liquid and gaseous phase in Eulerian coordinates, the less computational expensive Eulerian-Lagrangian approach is used

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Project Term
2022 - 2023

Clusters
Lichtenberg II Cluster Darmstadt

Software
OpenFOAM

Additional Software
ULF, ParaView, OpenMPI

Institute
Simulation of Reactive Thermo-Fluid Systems

University
Technische Universität Darmstadt

JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN
TECHNISCHE UNIVERSITÄT DARMSTADT
UNIKASSEL VERSITÄT
Philipps Universität Marburg

in this project. In this approach, the gaseous phase is solved in Eulerian coordinates and the liquid phase is described by lagrangian particles that interact with the gas phase. Each particle, a so-called parcel, represents a number of droplets that share the same properties (temperature, size, velocity). The coupling between parcels and gas phase involves momentum and evaporation source terms. In spray combustion, the mixture formation is an important quantity. The quality of the mixture field determines the accuracy of the combustion and pollutant formation simulation. Therefore, high fidelity Large Eddy Simulations (LES) are frequently used in literature. A large amount of the turbulent structures/eddies are resolved (high grid resolution), only a smaller amount of turbulence has to be modeled using appropriate turbulence models, leading to the need of HPC-resources. The last part in the simulation is the auto ignition process in spray flames. Chemical reactions are often computed using detailed chemistry solver, but in this project the so-called flamelet model is used, which allows to speed up the simulation significantly. The idea behind the flamelet model is that a turbulent flame can be represented by a manifold of one-dimensional flame structures, so-called flamelets. The great advantage of the flamelet model lies in the ability to precompute the flamelet solutions for all relevant thermo-chemical states and store them in look up tables. During the simulation the chemical source terms can be looked up, instead of solving a large amount of additional differential equations, using appropriate access variables.

Results

This project delivered important information on the diesel relevant spray combustion of biogenetic and synthetic fuels. The influence of significantly different thermophysical properties of renewable diesel fuels have been elucidated in detail. The influence of the increased latent heat of evaporation on ignition has been discovered and a new combustion model has been developed. Furthermore, the cause effect chain of different injector nozzle sizes has been elucidated and explained. Lastly, a new combustion model for “dual-fuel” combustion systems has been developed.

Discussion

The findings of this project are crucial for the further development of combustion engines using renewable fuels. As a novelty in this work, the influence of thermophysical properties of biogenic and synthetic fuels on mixture formation and combustion have been elucidated. For the first time the cause effect chain of mixture formation and combustion has been elucidated in great detail.
The new models can be utilized to reduce the computational cost for predevelopment of combustion devices that use renewable biofuels. The “dual-fuel” combustion model can be utilized to accelerate the development of retrofit solutions in large marine engines to reduce emissions.

Figures

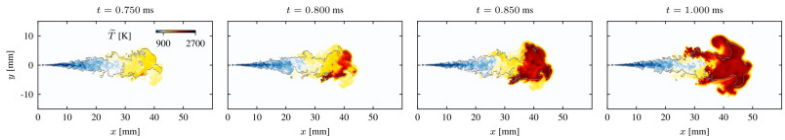


Figure 1: Time series of the temperature field of a reactive 1-Octanol spray combustion Large Eddy Simulation in the ECN Spray A3 configuration.

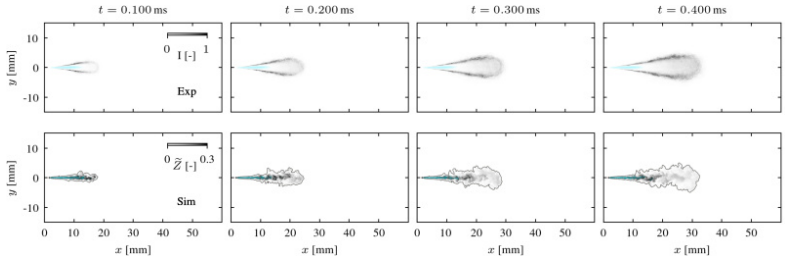


Figure 2: Comparison of experimental Schlieren images (top row) and the mixture fraction field from the Large Eddy Spray Simulation (bottom row) for 1-Octanol under inert conditions in the ECN Spray A3 configuration. The liquid phase is shown in blue.

Publications

Haspel, P; Gierth, S; Popp, S; Scholtissek, A; Rieß, S; Wensing, M; Hasse, C. Large eddy simulation of OME3 and OME4 spray combustion under heavy-duty conditions. Fuel, Vol. 352, 129097 (2023). https://doi.org/10.1016/j.fuel.2023.129097

Haspel, P. PhD: Comparison of turbulent reactive spray characteristics of different renewable fuels using Large Eddy Simulation, Simulation of reactive Thermo-Fluids (STFS), Department of Mechanical Engineering, TU Darmstadt (2023)

Haspel, P. Combined numerical and experimental study of 1-octanol spray flames at ECN Spray A conditions using measured Vapor Liquid Equilibrium data, 18th International Conference on Numerical Combustion, San Diego (2022)

Haspel, P. Evaluation of the Unsteady Flamelet Progress Variable Approach in Large Eddy Simulation of the ECN Spray A, ECN Webmeeting, ECN Webmeeting (2022)

Reference

Fechter, M.; Haspel, P.; Hasse, C.; Braeuer, A. Vapor pressures and latent heats of vaporization of Poly (oxymethylene) Dimethyl Ethers (OME3 and OME4) up to the vicinity of the critical temperature. In: Fuel, 303, S. 121274, Elsevier, ISSN 0016-2361 (2021) https://doi.org/10.1016/j.fuel.2021.121274

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