Injection, Mixing and Auto-ignition of E-fuels for Compression Ignition Engines

WRITTEN BY

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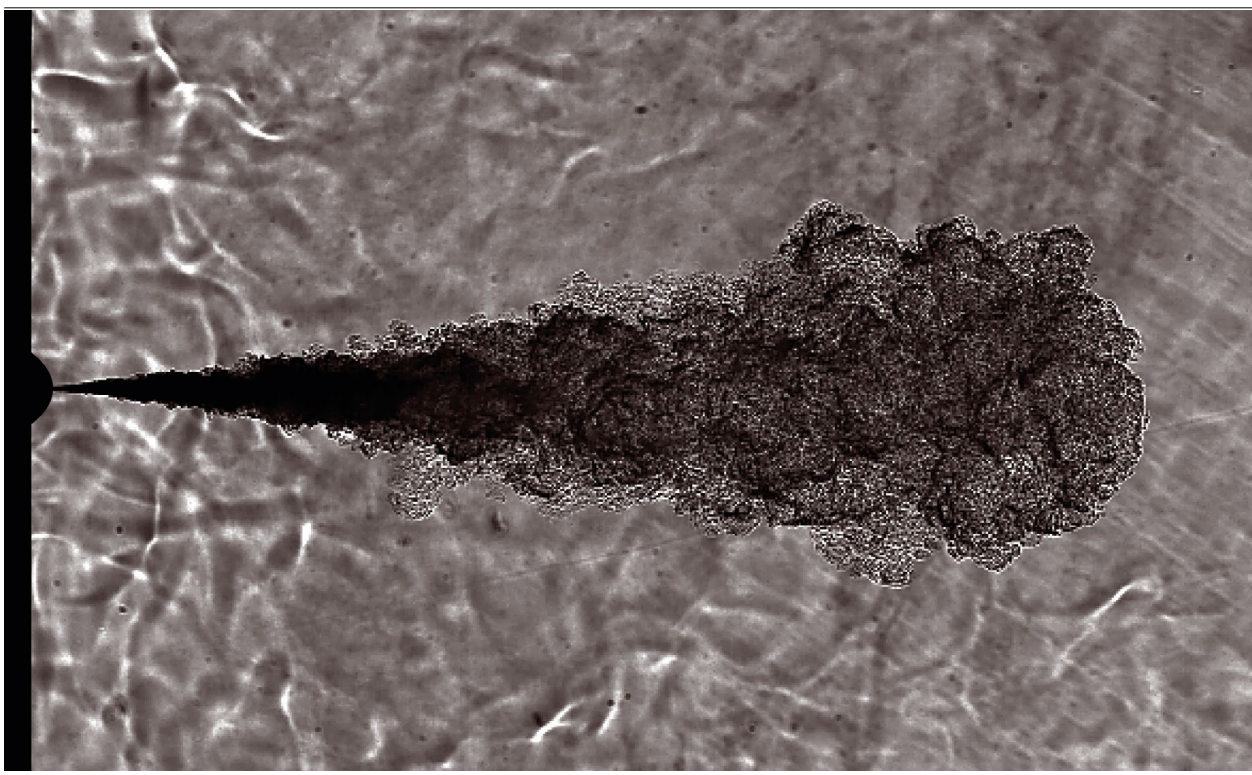
In order to achieve the best engine efficiencies while minimizing pollutant emissions, the physical and chemical behavior of liquid hydrocarbons from renewable energies during their mixture formation and combustion must be understood. In the FVV project “eSpray” (no. 1403), the injection, mixture formation and ignition of OME_{3-5} and 1-octanol are investigated in comparison to diesel-like n-dodecane. In this project, four other international research institutes are working together with Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU).



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1 RESEARCH NETWORK

Liquid hydrocarbons from renewable energies will make a significant contribution to carbon-neutral mobility and play an important role in the future energy supply. Because of their high energy densities, the so-called e-fuels have great potential in combination with efficient Compression Ignition (CI) combustion engines, particularly in mobile applications. Oxygenated e-fuels such as OME_{3-5} or 1-octanol promise a clean combustion. Their physical and chemical behavior in the combustion engine must be understood and modeled correctly in simulation tools in order to achieve optimal efficiency with minimized pollutant emissions when developing and adapting engines.

The aim of the research project is about creating a detailed understanding of the behavior of oxygenated e-fuels in CI engines. A total of five institutions are involved in the international research network: the Professorship for Fluid System Technology (FST) at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), the Combustion Research Facility at the Sandia National Laboratories (SNL), the Institute for Energy and Materials Processes (EMPI) of the University of Duisburg-Essen (UDE), the Institute of Powertrains and Automotive Technology (IFA) of TU Wien (TUW) and the Institute of Advanced Energy and Powertrain Technology at Shanghai Jiao Tong University (SJTU). The participation of these institutes with their different methods and resources as well as their close cooperation together succeed in creating deep insight and new findings.

2 METHODOLOGY

The very basic free-jet investigations are carried out at the FAU's optical combustion test rig with two different research injectors sized for a passenger car. Here, experiments are carried out under constant thermodynamic conditions similar to those in a diesel engine but without charge movement. Under inert conditions, the gas and liquid phase of the spray are recorded using Schlieren and Mie scattering optical measurement techniques. The images taken with high-speed cameras are analyzed with the help of specially developed software and provide information about the geometric dimensions of the fuel spray. In the reactive case, the ignition delay of the high-temperature combustion is evaluated via the chemiluminescence of the hydroxyl radical (OH*). In order to evaluate the sooting behavior of the investigated fuels qualitatively, the visible flame luminosity is recorded. In addition, the mass flow rates of the research injectors are determined at the FAU. Based on these data, the mixture and temperature distribution in the inert spray can be calculated with models.

The SNL also conduct free-jet experiments but with a conceptually different test rig and with different optical techniques. Namely, both the liquid phase and the soot are detected here using diffuse backlight illumination. The gas phase is characterized via Rayleigh scattering and thus the fuel-air mixture fraction is measured quantitatively. In addition, laser-induced fluorescence is used to detect formaldehyde, which characterizes the ignition delay of the low-temperature combustion. High-temperature ignition is determined via OH* chemiluminescence like at the FAU.

The comparison of the results from both institutes shows very good agreement, which reduces experimental uncertainties. Since the free-jet experiments only approximate real engine operation, further measurements are carried out. As part of the project, the UDE investigates the mixture formation and combustion of the e-fuels in an optically accessible single-cylinder engine. The ignition delay, ignition location and burnout phase are characterized via multi-spectral imaging. With the help of different bandpass filters, different gases are visualized – in particular, the gaseous fuel and thus also the penetration depth of the jet. In parallel to the investigations in the engine and the injection vessels, the reaction kinetics of the OME_{3-5} combustion are analyzed at the SJTU. The different species that occur and the ignition delay are investigated in a jet-stirred reactor and a mechanism for OME_{1-6} available in literature is adapted to the fuel under study. The newly developed reaction mechanism is implemented in

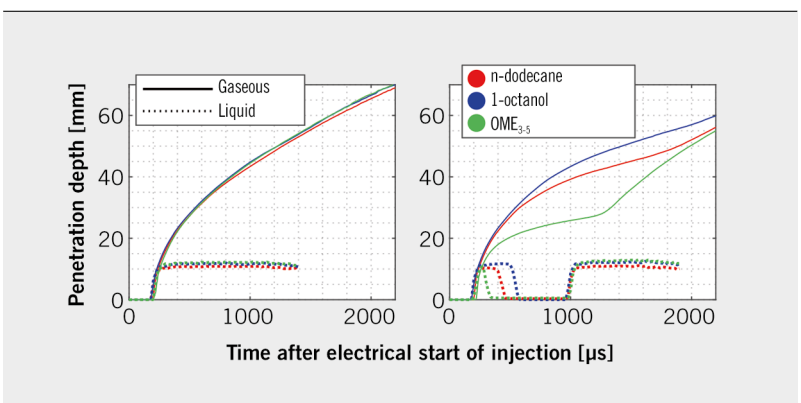

FIGURE 1 Liquid and gaseous penetration depth for ECN Spray A conditions: 1500 bar fuel pressure, 62 bar ambient pressure, 627 °C ambient temperature for single (left) and multi-injection (right) (© FAU)

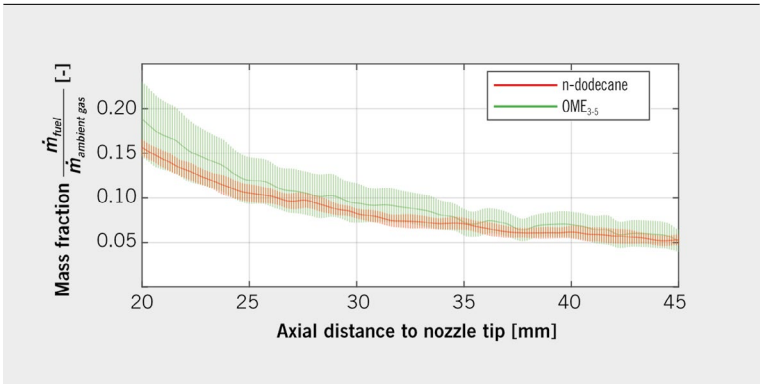

FIGURE 2 Quasi-stationary mixing ratio along the spray axis at ECN Spray A conditions (© SNL)

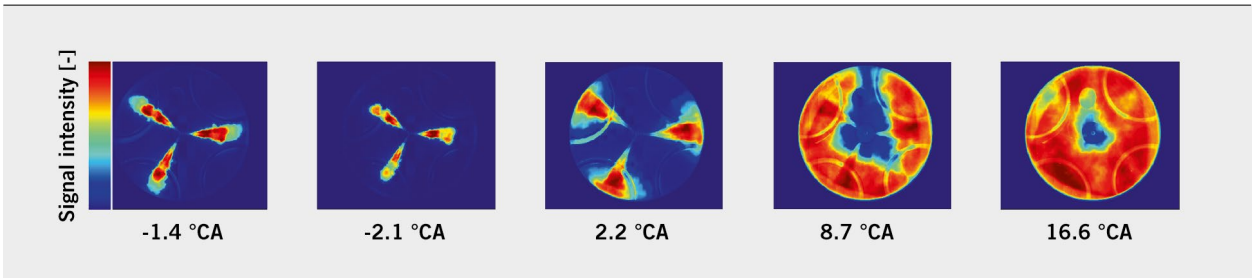

FIGURE 3 Intensity distribution of an inert OME_{3-5} injection in the optical engine recorded through a bandpass filter with a passband of 3365 ± 160 nm (for the detection of hydrocarbons) (© UDE)

a Computational Fluid Dynamics (CFD) simulation model, which is validated using the experimentally determined spray and engine data. Both the free-jet experiments and the engine investigations are simulated in AVL Fire. All numerical work is carried out by the TUW.

3 SUMMARY OF THE MOST IMPORTANT RESULTS

The basic spray experiments show that the vapor penetration depth of the different fuels does not differ under identical ambient conditions. However, there are clear differences in the liquid phase penetration length. Locally, OME_{3-5} and 1-octanol take significantly longer than n-dodecane to completely evaporate. **FIGURE 1** (left) displays this behavior as an example for the Spray A operating point defined by the Engine Combustion Network (ECN) [1]. In addition to that standardized operating point, at the FAU, multi-injections are also investigated. Here in particular, the influence of the e-fuels on the hydraulics of the injectors can be observed. For very short pre-injections, where the injector is operated in the ballistic range, the opening and closing behavior deviates from the diesel substitute n-dodecane, which leads to different injection durations for the same actuation time, **FIGURE 1** (right) [2].

The mass distributions of the e-fuels in the spray are calculated by the FAU using the models of Naber and Siebers [3] as well as Musculus and Kattke [4] for a steady-state spray jet. They show that there are no changes compared to n-dodecane or diesel. However, a different combustion air ratio occurs due to the different stoichiometric air requirements. The results from the models are confirmed by measurements from experiments performed at the SNL. **FIGURE 2** displays the quasi-stationary fuel-air mixture fraction for OME_{3-5} and n-dodecane along the spray axis. The deviations are within the experimental error.

Not only in the free-jet experiments at the FAU but also in the measurements in the engine at the UDE, it is observed that the e-fuels investigated burn further away from the nozzle tip. With OME_{3-5} more of the reaction happens on the spray axis than with n-dodecane. For use in existing diesel engines, this means that pistons with an adapted bowl geometry must be used to reduce the heat load. OME_{3-5} has a shorter ignition delay time than n-dodecane and the burnout phase for the same fuel mass is also shorter compared to n-dodecane. Therefore, in an existing engine, the start of injection must be adjusted.

Another important result of the project is the successful use of mid-infrared imaging technology in the optical engine. With an appropriate filter, the gaseous fuel penetration depth in the inert case can be determined much more easily than with

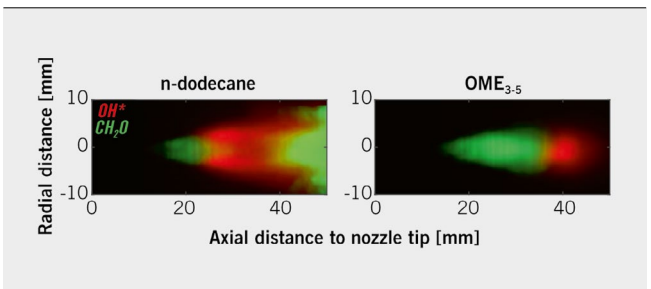

FIGURE 4 Laser-induced florescence of formaldehyde and PAH (green) and OH* signal (red): n-dodecane (left) and OME_{3-5} (right) at ECN Spray A conditions (© SNL)

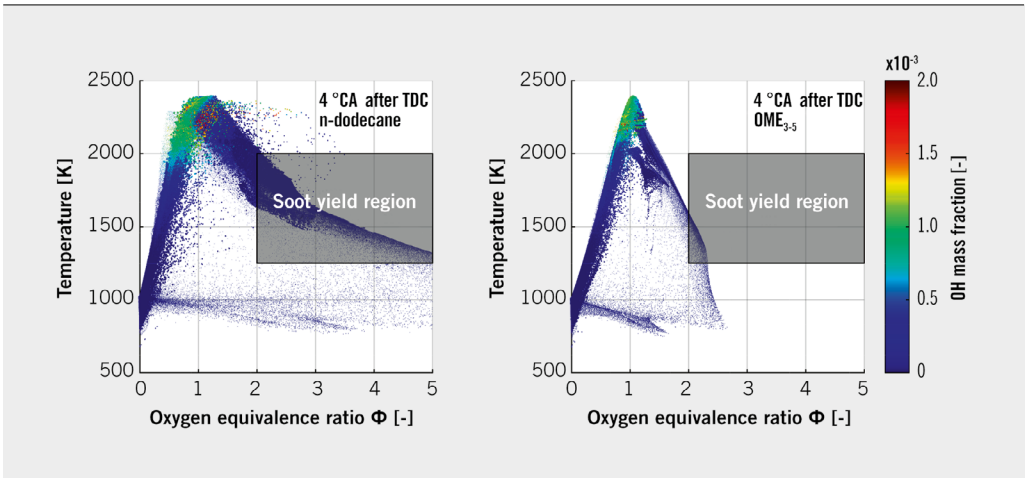

FIGURE 5 Simulated reactive mixture formation in the engine combustion chamber: n-dodecane (left) and OME_{3-5} (right) (© TUW)

conventional measurement techniques. **FIGURE 3** shows the spray plumes at different times of injection taken through a piston window. More details on the engine experiments and simulations can be found in [5].

All experiments show that OME_{3-5} burns soot-free for any operating condition investigated here. Soot precursors such as Polycyclic Aromatic Hydrocarbons (PAHs) are not formed during combustion of this fuel due to the lack of carbon-carbon bonds. PAHs fluoresce after excitation with a laser at a similar wavelength as formaldehyde. The only ways to distinguish between them is by their position in the spray, as well as by timing in the case of high-speed measurements. The signal closer to the nozzle tip can be attributed to formaldehyde, whereas the signal further away stems from the soot precursors. **FIGURE 4** displays a comparison of the formaldehyde and PAH fluorescence (green) and OH* chemiluminescence (red) for OME_{3-5} and n-dodecane combustion. It can be seen that in the area of potential soot formation – downstream of the OH* (to the right) – PAHs are not detected for OME_{3-5}.

The CFD simulation also shows that the entire combustion process from OME_{3-5} occurs very closely around the stoichiometric combustion air ratio. There are almost no reactions at mixing ratios that could lead to soot formation [6]. **FIGURE 5** displays the temperatures of all cells of the engine combustion chamber over the oxygen equivalence ratio calculated in the CFD simulation. The data points are color-coded according to the OH mass fraction, which can be understood as an indicator of combustion, or more specifically, the local heat release.

The project results provide physical insight into engine combustion and yield design aids for future CI engines to use the full potential of the e-fuels investigated. Due to the soot-free combustion of OME_{3-5}, high exhaust gas recirculation rates are possible reducing NO_x emissions significantly. Thus, powertrains that are not only carbon-neutral, but also have ultra-low toxic emissions can be realized with e-fuels.

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