Progress in FGM-LES modeling of igniting n-heptane sprays in a constant volume

Progress in FGM-LES modeling of igniting *n*-heptane sprays in a constant volume

C. Bekdemir[1]*, L.M.T. Somers[1], L.P.H. de Goey[1], J. Tillou[2], C. Angelberger[2]
[1]Department of Mechanical Engineering, www.combustion.tue.nl
Eindhoven University of Technology, The Netherlands
[2]IFP Energies Nouvelles, Rueil Malmaison, France

A study will be presented on the application of a tabulated chemistry technique to model fuel spray ignition. The objective is to predict correct spray combustion physics. The FGM approach is applied to take into account detailed chemistry. This chemistry tabulation technique has been applied to RaNS simulations of sprays and engine combustion before and proved to be effective in predicting the correct macroscopic behavior (Bekdemir et al. PROCI 33 (2011) 2887-2894, Bekdemir et al. SAE 2010-01-0358). However, to gain more insight in the effect of for instance the way the chemistry table is generated, different engine operating points, used reaction mechanism on the ignition process and the f ame structure (premixed, partially-premixed, non-premixed), one needs spatially better resolved simulations. LES can give such detail and becomes increasingly feasible for these applications. In this abstract we present the f rst results of FGM-LES applied to combusting *n*-heptane sprays in a constant volume chamber.

Numerical code

The code that has been used in this study is AVBP (which is owned by CERFACS and IFP Energies Nouvelles). AVBP is a parallel CFD code for reactive unsteady f ow simulations on hybrid grids. It can handle two-phase f ows with an Eulerian formulation and has an injection model specially developed for full cone spray simulations. The injection model relates injector parameters to two-phase boundary inf ow conditions that apply typically 10 times the nozzle orif ce diameter downstream of the nozzle exit (Martinez et al. Fuel 89 (2010) 219-228).

FGM: tables and implementation

Flamelet Generated Manifolds are pre-processed chemistry tables that contain information from detailed chemistry (DNS) simulations of 0D or 1D model problems. From experiments it can be concluded that non-premixed combustion is a major process in direct injection combustion. Therefore, in this analysis, 1D counterf ow diffusion f ames have been solved with our in-house code CHEM1D (www.combustion.tue.nl) to generate the FGMs. Unsteady diffusion f ames have been used additionally to steady diffusion f ames at a broad range of strain rates ($0.1 < a < 500$). The igniting f ame has been solved for a single strain rate value of 500 [1/s]. All needed quantities (may be chemical source terms, species mass fractions, thermodynamic properties etc.) are stored as function of mixture fraction $\mathcal{Z}$ and progress variable $\mathcal{Y}$ (here def ned as the sum of CO_2, CO and HO_2).

ambient oxygen	12, 15, 21 [mole% O_2]
ambient temperature	1000 K
ambient density	14.8 kg/m^3
nozzle orif ce diameter	0.100 mm
injection pressure	150 MPa
fuel	*n*-heptane
fuel temperature	373 K

Figure 1: Conditions baseline n-heptane (http://www.sandia.gov/ecn/index.php)

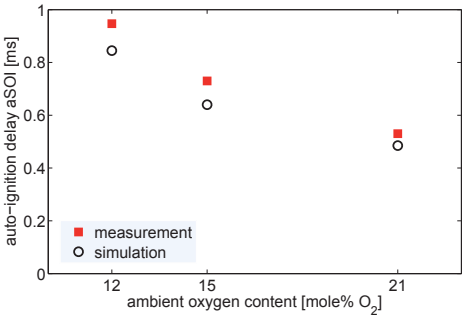

Figure 2: Auto-ignition delay as function of the ambient oxygen content.

In this study a very compact reaction mechanism is used that is based on the *n*-heptane mechanism of Peters et al. (C&F 128 (2002)38-59). The size is reduced leading to a mechanism with 248 reactions among 48 species. During the LES simulations transport equations for $\mathcal{Z}$ and $\mathcal{Y}$ are solved, which are used to look-up desired quantities from the FGM table. So, for now, the variances are neglected.

*Corresponding author: c.bekdemir@tue.nl

Preliminary results

In this section, the simulation results of Sandia's baseline *n*-heptane cases are compared to experimental data. All simulations have been performed on an unstructured grid with a mesh size of 80 μm at the nozzle exit that gradually increases to 800 μm downstream. The case conditions are summarized in Fig. 1.

Ignition delay in experiments is def ned at rapid pressure rise marking the beginning of second-stage high temperature chemistry. This point is not easily identif ed from simulations. Therefore, for now, the ignition delay from simulations is def ned at the steep increase of maximum temperature in the domain, which is a sharp mark in temporal space. If one would take the experimental def nition the numerical ignition delays would resemble the experiments better, but as said, this would be more arbitrary. Measured ignition delays increase with decreasing oxygen content. The same trend has been found for simulations as well. A comparison can be seen in Fig. 2.

Lift-off length in experiments is def ned at excited-state OH (OH*) which is found in high-heat-release regions. Since we do not have simulated OH* data readily available, for the time being an indicative comparison can be made on basis of the chemical source term, which is also a measure for heat-release. In experiments the lift-off length increases with decreasing oxygen content. This behavior is observed in simulations as well, as can be seen qualitatively from Fig. 3. In this f gure the instantaneous cross-section contours of the simulated cases shortly after auto-ignition are shown. The progress variable source is indicated with the colors up to 10000 [1/s], for clearness everything above that value is clipped to the red color, and the white lines mark the stoichiometric mixture fraction contours.

A similar picture is shown for temperature contours in Fig. 4. It is clear that a lower oxygen content in the ambient air suppresses combustion temperatures considerably.

Ignition delay is predicted quantitatively well and f ame lift-off trend is captured correctly. Altogether, these f rst FGM-LES simulation results of igniting *n*-heptane sprays and the comparison with experiments are encouraging.

Outlook

Developments in FGM-LES modeling of combusting fuel sprays will clearly benef t from more in depth analysis of simulation results. Detailed analyses will be done to investigate for instance the effect of pre-tabulation on the f ame structure and the effect of different fuels and reaction mechanisms on the auto-ignition behavior.

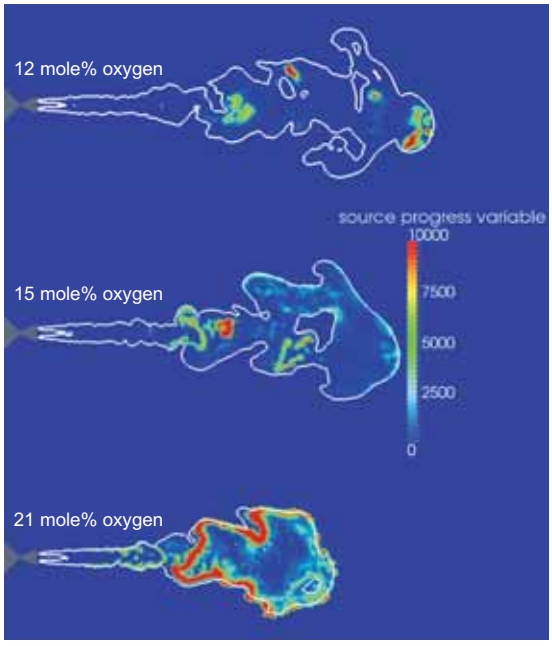

Figure □: □nstantaneous spray cross-sections of □ different cases showing $\mathcal{Y}$-source contours shortly after auto-ignition.

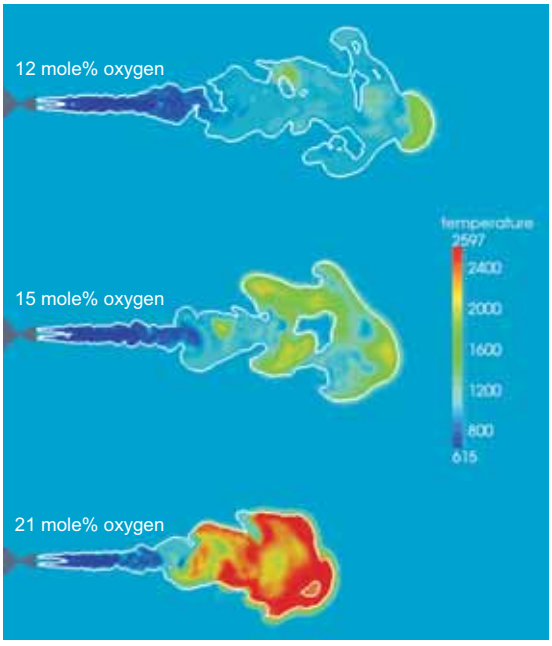

Figure □: □nstantaneous spray cross-sections of □ different cases showing temperature contours shortly after auto-ignition.