Simulation of Lifted Diesel Sprays using a newly developed Combined Level-set Flamelet Model

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Under lower temperature or very high Exhaust Gas Recirculation (EGR) the stabilization at the lift-off length (LOL) is caused by premixed flame propagation. A newly developed G-equation model coupled with Multiple Representative Interactive Flamelets (G-MRIF) is used to predict multiple auto-ignitions as well as premixed flame propagation. However at high temperatures the numerical simulations strongly indicate that the lift-off length (LOL) is defined by auto-ignition.

Introduction

This paper deals with the improvement of models for Diesel sprays. Pickett et al. [1, 2] observed that for very small Diesel sprays no detectable amount of soot is formed inside the flame. The reason for this is the spatial separation of the fuel-rich zones in the spray from the diffusion flame downstream. Because the lift-off length (LOL) is large there is enough time available to premix oxidizer and fuel. This results in a leaner and more premixed-like combustion, where little soot is formed. For this beneficial kind of combustion mode to occur, it is necessary that the resulting LOL is much larger than the liquid penetration length of the fuel.

Computational Model

The CFD code used in this work is AC-FluX (formerly known as GMTEC), a flow solver based on Finite Volume methods [3] which employs unstructured, mostly hexahedral meshes. AC-FluX is documented in detail by Khalighi et al. [4] and in particular by Ewald et al. [5]. AC-FluX solves for the partial differential equations of continuity, the Navier-Stokes equations, an equation for the total enthalpy, and two equations modeling the turbulence (k-epsilon-model).

The applied spray model is a Discrete Droplet Model (DDM) and is the standard technique for current combustion codes. The applied breakup model (Kelvin-Helmholtz-Rayleigh-Taylor) was developed at the Engine Research Center (ERC), and was first introduced by Patterson and Reitz [6]. Collision and evaporation are based on the work by Amsden et al. [7].

A surrogate fuel for Diesel called IDEA consisting of 70% n-decane and 30% α-methyl-naphthalene (in volume) was developed within the Integrated Development on Engine Assessment (IDEA) project. IDEA has nearly the same chemical and physical behavior as European Diesel. The complete chemical reaction mechanism comprises 999 elementary reactions and 116 chemical species. The formation, growth, and oxidation of soot particles is described by a kinetically based model. A method using statistical moments is employed according to Mauß [8] and Frenklach and Harris [9].

Laminar flame speeds were calculated using the in-house code Flamemaster [10]. For these calculations the previously described IDEA mechanism was used. These calculations show that n-decane is consumed during first auto-ignition, in contrast to α-methyl-naphthalene, which is quite stable. During this investigation, flame speeds then were calculated based on the full mechanism for situations before and after first-stage auto-ignition. A similar investigation for n-heptane has been done by Honnet and Peters [11]. If the upstream conditions are those after first-stage ignition, calculations fo n-heptane at 1 atm had shown a significant increase in laminar flame speed. The resulting flame speed at the elevated pressures for the IDEA fuel is not very different for the two cases; therefore it is possible to use the speed before auto-ignition. Hence, only one laminar flame speed table was used in this paper; an example for 50 bar is shown in Fig. 2. This flame speed calculations are used to fit splines for a flame speed table according to Ewald [12]. Therefore gaps as they appear in Fig. 1, which are caused by non-converging calculations, are filled.

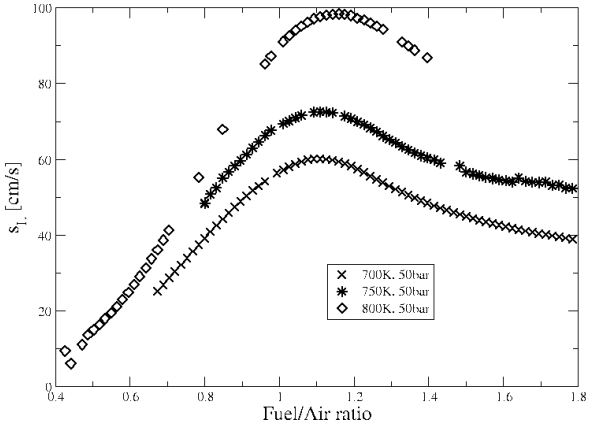

Fig. 1: Laminar flame speeds at 50 bar

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For non-premixed combustion, oxidator and fuel are mixed during combustion. In conventional Diesel modes, the heat release is mainly controlled by diffusion and evaporation. Evaporation is controlled by the injection rate (mass-flow rate, injection velocity) and by the resulting breakup effect. The Representative Interactive Flamelet concept (RIF) [13] allows taking elementary chemistry into account by solving the flamelet equations for the temperature and many chemical species. Therefore, a much more complex chemistry can be solved. The turbulent flow provides the scalar dissipation rate which is a parameter in the flamelet equations χ and the average pressure p. The extended RIF concept G-equation model coupled with Multiple Representative Interactive Flamelets (G-MRIF) to be used here subdivides the injected fuel mass during the time of injection and thereby defines different flamelets. Additionally it also describes the flame propagation through the G-equation which tracks the turbulent flame front The injected fuel is portioned by injection timing into different fuel classes, which can be seen in Fig. 2.

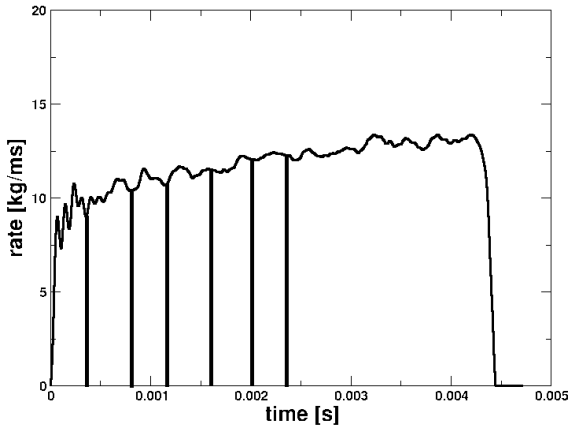

Fig. 2: Definition of the flamelets according to the injection time, based on mass criteria

The G-equation model is based on the assumption that the instantaneous, turbulent flame, being an ensemble of laminar flamelets, is a thin reactive-diffusion layer, embedded in an inert turbulent flow field. The structure of the laminar flame is resolved by the laminar flame speed calculations employing finite-rate chemistry, which provide the laminar bruning velocity s_L and the laminar flame thickness l_F. The G-equation model is not only applicable in the corrugated flamelet regime, but also in the thin reaction zone regime, since the effect of turbulence on the structure of the flamelets can be taken into account [13]. After a certain temperature is reached through auto-ignition, a flame front is initialized using the G-equation approach. In the G-MRIF model two chemical states are present for every injected flamelet. One is the solution in front of the flame front (in the stage of auto-ignition), and the other state is behind the flame front (burning). The two flamelet solutions are identical untill a significant fuel mass of a certain injection reaches a flame front. If a certain amount gets burnt by the turbulent flame front, one of the flamelet pairs is artificially auto-ignited. The remaining fuel mass is still able to auto-ignite. If a natural auto-ignition happens, the G-field is reinitialized.

Experimental setup of the Aachen vessels

The Aachen measurements presented in this work were conducted in two different constant-flow, high-pressure, high-temperature vessels. The pressure was set up to 50 bar and the temperature to 800 K. The energizing duration was 3.5 ms for all investigated cases. The air stream consisted of pure air and Diesel was used as fuel. The data was acquired from two different vessels. One was operated by the Lehr- und Forschungsgebiet Laser-Messverfahren in der Thermofluiddynamik (LTFD) and the other by the Lehrstuhl für Wärme- und Stoffübertragung (WSA). Data on the investigated nozzles may be found in table (1).

Parameter	Value
Nozzle type	Mini sac
Number of holes	3
	120° spacing
Orifice diameter	85 µm, 118 µm, 131 µm
ks-factor	1.3
Cone angle	148°

Tab. 1: Investigated nozzles

OH was measured using chemiluminescence as described in Pauls et al. [14]. The soot measurement was made using Laser Induced Incandescence (LII) as described in Vogel et al. [15]

Simulation setup

The computational domain is 18 cm long and has a diameter of 12 cm. The grid has a resolution of about 2.4 mm at the investigated area. Through local refinement using a maximum level of 3, the resulting grid dimension is about 0.3 mm within the main combustion region. Fig. 3 shows the computational domain and the applied local refinement, which allows a very good grid resolution in the area of interest. The 131 µm nozzle at 1350 bar injection pressure was used to calibrate the injection parameter. The initial injection parameters were applied according to Weber et al. [16].

A slight recalibration was necessary to adopt the spray parameters to the used grid. The values are sufficient for the used application. An improved

calibration is made impossible by computational restrictions (runtime is over two weeks for a single case). The ambient condition was chosen as T = 800 K and p = 50 bar according to the experiment. The injection quantities and the injection rates were taken from Bosch-Tube data at p = 600 bar, 900 bar, and 1350 bar injection pressure using standard Diesel fuel. The spray parameters were adopted to match the simulated liquid and gaseous penetration with the experiment and were applied for the whole pressure range. The temperature at which the turbulent flame front is initialized is chosen to predict the LOL. This temperature is kept constant for all Aachen simulations. The LOL is defined as the shortest distance between the nozzle and the mean turbulent flame front.

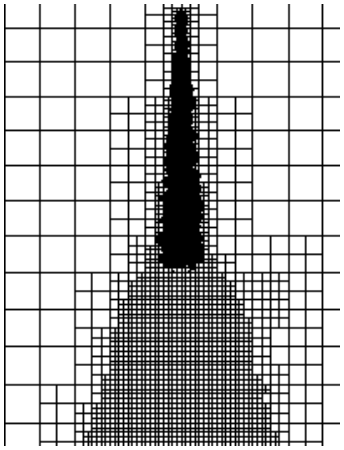

Fig. 3: Cutout of the computational grid

Results and Discussions

	600 bar	900 bar	1350 bar
131 µm Exp. (Diesel)	17.0 mm	19.8 mm	21.9 mm
131 µm Sim. (IDEA)	20.0 mm	22.0 mm	24.0 mm
118 µm Exp. (Diesel)	19.8 mm	24.1 mm	25.8 mm
118 µm Exp. (IDEA)	21.5 mm	27.5 mm	35.1 mm
118 µm Sim. (IDEA)	22.0 mm	20.0 mm	27.0 mm

Tab. 2: Experimental and simulated LOL

All results are shown in Tab. 2. The results show the right general trend. There are two things noticeable. First, the LOL is increasing with decreasing nozzle diameter. Second, the decrease of the LOL for the 118 µm nozzle in the simulation is obvious. In the experiments, a decrease of the LOL for 270 the 118 µm nozzle was found at 750 bar for Diesel and at 1100 bar for the IDEA mixture. For all investigated conditions of the Aachen combustion vessel, the turbulent premixed flame is stabilized by auto-ignition and therefore this kind of combustion mode is called Auto-Ignition-Induced Flame Front (AIIF) by the authors. Recent results show separated second auto-ignition spots between the flame front and the nozzle, which is a strong indicator that in the experiments the LOL is also stabilized by auto-ignition, rather than by turbulent flame propagation.

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