Large-Eddy Simulation of an Auto-Igniting Liquid Diesel-Type Spray

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1 Introduction

In the context of increasing concern about global warming, Diesel engines represent a high interest technology route. Using computational fluid dynamics (CFD) appears as a key tool for improving Diesel engines consumption and pollutant emission

Many published work are devoted to RANS (Reynolds averaged Navier-Stokes) techniques and models for the prediction of Diesel spray combustion [1]. Large-Eddy Simulation (LES) has recently received some interest for studying Diesel spray combustion, as a result of its potential for more detailed description of spray entrainment and mixing and thus improved combustion predictions [2]. The objective of the present work was to undertake first steps towards a detailed exploration of the predictive capabilities of LES in terms of Diesel-spray mixing fields and auto-ignition. The AVBP LES code [3] was applied to the simulation of a single hole liquid spray injected into a constant volume vessel exhibiting temperatures and pressures representative of Diesel engine conditions, and LES predictions were compared with experimental findings. Auto-ignition and combustion were described with the TKI model, which has successfully been used in RANS of Diesel engines, yielding satisfactory [4]. The aim of this first study was to explore whether this model would perform accurately in LES, where mixture fluctuations should play a lesser role due to the usage of finer meshes and the fact that instantaneous flow structures are directly resolved.

1 The TKI-LES combustion model

The TKI (Tabulated Kinetics Ignition) model [5] has initially been developed to predict the auto-ignitions in RANS simulations of piston engines. It is based on the *a priori* construction of look-up tables based on complex chemistry computations of adiabatic auto-igniting homogeneous reactors at constant pressure. It has been applied to RANS simulation of conventional and HCCI Diesel engines [4].

The first stage of the model describes the time occurrence of first noticeable chemical reactions due to auto-ignition by solving a transport equation for a scalar Y_{ir} which reaches 1 at the time for which the

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progress variable reaches $\widetilde{c}_{TKI} = 10^{-3}$. The second stage of the model is then switched on, dealing with auto-ignition (including cold flame phenomena) and main combustion.

The combustion is described based on a progress variable $\widetilde{c}_{TKI}$, the reaction rate of which is taken from the look-up tables. It is defined as:

$$\widetilde{c}_{TKI} = 1 - \frac{\widetilde{Y}_F}{\widetilde{Z}} \tag{1}$$

where $\widetilde{Y}_F$ is the filtered fuel mass fraction and $\widetilde{Z}$ is the filtered mixture fraction. The starting point of the proposed approach is to distinguish fresh and burnt gases states in each cell. The tabulated filtered reaction rate $\widetilde{\dot{\omega}}_c$ of $\widetilde{c}_{TKI}$ is used to compute the reaction rate $\widetilde{\dot{\omega}}_i$ of species i as:

$$\widetilde{\dot{\omega}}_i = \left(Y_i^{eq} - \widetilde{Y}_i^u\right) \widetilde{\dot{\omega}}_c + \widetilde{c}_{TKI}\ \widetilde{\dot{\omega}}_i^b \tag{2}$$

The first term on the right-hand side models the consumption of fresh gases, and thus production of burnt gases, by combustion. It is addressed via a TKI approach, whereby $\widetilde{Y}_i^{eq}$ denotes the equilibrium mass fraction of species *i* extracted from the TKI look-up tables, and $\widetilde{Y}_i^u$ is the unburnt state obtained by solving model transport equations. The TKI model assumes that the species mass fractions evolve linearly with the progress variable. This strong assumption is acceptable in the context of fast auto-ignition phenomena with very fast combustion.
The second term models the evolution of the burnt gases composition. In former formulations, this was addressed using equilibrium calculations or reduced kinetic schemes. The present work takes advantage of the homogeneous reactors simulated for building TKI to build a FPI [6] look-up table. The resulting table contains values of Y_i as function of the FPI progress variable defined as:

$$\widetilde{c}^{FPI} = \frac{\widetilde{Y}_{CO} + \widetilde{Y}_{CO_2}}{\widetilde{Y}_{CO}^{eq} + \widetilde{Y}_{CO_2}^{eq}} \tag{3}$$

, mixture fraction, pressure and temperature. Following the work of Michel et al. [7], the species reaction rates in the burnt gases are then estimated using a linear relaxation:

$$\widetilde{\dot{\omega}}_i^b = \frac{Y_i^{FPI}\left(\widetilde{c}^{FPI} + \delta\widetilde{c}^{FPI}\right) - Y_i^{FPI}\left(\widetilde{c}^{FPI}\right)}{\tau_r} \tag{4}$$

where Y_i^{FPI} is the tabulated FPI mass fraction and $\delta\widetilde{c}^{FPI}$ is the progress variable increment computed as in [7] for the characteristic time τ_r.
Finally, temperature is computed by inversing the species enthalpies.

2 Experimental setup

The TKI model is applied to the LES of a liquid spray experiment studied by Bruneaux [8]. Liquid fuel is injected via a single hole nozzle into a constant volume cubic vessel of 112mm edge length. The vessel is pressurised and preheated by a pre-combustion allowing to reach pressure and temperature levels representative of those found in a Diesel engine. Table 1 lists the initial pressure and temperature at injection, the injection pressure, as well as the composition of the injected fuel.

Available experimental results include Laser Induced Exciplex Fluorescence (LIEF) for quantifying local fuel vapour concentrations, Laser Induced Fluorescence excited at 355 nm (LIF 355) and OH LIF for tracing auto-ignition locations, and Particle Image Velocimetry (PIV) for gas velocities at the jet edge. Simulated cases include a non reactive case with N_2 filling the vessel, and a reactive case with air.

P_0	T_0	P_{inj}	Injected fuel
66.75 bar	900 K	1200 bar	30% α-methylnaphtalene 70% n-decane

Table 1: Operating conditions

3 Numerical setup

The simulations are performed with the fully compressible AVBP LES solver [3] using a second order Lax-Wendroff centered scheme coupled with an explicit time advancement allowing a good compromise between numerical diffusion and CPU time. Subgrid fluxes were modelled via a constant coefficient Smagorinsky model.

Combustion is described by the TKI-LES model. The liquid spray is simulated using a mesoscopic Eulerian spray model [9]. The used DIturBC approach of Martinez et al. [9] is a deported boundary condition that initiates the spray physics close to the nozzle exit whilst avoiding resolving the liquid core, cavitation and primary break-up close to the injector.

The computational mesh consists of 1.8 million tetrahedra, refined towards the injector outlet where the cell size is around $80\mu m$. The computation of 1 ms of physical time required 13 hours of CPU time on 64 AMD Barcelona 2.3 GHz processors for the non reactive case and 28 hours for the reactive case.

4 Results

4.1 Non-reactive case

The modelling approach for the liquid jet was validated by comparing its predictions with experimental findings for the non-reacting case. To this purpose 9 individual realisations (differing by the random selection of turbulence on liquid and gas velocity profiles at injector outlet) were performed using LES, and resulting ensemble averages compared with measurements. Instantaneous snapshot of fuel mass fraction fields are shown at $t = 500\mu s$ for two differents realisations (fig. 1)

The comparison of the fuel partial density along the axis (Fig 2) shows that LES allows a satisfactory reproduction of experimental data in terms of fuel concentration and penetration length. The shown instant corresponds to $150\mu s$ after the end of the injection, leading to a somewhat unusual fuel mass fraction profile exhibiting larger concentrations in the downstream region than close to the injector. This is a direct result of the fast decrease of injection rate, which induces a phenomenon called entrainment waves [10], that leads to increased small scale vorticity near the injector. These enhance mixing in this region, thus leading to lower partial densities close to the injector, which are accurately reproduced by LES.

Radial profiles also show a very good agreement between LES and measurements (Fig 2) with an accurate reproduction of the spray angle. Even if the RMS of fuel partial densities are very large (of the order of the mean value), 9 realisations appear sufficient to satisfactory reproduces the mean profiles. Similar good results were obtained at locations 10 and 20 mm from the injector.

4.2 First combustion results

A TKI look-up table was generated using the detailled chemical scheme of Wang et al. [11] including 3684 reactions and 662 species. Up to now only one realisation of the auto-igniting case has been

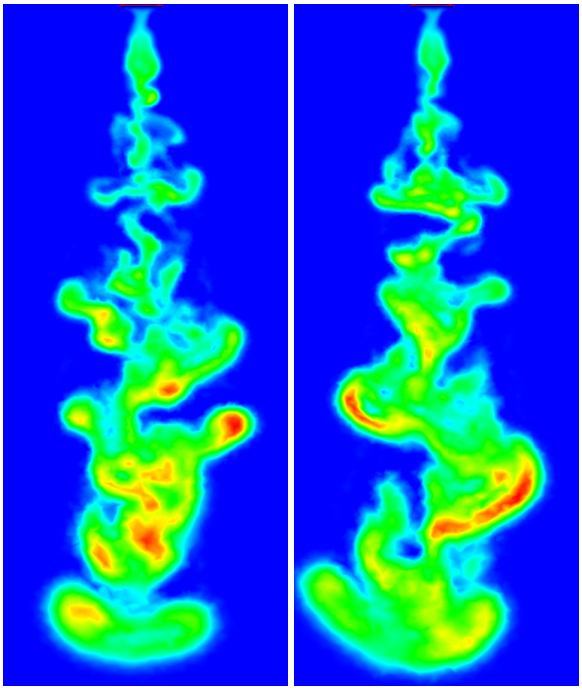

Figure 1: Snapshots of the partial fuel density at $t = 500\mu s$ for two different realisations (i.e. different initial turbulence)

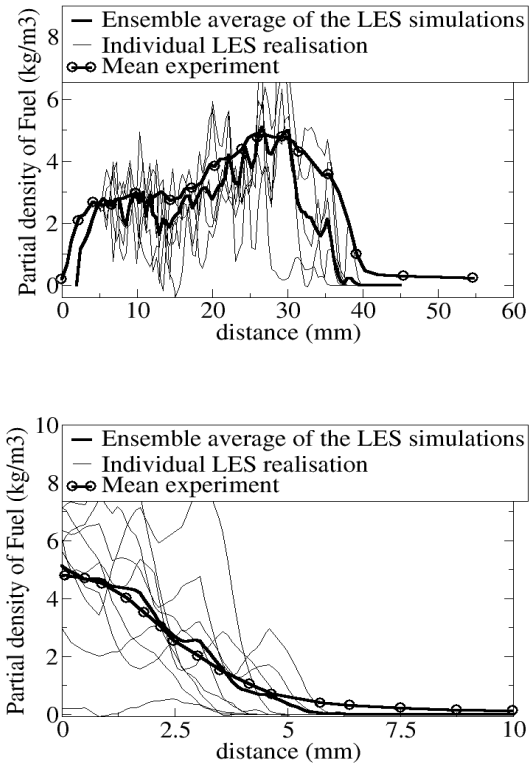

Figure 2: Comparison of the fuel partial density along the injector axis (top) and along a radial profile (bottom) located 30 mm downstream of the injector at $t = 500\mu s$

performed and is displayed in Fig 3.

The auto-ignition is found to take place very close to the injector. Moreover, the flame is located close to the stoichiometric value of the mixture fraction and the combustion appears in slightly rich mixtures. Nevertheless, even if this evolution seems to qualitatively agree with the physical analysis presented by [12], our LES predicts auto-ignition at $280\mu s$, much earlier than the experimental value of $600\mu s$. This too short ignition delay predicted by the TKI model could be explained by the fact that TKI does not account for strain effects, each cell being considered as a homogeneous reactor. In order to verify this analysis, the filtered local scalar dissipation rate $\widetilde{\chi}$ was estimated using the model proposed by De Bruyn et al. [13] based on a simple equilibrium assumption:

$$\widetilde{\chi} = \left(\frac{\nu}{Pe} + \frac{\nu_t}{Sc_t}\right)\left(\nabla\widetilde{Z}\right)^2 \tag{5}$$

Assuming a flamelet structure and a β-pdf for the P(Z) function, this quantity gives access to the strain rate value. As shown in Fig. 4, the first auto-ignition events take place in highly strained regions. Steady strained 1D flamelet calculations under present conditions lead to an estimation of the auto-ignition maximal strain rate value of about $17000s^{-1}$ (Fig. 5).

Fig. 4 shows that less than 6% of the significant reaction rates occur for strain rates lower tan this estimation. Even if values of unsteady strain rates cannot be directly compared to an 1D strained flamelet,

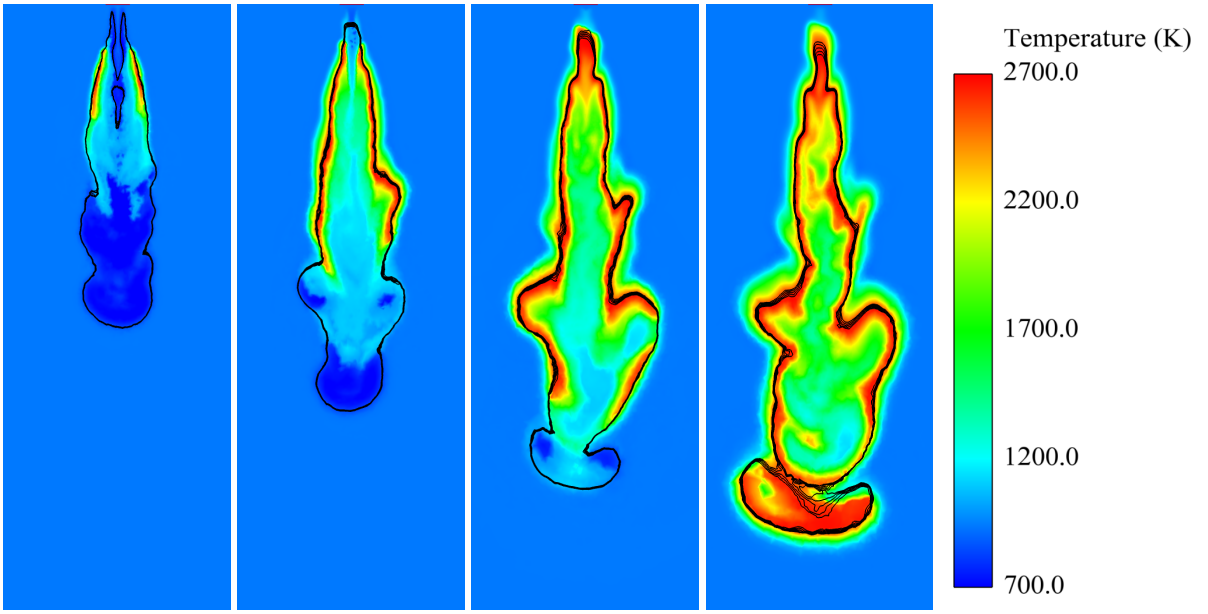

Figure 3: Temperature evolution for time $t = 300\mu s$, $t = 400\mu s$, $t = 500\mu s$ et $t = 600\mu s$. The black line represents the stoichiometric mixture fraction

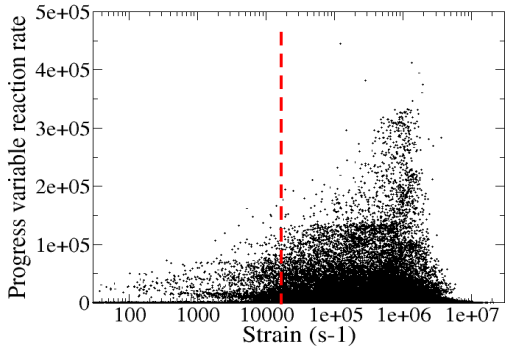

Figure 4: Scatter plot of $\widetilde{\omega}_c$ as a function of the strain at $t = 300\mu s$ (just after start of auto-ignition). The red line represents the limit of auto-ignition as shown in fig. 5

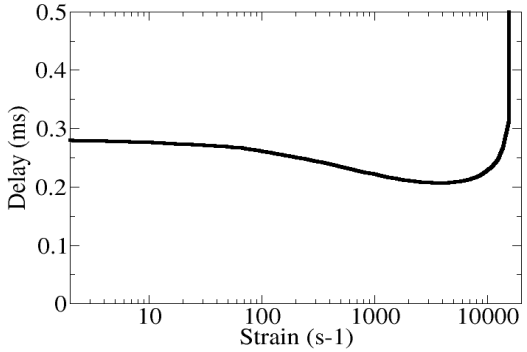

Figure 5: simulation of a 1D flamelet auto-ignition delay at the stoichiometric mixture fraction showing strain limit value of 17.000 s^{-1}.

they nevertheless give indications on the order of magnitude of the auto-ignition strain rate limit. Using a model taking into account the strain rate seems therefore to be essential to predict the correct ignition delay in such configurations.

5 Conclusions

The aim of the presented work was to undertake first steps towards a detailed evaluation of the capabilities of LES to predict Diesel sprays in terms of liquid jet structure, mixing and auto-ignition. To this purpose, a mesoscopic Eulerian spray model was combined with a TKI model for auto-ignition and

combustion to perform LES of a single hole liquid spray of α-methylnaphtalene/n-decane injected into a constant volume vessel under Diesel-like conditions.

Comparisons of nine LES realizations with experimental findings for a non-reactive case showed that the proposed modelling approach allowed an accurate reproduction of the spray angle and gaseous penetration, and predictions are qualitatively similar to recent results reported in the literature. A single LES realization of a reactive case indicated that the modelling approach largely under-estimated the experimentally observed ignition delays and lift-off lengths. First analysis indicates that the auto-ignition locations predicted by TKI correspond to zones with very high scalar dissipation rates, the efffect of which is not rendered by the present approach. Work to come will concern the implementation of a LES formulation of the ADF-PCM [14] model to improve auto-ignition and combustion predictions by accounting for scalar dissipation effects in LES.

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