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Lagrangian–Lagrangian Modelling of an N-heptane Jet at Diesel Engine Conditions

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Abstract

The composition Probability Density Function (PDF) model is coupled with a standard Reynolds-averaged $k-\varepsilon$ turbulence model and a reduced chemical mechanism to simulate transient n-heptane spray injection and ignition in a high temperature and high density ambient fluid. The molecular diffusion is modelled by a Modified Curl (MC) mixing model. The liquid phase is solved by a Discrete Phase Model (DPM). This represents the first application of the Lagrangian-Particle Lagrangian-Fluid (LPLE) implementation of the PDF method applied to practical diesel engine conditions. A non-reacting case was first considered, with the focus on the ability of the model to capture the spray structure, e.g., vapour penetration and liquid length, fuel mixture fraction and its variance. The predictions of lift-off length and ignition delay for reacting cases were then compared to experiment and to a set of results from a well-mixed model that ignores turbulence-chemistry interactions, which is the de facto standard for diesel engine modelling today. Significant structural differences in the modelled flame are revealed comparing the PDF method with the well-mixed model. Quantitatively, the PDF model performs better than the well-mixed model in most cases.

Introduction

Modelling of diesel spray combustion is very challenging due to complicated sub-processes involved, especially due to the highly non-linear finite-rate chemical kinetics and the different combustion modes (premixed and nonpremixed) existing in the same flame [1]. The traditional Lagrangian-Particle Eulerian-Fluid (LPEF) method is widely used in the spray community, with the liquid phase solved by tracking an ensemble of discrete particles interacting with the gas phase, which is treated by the typical Eulerian approach. For modelling in practical diesel engine conditions, it is usually assumed that there are no turbulent fluctuations of thermo-chemical state, i.e. the fluid is well-mixed [2–6]. Due to the nonlinearity of the chemical source terms, this approach can obviously lead to significant errors if in reality turbulent fluctuations of the thermochemical state are non-negligible. The present work is aimed at improving this modelling by adopting the Lagrangian Probability Density Function model for the gas phase [7], in which the source term appears in closed form. The work extends our previous study in which we did not model the liquid spray, instead replacing it with an equivalent gas-jet [8]. This Lagrangian-Particle Lagrangian-Fluid (LPLF) method has been previously applied to an evaporating polydispersed spray [9], encouraging application for reacting cases.

Recently, an experimental dataset of considering spray and combustion in practical diesel engine conditions were made available through Engine Combustion Network, named "Spray H" [10]. The experiments include non-reacting and reacting cases with well-defined initial and boundary conditions. More than 15 research groups worldwide are involved in modeling this dataset with different chemical kinetic and combustion models in various codes [2–6, 8, 11].

The objective of the present study is to evaluate the Lagrangian-Particle Lagrangian-Fluid method against "Spray H" with the focus on the performance of PDF model compared to a well-mixed model. The composition PDF was coupled with a standard $k-\varepsilon$ Reynolds-averaged turbulence model in the Fluent version 14.0 commercial code. The Modified Curl (MC) [12] was adopted for modelling the molecular diffusion. The vapour-liquid equilibrium theory was adopted to account for the two phase interaction. Breakup and collision models were ignored to simplify the spray modelling. Non-reacting cases were first considered with the focus on the ability of the method to predict the spatial and temporal structure of the mixture fraction mean and variance. Reacting cases were then studied using a reduced chemical kinetic model [13] for n-heptane coupled with the ISAT (In-Situ Adaptive Tabulation) chemistry acceleration scheme [14]. The prediction of ignition delay and flame lift-off length is compared to experimental results and to a set of results from a well-mixed model.

Methodology

Experimental setup

The experiments were conducted in an optically accessible constant-volume combustion chamber at simulated conditions that are relevant to practical diesel engines. Briefly, the vessel was pre-filled with a combustible mixture, ignited and mixed for a relatively long period (seconds), slowly cooling down to the expected ambient condition. A liquid fuel spray was then injected from a centrally located single-hole injector, and the subsequent combustion behaviour depended upon the composition of the gases in the chamber, which was controlled by varying the composition of the initial mixture. In the case of liquid spray in non-reacting conditions, the composition of the precursor charge was chosen to result in negligible residual oxygen. The experiments are fully described on the website of the Engine Combustion Network [10]. The baseline non-reacting and reacting conditions of the experiments are listed in Table 1.

O_2%	T (K)	Density (kg/m^3)	Pressure (MPa)
0	1000	14.8	4.33
21	1000	14.8	4.21
15	1000	14.8	4.25
12	1000	14.8	4.27
10	1000	14.8	4.28
8	1000	14.8	4.29

Table 1: Experimental conditions.

Numerical setup

The Lagrangian-Particle Lagrangian-Fluid method was implemented into the Fluent version 14.0 commercial package. A 2-D axisymmetric mesh with dimension of 100 *mm* by 63 *mm*

was adopted. The mesh has a total of 2385 cells, which was found after extensive grid dependence studies to be sufficient and was considered as the baseline mesh. Table 2 describes the numerical setup for the model. A pressure-based transient solver was coupled with the standard turbulence model. It is noted that $C_{\varepsilon 1}$ was adjusted to fix the round-jet anomaly [15]. For considerations of numerical stability, the standard discretisation for pressure and SIMPLE for pressure-velocity coupling were adopted. The first order upwind solution was implemented as it tends to dampen the effects of statistical error compared to the second order solution. A more detailed description of these schemes can be found in the Fluent manual [16].

Domain	2D axisymmetric
Solver	Transient, pressure based
Turbulence model	Standard $k-\varepsilon$ model with $C_\mu = 0.09$, $C_{\varepsilon 1} = 1.46$, $C_{\varepsilon 2} = 1.92$, $\sigma_k = 1.0$, $\sigma_t = 1.3$, $\sigma_\phi = 1.2$
Droplet diameter	0.01 *mm*
Time step	4×10^{-6} *seconds*
ISAT error tolerance	$1.0e-5$
Discretization	Standard for pressure, SIMPLE for pressure-velocity coupling , first order upwind on momentum, density, k and ε

Table 2: Numerical conditions.

Results

In this section, the baseline non-reacting case is first examined, with the focus on the prediction of the spray structure, which is a necessary precursor for accurately predicting the reacting cases. Convergence studies were conducted, with respect to the mesh, time step and number of particles per cell, which showed that the current case is sufficiently converged.

The lift-off length and ignition delay for the reacting cases were then extracted and are compared to the experimental results and a set of results from a well-mixed model. Similar convergence studies as performed for the non-reacting cases were also conducted. In addition the sensitivity to the ISAT error tolerance was assessed. Detailed results for convergence studies cannot be shown here due to the limited space.

Non-reacting results

Figure 1 plots the vapour penetration and liquid length comparison with experimental results for different mixing constants. The vapour penetration length was defined computationally as the length from the injector to the location of 0.1% fuel mass fraction. The liquid length was defined as the length from the injector to the location of 0.15% volume fraction of liquid particles. As one can see, the prediction of vapour penetration and liquid length have very good agreement with the measurement. Moreover, the difference between different mixing constant is hardly noticed, which proves that the mixing constant has no direct influence on spray penetration.

The radial profile of fuel mixture fraction is compared with experiments and reported in figure 2 at four different axial locations. It can be seen that very good radial profiles of fuel mixture fraction are obtained. The mixing constant has minimal effect on the mean fuel mass fraction, which is expected as the mixing constant controls the mixing intensity within a cell and leaves the mean scalar value unchanged [7].

The variance of fuel mass fraction is another matter entirely as reported in figure 3 and figure 4, respectively. The experimental variance was extracted from instantaneous Rayleigh scattering images, while the computational variance was extracted from instantaneous particle data; both were smoothed by cubic smoothing splines to remove some statistical noise [7]. Figure 3 shows radial profile of variance on four different axial stations, while figure 4 plots variance on the centre-line versus axial station. The MC mixing model and different mixing constants C_ϕ from 2 to 4 were used for this modelling results. Figure 3 and figure 4 clearly show that the variance is strongly dependent on the mixing constant, with larger constants obviously leading to lower variances and a stronger axial decay. The mixing constant of 2.5 is found to give the best overall agreement, and exhibits a good prediction of the variance except at stations before around 20 *mm*. This over-prediction could not be explained by the statistical uncertainty as shown in figure 4. It might be a systematical experimental error and is probably because of a median-filter smoothing applied to the raw data to remove spurious signals due to particles in the fluid [17]. This selection of the value of mixing constant is the same as the previous study with gas-jet PDF method that applied to the same spray [8].

Overall, very good results are obtained for the non-reacting case compared to experiments, which is essential for the studies of reacting cases.

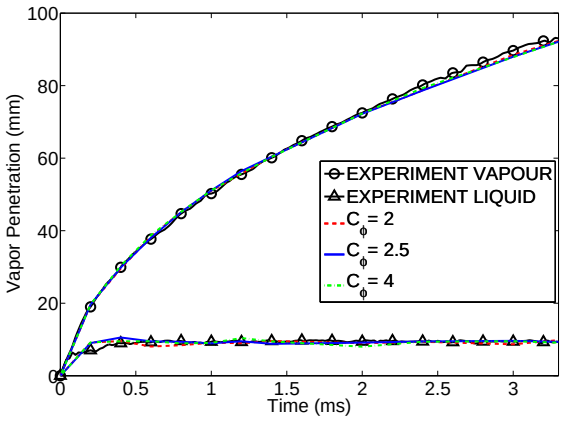

Figure 1: Vapour penetration and liquid length from experiments and computations with different mixing constants, MC mixing model.

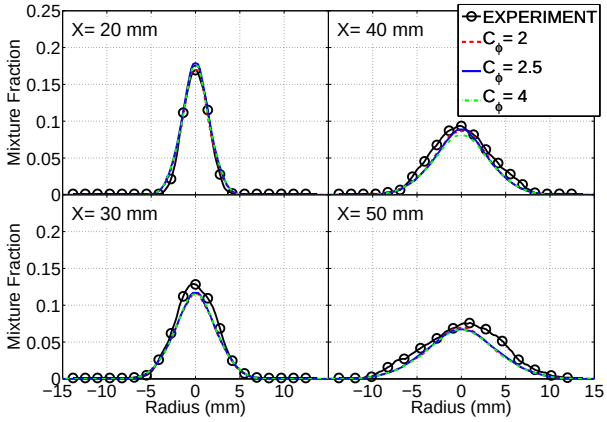

Figure 2: Radial profile of fuel mixture fraction from experiments and computations with different mixing constants, MC mixing model.

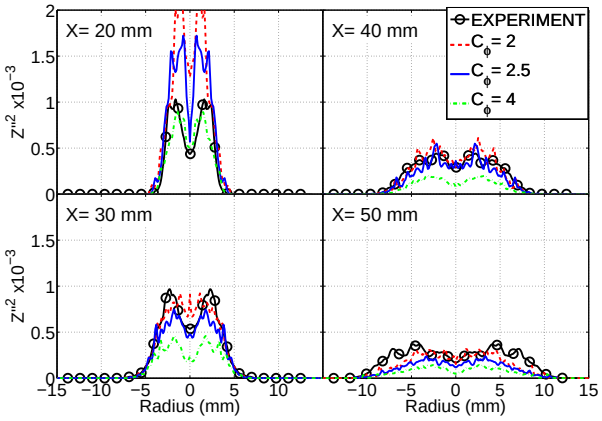

Figure 3: Radial profile of fuel mixture-fraction variance from experiments and computations with different mixing constants, MC mixing model.

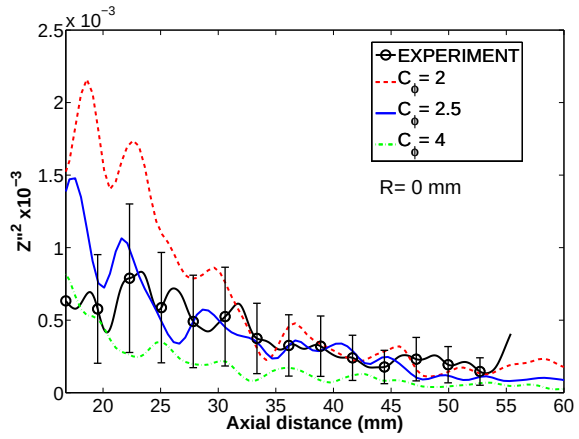

Figure 4: Axial profile (R = 0 mm) of fuel mixture-fraction variance from experiments and computations with different mixing constants. The 95 % confidence interval is shown for the experimental data.

Reacting results

In this section, the baseline reacting cases are considered and compared to a set of results obtained from a well-mixed model and to the experiments. The qualitative comparison of OH structure between the PDF and well-mixed models at 4 ms ASI is shown in figure 5. Significant difference can be observed between the PDF and well-mixed models. A broader region with high mean OH mass fraction and lower peak mean values is found for the PDF model, while the well-mixed model presents a thin profile of OH mean values, with higher peak value. This significant difference is expected and is due to the consideration of thermal-chemical fluctuations in the PDF model [8].

Quantitatively, the lift-off length (LOL) was defined as the distance from the injector to the axial position of 2% of its steady-state OH mass fraction. Ignition delay (IG) was defined as the time from the start of injection to the time where the maximum rate of maximum temperature rise happens. These two definitions were both suggested from Engine Combustion Network workshop 1 [18] and the follow-up web meetings.

Figure 6 presents comparison of the temporal evolution of lift-off length between the PDF and well-mixed models at 15% O_2 ambient condition. Again, a remarkable difference can be observed. First, the PDF model quantitatively exhibits better results than well-mixed method at this ambient condition com-

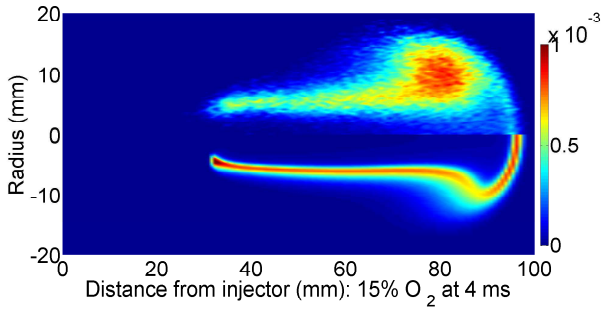

Figure 5: Comparison of OH mass-fraction contour between well-mixed (down) and PDF (up) models under 15% O_2, 14.8 kg/m^3 at 4 ms, PDF model with MC mixing model and $C_\phi = 2.5$.

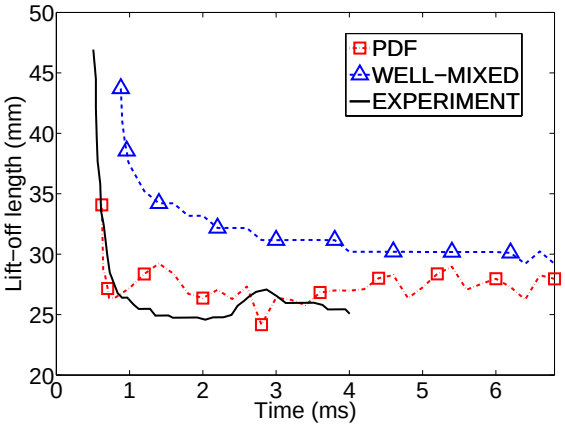

Figure 6: Comparison of temporal evolution of lift-off length between the well-mixed and PDF models under 15% O_2, 14.8 kg/m^3 , MC mixing model with $C_\phi = 2.5$.

pared to experimental results. Second, A meandering flame stabilization point can be observed for the PDF model, while the curve of the well-mixed model shows a smoother trend and the stabilization point is gradually moving downstream.

Lastly, the comparisons were expanded to different ambient O_2 conditions. The lift-off length and ignition delay are compared between the PDF and well-mixed methods, along with the experimental results in figure 7 and figure 8, respectively.

From figure 7, one can see that the PDF model with $C_\phi = 2.5$ shows quantitatively better results than the well-mixed in most cases. A smaller value of $C_\phi = 1.3$ for the PDF model was also studied and much better results were obtained as shown in figure 7, with excellent agreement with the experimental results at lower ambient O_2 conditions and slight over-prediction at higher ambient O_2. It can also be noticed from figure 7 that the effect of C_ϕ is more significant at lower ambient O_2 conditions.

For the ignition delay reported in figure 8, the PDF model shows much better results than the well-mixed model in all cases for both $C_\phi = 2.5$ and 1.3. Not much difference for ignition delay is noticed when varying the mixing constant.

Conclusions

An n-heptane spray at diesel engine conditions has been modelled for the first time with the Lagrangian-Particle Lagrangian-

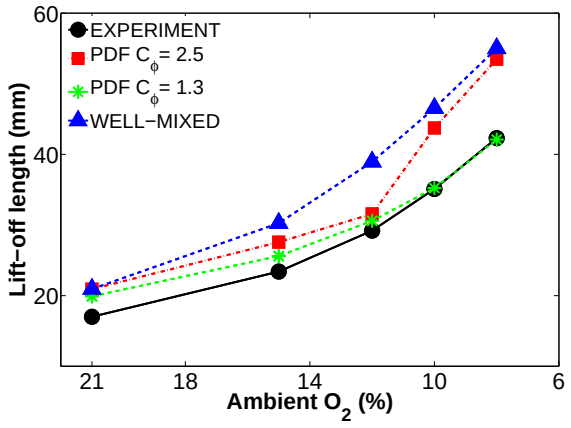

Figure 7: Comparison of lift-off length between the well-mixed and PDF models under different ambient O_2 conditions at 14.8 kg/m^3, PDF model with MC mixing model and different mixing constants.

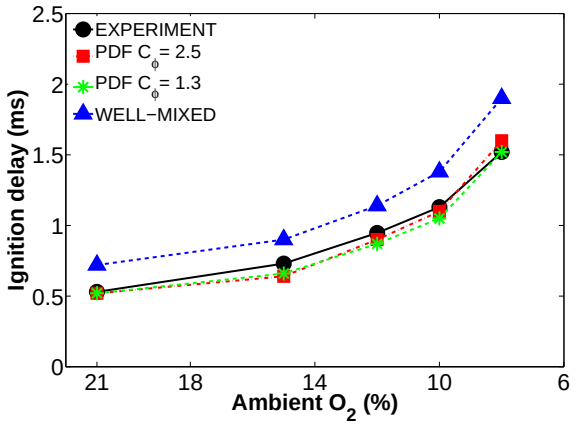

Figure 8: Comparison of ignition delay between well-mixed and PDF models under different ambient O_2 conditions at 14.8 kg/m^3, PDF model with MC mixing model and different mixing constants.

Fluid method, with the continuous phase solved by the transported probability density function approach. Good predictions of the non-reacting, transient fuel-jet structure have been obtained, including vapour penetration and liquid length, and radial profiles of mean mixture fraction and its variance. The value 2.5 for C_ϕ gave the best prediction for the variance except in the region $x < 20$ mm. Reacting cases coupled with a reduced mechanism were also reported, with the focus on the comparison of the model's lift-off length and ignition delay to a set of results from a well-mixed model and to the experimental results. The PDF model shows qualitatively correct flame details and performs quantitatively better than the well-mixed model in most cases.

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