

Development and Experimental Validation of a Fast Spray Ignition Model for Diesel Engines Using Insights from CFD Spray Calculations

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ABSTRACT

Modern Diesel engines have become ever more complex systems with many degrees of freedom. Simultaneously, with increasing computational power, simulations of engines have become more popular, and can be used to find the optimum set up of engine operation parameters which result in the desired point in the emission-efficiency trade off. With increasing number of engine operation parameter combinations, the number of calculations increase exponentially. Therefore, adequate models for combustion and emissions with limited calculation costs are required. For obvious reasons, the accuracy of the ignition timing is a key point for the following combustion and emission model quality. Furthermore, the combination of mixing and chemical processes during the ignition delay is very challenging to model in a fast way for a wide range of operation conditions. This work focuses on the description of a physics-rich diesel engine spray ignition model, which offers the possibility of real-time calculation.

The spray ignition model uses a simplified 3-Arrhenius approach for the modelling of chemical reactions, with time-variant conditions of temperature and mixture fraction replicating the history of the igniting fuel portion. To identify the mechanisms for fuel mixing and ignition conceptually, 3D computational fluid dynamics simulations were performed using a conditional moment closure (CMC) combustion model. A Lagrangian tracking method which is capable of capturing spray pattern and fuel trajectory in liquid and vapour phases was applied to characterise the mixing history of the fuel. The result of the tracking is the information of local equivalence ratio and temperature along the trajectory of the igniting fuel portion of the spray, from injection to ignition. A variation in operating conditions (changing nozzle diameter, injection pressure, ambient temperature and fuel temperature) including reactive and non-reactive calculations provided a broad understanding of the role of mixing and low temperature reactions in the trajectory of the igniting fuel. For the spray ignition model, this trajectory has been deduced in a conceptual way, using distinct phases that could be identified from the CFD simulation. The resulting equivalence ratio and temperature evolution has been used to complete an ignition integral using a simplified 3-Arrhenius approach. The final model contains 6 parameters, which need to be adapted for operation in a Diesel engine.

The model has been calibrated on a medium-speed diesel engine and validated for a broad variation of engine operating conditions (load, boost pressure, start of injection, EGR, intake temperature, intake valve timing, etc.) in two different engines. The accuracy of the modelled versus the measured ignition delay is very good. The dominant effects of the spray ignition process have been identified and successfully transformed into a simplified description, which can be used for real-time calculations.

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INTRODUCTION

Diesel spray ignition is a complex process which involves simultaneous spray atomisation, fuel-air mixing, heat transfer and chemical reactions. All abovementioned processes are complex enough to warrant detailed dedicated experimental and numerical studies ranging from single droplet ignition experiments and direct numerical simulations (DNS) [1, 2, 3, 4] to spray morphology and autoignition in optically accessible engines and test-rigs [5, 6, 7].

Recent investigations have highlighted the importance of low temperature reactions on diesel (or diesel-like hydrocarbon fuels showing two-stage ignition) spray ignition. In recent investigations using DNS Borghesi and Mastorakos [2] showed that cool flame reactions initiated at the lean part of a single droplet resulted in an increase in the local temperature in richer regions, which led to the high temperature ignition. Similarly, Krisman et al. [4] showed that this cool-flame propagation towards richer mixtures resulted in a significant decrease of their high-temperature ignition delay.

Most phenomenological/0D ignition delay (ID) models found in the literature [8, 9, 10] take into account a mixing and a chemical delay which are typically added, in order to capture as well as possible the processes found in the engine [11]. The mixing factors are typically dependent on injection parameters, whereas chemical factors are typically expressed with an Arrhenius-type expression. Until now very few 0D models have taken into account the effect of cool flame, which leads to a commonly seen over-prediction of ID under low temperatures or high levels of EGR (eg. [12]).

In terms of simplified, computationally efficient mathematical formulations of chemical reactivity, the 3-Arrhenius Model has been extensively used. Proposed initially by Weisser [13] and expanded by Vandersik [14] and Blomberg [15], the 3-Arrhenius model has its roots in the complex hydrocarbon oxidation chemistry.

It is important to note that the 3-Arrhenius model was originally developed for premixed conditions in a shock tube. To calculate the ignition delay, the reaction rate is integrated over time, using a method was proposed by Livengood [16].

This paper presents a novel approach for fast diesel spray ignition modelling based on a physical description of the spray mixing. This study is split in two parts: first is a numerical investigation using 3D CFD to determine a valid concept for the simplified modelling by investigating the local evolution in temperature and equivalence ratio of the igniting fuel. This is followed by the formulation of a simplified mixing and chemistry model capable of real-time estimations and its application on two different diesel engines with a broad variation of engine operating parameters, including low end-of-compression temperature conditions.

NUMERICAL METHODOLOGY

Concept

By inserting notional gas particles into the transient flow-field obtained by CFD simulation, one can track local evolutions in space and time in a Lagrangian reference frame, which moves with these tracker particles. Each tracker coincides uniquely with one liquid parcel injected into the domain from the nozzle location. Upon complete evaporation of the liquid parcel, the trackers continue to follow the local flow, being driven as massless particles carried by the underlying local velocity. Important quantities such as mixture fraction, temperature and intermediate species mass fractions are thus recorded over the entire trajectory, starting from the nozzle outlet.

The trajectory of the tracker particle which is found at the ignition location at the ignition time is selected for investigation, to extract insights into the local developments leading to auto-ignition.

Computational Fluid Dynamics

The commercial CFD solver STAR-CD version 4.22 is used in this study, coupled with an in-house research code implementing the combustion model. The Navier-Stokes equations for continuity, momentum and energy are solved using finite-volume discretization using the PISO algorithm. A RANS approach to turbulence is employed using the standard k - ϵ model, which solves two additional equations for turbulent kinetic energy k and dissipation rate ϵ respectively.

Spray modelling of the liquid phase is treated by Lagrangian-Eulerian approach for the two-phase process, where the blob model accounts for the atomization with the cone angle θ prescribed to be 10 degrees as a constant, and the Reitz-Diwakar model governs the secondary break-up. The droplets are subject to turbulent dispersion based on a stochastic model. The number of parcels injected is set to 5000/ms. Thermo-physical properties of the fuel (n-heptane) are computed in the solver as a function of temperature.

The mixture fraction ζ characterizes the state of mixing between the fuel and ambient air. Transport equations are solved for the evolution of mixture fraction and its variance. The mixture fraction together with its variance is used to construct the probability distribution function (PDF), which conveys information about the turbulent mixing field to the combustion model.

Combustion Modelling

In this study, we employ the conditional moment closure (CMC) combustion model [17]. This approach has been extensively applied to a number of generic test rigs [18, 19, 20, 21, 22] and diesel engines

[23, 24] and has shown excellent reproducibility of ignition delays, lift-off lengths, and heat-release rates. The influence of turbulence-chemistry interaction using the CMC model over a well-mixed approach is discussed in detail in Ref. [22]. The CMC model solves transport equations for the conditional mean of temperature and all chemical species, which are weighted with a (presumed shape) beta-PDF function to yield the physical temperature and species fields. The conditioning is performed upon the mixture fraction ζ , for which η denotes the sample space variable, which is resolved with 101 points between the oxidiser and fuel sides ($\zeta=0$ and $\zeta=1$ respectively) and clustered around the stoichiometric mixture fraction.

Conditional expectations of the α -th species mass fraction, Q_α , and temperature, Q_T , evolved by solving transport equations. Detailed derivations of the governing equations are found in [17]. The broad methodology of implementation and CFD-CMC coupling is discussed at length in [23] and is not repeated. A number of sub-models are still required for full closure of the governing equations. The conditional scalar dissipation rate is treated by the AMC model [25] while a linear relationship is used for the conditional velocity terms. Turbulent fluxes are closed with a gradient flux assumption. The governing equations are discretised with a second-order central differencing scheme for the diffusion terms and an upwind scheme for convective terms. A full operator splitting between the transport in physical and mixture fraction space and chemistry is employed [18].

A simplified reaction mechanism for n-heptane consisting of 22 chemical species in 18 reaction steps is applied [26] based on good agreement with experimental data obtained with this compact

description in previous studies in constant-volume chambers [19, 20, 21] as well as engines [27, 28]. Conditional chemical sources are closed at first order; this approach has shown very good results in diesel spray simulations [18, 19, 21, 23, 24]. The computational mesh for solving the conditional transport equations is coarser than the flow-field mesh; this is possible due to the much weaker spatial dependence of conditional quantities compared to their unconditioned counterparts, as shown in [19, 23]. Data mapping between the two meshes is performed at each time step using PDF-weighted averages. Further, as described in detail in [23], the mesh for CMC computations is two-dimensional where the cells have been collapsed azimuthally into a single vertical plane.

Lagrangian Tracking

A centre-line tracking approach has already been applied previously [22] to study the temporal history of ignition activity in an n-heptane spray. A generalized particle tracking approach is adopted here: a notional particle is spawned the instant a liquid parcel is fully evaporated and reaches a diameter of zero; this particle is driven subsequently by the local velocity of the underlying flow field as a massless tracker, recording local quantities (notably mixture fraction, temperature, and important intermediate species) as it moves. The number of tracker particles is equal to the number of liquid parcels injected (presently 5,000 parcels per millisecond of simulation) since each tracker corresponds to an evaporated liquid parcel. Turbulent dispersion is neglected for computing their trajectories. The method is numerically non-intrusive, i.e. it does not affect the computation of the underlying flow field. Further details are found in [29].

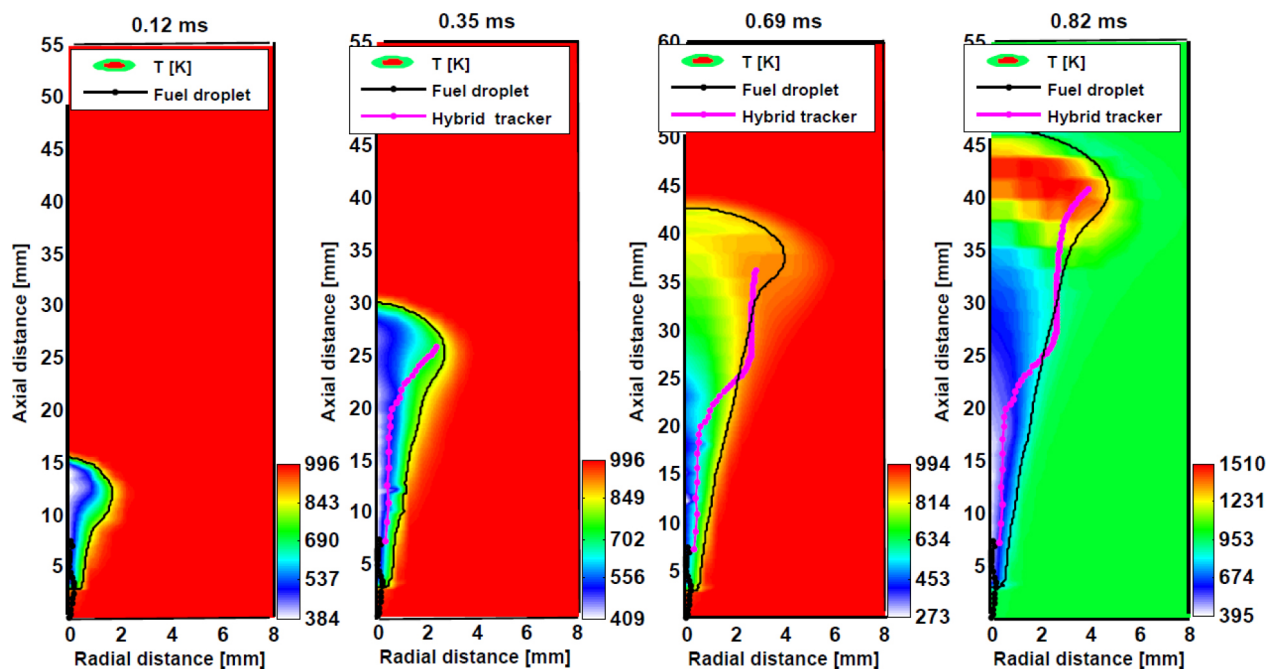


Figure 1. The evolution of the local temperature distributions at time 0:12ms, 0:35ms, 0:69ms, 0:82ms with the trajectory of the corresponding tracker which is traced back from the auto-ignition site.

One such resulting trajectory is shown in Figure 1 at four different time instants along its evolution. The trajectory shown here is the one which is found at the ignition location at the time of ignition.

Numerical Setup

A two-degree wedge angle, 2D CFD grid is employed due to the axisymmetric nature of the spray. The time-step for the CFD simulation is set to 10^{-6} s as a constant. The CFD mesh is in a 2D-axisymmetric arrangement with 108mm in axial length and 60mm in radial width. A mesh resolution of $0.5\text{mm} \times 0.5\text{mm}$ in the first 15mm along the radial direction and $1\text{mm} \times 1\text{mm}$ beyond is employed, with a total of 17,820 cells in the computational domain. The spatial resolution of the CMC mesh is $2\text{mm} \times 1\text{mm}$. The mixture fraction domain is discretized into 101 nodes between 0 and 1, clustered around the stoichiometric mixture fraction.

The Engine Combustion Network (ECN, see www.sandia.gov/ecn) coordinates efforts among research institutions around the world, ensuring consistent and well-defined experimental conditions and methods. The operating point relevant for this study is the *spray H* condition of the ECN using n-heptane, with $T_{\text{bulk}} = 1000\text{K}$, $\rho_{\text{bulk}} = 14.8 \text{ kg/m}^3$ and 21% O_2 . This well-known condition has been investigated numerically with a wide range of modelling approaches. A detailed study and validation using the CMC model is found in [20, 22].

In the CFD simulation, at the instant when the high temperature auto-ignition occurs, the tracker which is exactly found at the first ignition site will be identified and traced back to its initial location. In so doing, the complete temporal local quantities obtained by the tracker along its trajectory can be obtained. In line with ECN norms, the start of high temperature ignition is defined as the first time the mass fraction of OH reaches 2% of the maximum in the domain after a stable flame is established (≈ 0.004 as a constant). In this study, the first ignition sites are defined as the cells in which the mass fraction of OH is around the maximum value within the current domain at the start of high temperature ignition.

Results

For predicting the auto-ignition under inhomogeneous conditions of diesel sprays by means of the integrated 3-Arrhenius ignition model, the values of the temporal and spatial quantities should be precisely obtained in a Lagrangian scenario. In this chapter, the results from the adoption of the tracking method coupled with the 3-Arrhenius ignition model to predict the auto-ignition process in diesel sprays (n-heptane as surrogate), carried out using CFD simulation, will be presented and discussed. They include the evolutionary profile of temperature and equivalence ratio, sensitivity analysis and comparison of the ignition delay (ID) predictions with CFD simulation.

Tracking

Figure 2 depicts the evolutionary profile of the local temperature $T(t)$ and equivalence ratio $\phi(t)$ with the corresponding integral value of ID, based on the tracker from the first ignition site in the flow field of Figure 1. Time $t=0\text{ms}$ corresponds to the overall start of injection. During the entire evolution in Figure 2, four distinct periods can be observed, which have been marked at 0.12ms, 0.35ms, 0.69ms and 0.82ms, respectively.

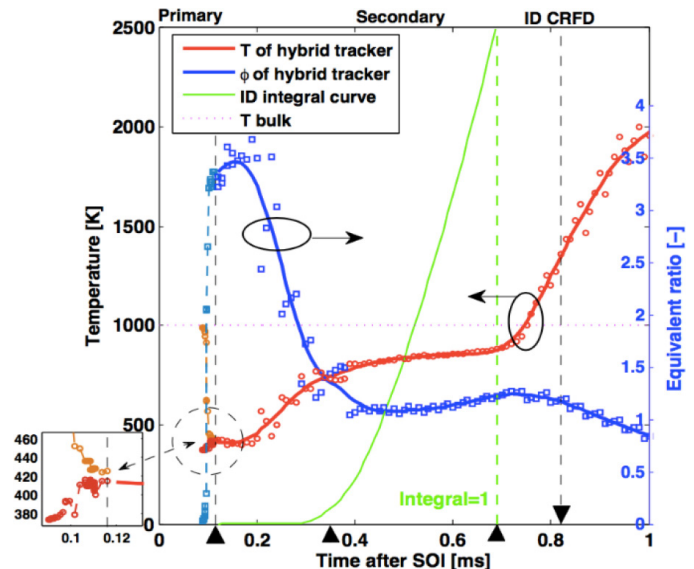


Figure 2. Evolutional profile of the local values of temperature and equivalence ratio by the tracker extracted from the surrounding flow (reference case). In the small sub-plot, the difference between the vapour temperature (orange) and the liquid temperature (red) at the same location is seen, until evaporation is complete.

The first period captures the state of this tracker which is injected at around 0.09ms and gets fully evaporated at 0.12ms. In this period, the tracker follows the liquid parcel's trajectory and is therefore identical with the latter, however it records both liquid-phase and vapour-phase local quantities. From the far left in Figure 2 it can be seen that the fuel droplet itself undergoes a slight increase of temperature (in red) and its surrounding flow shows a drastic decrease in temperature (in orange) from 1000K to around 420K which almost coincides with the fuel droplet temperature. It is also combined with a rapid increase of equivalence ratio (in blue) from zero to approximately 3.5. Along with the changing flow temperature this indicates a dense liquid core and an intensive evaporation process within this near nozzle region (within approx. 10mm from the nozzle). Note that during this period, the local quantities are not included in the integral ignition delay evaluation since (the local temperature being quite low) its effect on the chemical ignition is marginal.

The second period starts when the liquid fuel droplet has evaporated fully, at 0.12ms to the time 0.35ms. During this period, as seen from Figure 2, the local temperature from the tracker - which is now following the underlying vapour-phase velocity field - gradually increases from 420K to about 700K by the fuel-air mixing, while the local equivalence ratio reduces to a lower value around 1.5. These are consistent with the consequence of the local spray motion that forces the tracker towards the radial direction. Starting from this period, following the temperature increase due to mixing, the ignition integral starts depicting positive values.

Figure 3 shows the change of average concentrations of intermediate species over time, divided into the same four periods. A prominent lift of the integral curve is observed in the third period from the time 0.35ms to 0.69ms in which its value reaches one (predicted ignition delay). Within this period, the tracker enters a premixed-like fuel vapour environment where the equivalence ratio stays around 1.3. In the meantime, the temperature shows a slow increase from 700K to around 900K. Generation of intermediate species hydrogen peroxide (H_2O_2) and formaldehyde (CH_2O) implies that starting from the time at 0.35ms, low temperature combustion (cool flame) occurs leading to a certain amount of heat released.

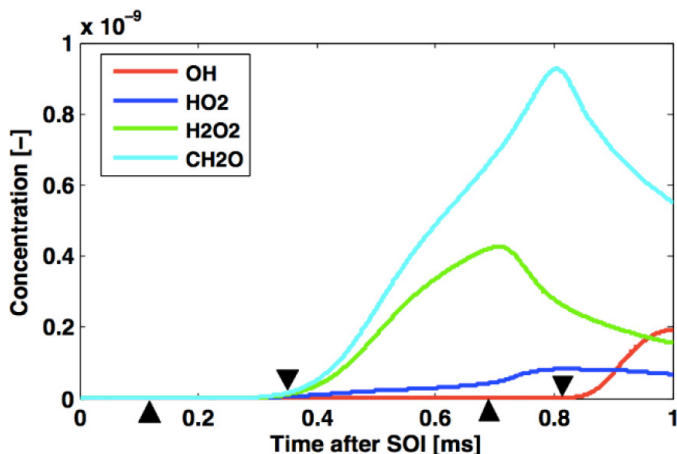


Figure 3. Concentrations of the intermediate species (bulk averaged).

The fourth period is designated from the instant the integral value reaches one until the global high temperature ignition happens (0.82ms) in the CFD simulation. Therefore, there is a slight underestimation of the high temperature ignition delay compared to results from the CFD simulation.

Reactive vs. Non-Reactive

Figure 4 exhibits the evolution for reactive and non-reactive cases for which the local temperature from a given trajectory shows a distinct trend. The non-reactive simulation considers 100% N_2 in

the background. The trajectory is the same as discussed in the previous section. Unlike the reactive case, the temperature from the non-reactive case presents an almost constant shape after 0.3ms. This is as expected since temperature is affected only by mixing, in the absence of reactions. This in turn strengthens the proposition that the gradual increasing of the temperature in the reactive case during this period is only because of the cool flame combustion. Specifically, the cool flame combustion leads to a contribution of approx. 100K over the non-reactive case at about 0.69ms. This reflects that the cool flame acts as an accelerator to precede the process of high temperature auto-ignition, consistent with [30]. This is also consistent with DNS data [2, 4] where cool flame reactions are shown to travel from leaner towards the richer zones of the mixture, leading to increases in temperature in the latter regions.

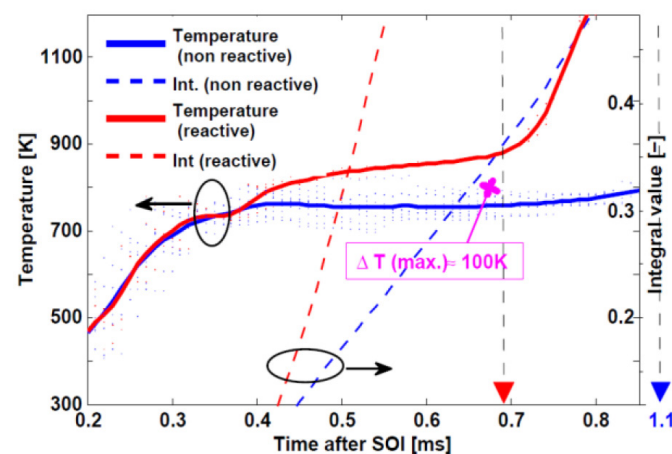


Figure 4. The comparison of local temperature and integral value from reactive and non-reactive cases.

The T- ϕ diagram in Figure 5 elucidates the scatter distribution of temperature in the equivalence ratio space represented by *all* the trackers in the non-reactive case (left) and the reactive case (right). During the first 0.3ms, all the data are near mixing line. In the interval between 0.6ms and 0.7ms, the global trackers' data show a slight increase in temperature, starting from the leaner parts of the jet. In particular, the first-igniting tracker in red, reveals a perceptible lift. These are interpreted as the influence of the cool flame combustion. At 0.85ms to 1.0ms, vigorous combustion takes place where the maximum temperature of around 2300K is reached as seen in the reactive case plots, while for the non-reactive case as anticipated, all the scatter data stay on the mixing line from beginning to end.