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Full Length Article

Modelling of spray and combustion processes by using the Eulerian multiphase approach and detailed chemical kinetics

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HIGHLIGHTS

- Euler Eulerian multi-continuum approach was used in combination with detailed chemistry.
- Liquid fuel injection and combustion processes were simulated.
- The influence various parameters was successfully tracked.
- The developed method can be used for simulation of highly turbulent sprays and combustion processes.

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ABSTRACT

This research deals with computational modelling of non-reactive and reactive turbulent spray processes. The spray process is modelled using the Euler Eulerian multiphase approach together with a size-of-classes model where the discrete phase is considered as continuum and divided into sub-classes. The combustion process is modelled by taking into account chemical kinetics and solving homogeneous gas phase reactions. The combustion model is implemented into a commercial computational fluid dynamics code, and used in combination with previously validated spray sub-models. Several non-reactive cases are modelled by comparing the fuel spatial and temporal development to the available experimental data. The modelled results show excellent agreement for fuel penetration and mixture distributions. Furthermore, the developed method is validated by modelling reactive spray processes within constant volume vessel, and by comparing results to the Engine combustion network experimental data. The vessel conditions correspond well to diesel-like conditions in terms of gas residuals, pressure and temperature. Finally, the given results show a good agreement for the lift-off length and the ignition delay trends compared to the experimental data, but a slight discrepancy in the combustion process occurrence is observed.

1. Introduction

As a result of better fuel-energy conversion compared to spark ignition engines [1], diesel engines have greater popularity on the transportation vehicle market. Their overall efficiency in terms of fuel consumption and pollutant emissions is highly dependent upon the fuel-air mixing which is strongly influenced by fuel atomisation and evaporation processes. The European Union promotes usage of different fuels for powering transportation vehicles [2]. Therefore, in order to remain the most used vehicle powering system, diesel engines must meet higher efficiency standards which can be achieved through their constant development [3]. Modern development methods combine experimental research with Computational Fluid Dynamics (CFD) tools which offer a cost-effective approach. The prerequisite for their reliable use is model accuracy achieved through the validation processes. In CFD modelling of diesel fuel combustion processes, the predictive spray model capabilities play the most important role [4]. Due to that fact, many researchers have invested their time in development of various spray modelling approaches.

In this research two modelling approaches for solving multiphase flows are mentioned: the Euler Eulerian (EE) and the Euler Lagrangian (EL) approach. The EL approach is the most widely used approach for engineering applications, but it suffers from several disadvantages as described in [5,6]. This approach is not able to adequately capture mass, momentum and energy inter-phase

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exchange in regions where the liquid void fraction dominates, i.e. the near nozzle region. To overcome the disadvantages of the EL approach, the EE modelling approach can be utilised. It provides a more reliable description of the physical processes in the nozzle vicinity. The EE approach represents a two-continuum flow description that can be further extended to a multi-continuum method dividing the dispersed phase into classes. The Eulerian conservation equations for mass, momentum and energy are solved for all classes, and the phase coupling is achieved through modelling of interphase exchange terms.

In Compression Ignition (IC) engines, the spray is formed due to high-pressure fuel injection through a small diameter nozzle. The liquid jet flows into the engine cylinder possessing a high momentum. This causes fuel jet disintegration into unstable ligaments and different sized droplets. In general, a spray can be divided into three different regimes: the dense, dilute and very dilute regime, depending on the concentration of the liquid phase. In the dense spray region, the liquid core disintegrates owing to turbulence induced forces and growing surface instabilities – this process is referred as the liquid jet primary atomisation. Such produced droplets are further influenced by relative inter-phase velocities and instabilities acting on the droplet surface. As a result, even smaller droplets are created – this process is called secondary atomisation process. It is essential to reliably model the spray process, since the IC engine combustion performance and emission formation are mainly influenced by the liquid fuel atomisation and the fuel-air mixing processes.

Reactive turbulent spray processes have been modelled by many authors employing various numerical approaches, such as eddy dissipation model, flamelet models, PDF method, and detailed reaction mechanisms. The use of the Eddy Dissipation Concept Model (EDC) was presented in [7], whilst combustion of diluted methanol and ethanol sprays was shown in [8–10]. The investigation to account for the influence of turbulence and nozzle geometry on spray combustion was performed in [11,12]. Furthermore, the influence of fuel injection timing on pollutant emission formation was shown in [13], whilst the prediction of NO and soot trends for various combustion parameters was shown in [14].

The modelling of reactive sprays by employing the EE approach was researched in the recent period, and a summary of relevant publications is briefly discussed. A diluted spray combustion process was modelled by employing the eddy breakup model, and results were presented in [15]. The PDF-Chemical equilibrium combustion model, without discretisation of the liquid phase, was presented in [16,17]. To avoid the difficulties of modelling the near nozzle region, a model for a turbulent inflow boundary condition located downstream was presented in [18]. The diluted spray combustion was modelled by employing the tabulated chemistry approach in [19], whilst combustion of monodispersed sprays was researched in [20]. The authors highlighted the influence of the dispersed phase on the flame propagation. Furthermore, the importance of poly-dispersed sprays on the combustion process was shown in [21].

From the given literature review it can be concluded that the EE approach extended to a multi-continuum model has not been extensively tested on its ability to capture highly turbulent spray and combustion processes. The main objective of this research was to develop a new computational method capable to model the combustion process of poly-dispersed sprays. The presented method is suitable for modelling of multiphase reactive flows, and it can be utilized for modelling the processes occurring in dense spray region. The given results imply that the developed method is adequate for prediction of atomisation, collision, evaporation, and combustion processes.

The Engine Combustion Network (ECN) experimental data [22] of fuel injection with non-cavitating nozzle flow conditions were used for validation of the developed method. ECN is a worldwide group of institutions that perform both, experimental and numerical research. Their ultimate goal is to enrich the knowledge of spray and combustion processes at IC engine-relevant conditions. As a result of their work, a large set of experimental data was generated.

The paper is structured as follows: initially, the description of the developed method for modelling reactive sprays is presented in Section 2. The used ECN experimental data and the numerical setup are described in Section 3. The comprehensive validation of the developed method is presented in Section 4. Next, the liquid and vapour penetration, mixture radial and spatial evolution, Lift-Off Length (LOL), Ignition Delay (ID), pressure rise, and Rate of Heat Release (ROHR) were investigated for different diesel-like conditions. Finally, the research conclusions are drawn in Section 5.

2. Mathematical model

RANS based numerical simulations of the spray and combustion processes were performed. The EE size-of-classes model was used for modelling the highly turbulent spray behaviour. In this approach both the liquid and the gas phases are treated as interpenetrating continua defined by their volume fraction. The liquid phase is further divided into n classes according to the droplet diameter sorted in ascending manner. The first class is always defined as gas phase consisting of the contributing gas species. The classes from 2 to $n-1$ are the droplet classes, whilst the last class n is defined as a bulk liquid class with a diameter corresponding to the nozzle hole diameter. For each Eulerian class a separate set of conservation equations is solved, Eqs. (1)–(3) [23]. The accuracy of the spray description depends on the number of classes. A higher number of droplet classes leads to a better resolution of the droplet size distribution function, but also to higher computational effort.

2.1. EE approach size-of-classes model

Employing the EE approach size-of-classes model a finite number of classes has to be defined together with the sources for the inter-phase exchange. The terms on the left-hand side of the conservation equations determine the property rate of change and the convective transport for class k. Terms Γ_{kl}, $\boldsymbol{M}_{kl}$ and H_{kl} on the right-hand side are the modelled interfacial terms for mass, momentum and enthalpy exchange. Eq. (4) represents the volume fraction compatibility condition that must be fulfilled in order to achieve property conservation.

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{v}_k) = \sum_{l=1, l\neq k}^{n} \Gamma_{kl} \tag{1}$$

$$\frac{\partial \alpha_k \rho_k \mathbf{v}_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{v}_k \mathbf{v}_k) = -\alpha_k \nabla p + \nabla \cdot \alpha_k (\boldsymbol{\tau}_k + \boldsymbol{\tau}_k^t) + \alpha_k \rho_k \mathbf{f} + \sum_{l=1, l\neq k}^{n} \mathbf{M}_{kl} + \mathbf{v}_{\text{int}} \sum_{l=1, l\neq k}^{n} \Gamma_{kl} \tag{2}$$

$$\frac{\partial \alpha_k \rho_k h_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{v}_k h_k) = \nabla \cdot \alpha_k (\mathbf{q}_k + \mathbf{q}_k^t) + \alpha_k \rho_k \mathbf{f} \cdot \mathbf{v}_k + \alpha_k \rho_k \theta_k + \alpha_k \boldsymbol{\tau}_k : \nabla \mathbf{v}_k + \alpha_k \frac{dp}{dt} + \sum_{l=1, l\neq k}^{n} \mathrm{H}_{kl} + h_{\text{int}} \sum_{l=1, l\neq k}^{n} \Gamma_{kl} \tag{3}$$