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Towards a more sustainable transport sector by numerically simulating fuel spray and pollutant formation in diesel engines

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ABSTRACT

Diesel engines account for approximately 50% of new passenger-car sales in the European market and are the major contributor to pollutants that adversely affect human health and the environment. The most adverse pollutants emitted by the combustion of diesel fuel are NO_x, soot, CO and HC. Numerous studies have been carried out to determine the influence of engine design, fuel injection, fuel-air mixing and combustion on pollutant emissions. Information gained through experimental research of in–cylinder processes is limited, and the body of knowledge can be improved by the use of numerical modelling and computer simulations. Computational Fluid Dynamics (CFD) has become a valuable tool that decreases the time and the cost of experimental research. Therefore, CFD is being increasingly used in development of combustion systems. This paper presents how the development of CFD models is the proper approach towards achieving a cleaner and more sustainable transportation sector. The physical models for the liquid fuel disintegration, evaporation and pollutant formation are used and implemented into the commercial CFD code FIRE. The models are capable of predicting complex in–cylinder processes and, ultimately, the formation of pollutant emissions. The results from numerical simulations, such as NO_x and soot concentrations, in–cylinder pressure and temperature are found to be in good agreement with the existing experimental data.

1. Introduction

In modern society, cleaner and more sustainable production in all industrial sectors, particularly in the transportation sector, is becoming an increasingly important issue (Klemeš et al., 2012). It is well known that a vast amount of the worldwide CO_2 emissions are released into the environment as a result of fossil fuel combustion. According to Vad Mathiesen et al. (2011) greenhouse gases, including CO_2 must be reduced to 50–85% of the year 2000 levels by 2050. The transportation sector is one of the most challenging sectors to achieve sustainable development since it is highly dependent on fossil fuel products and increasing energy demands (Liu et al., 2013). Diesel engines characterized by better fuel efficiency and lower pollution are becoming a more popular choice in the transportation vehicle market (Hussan et al., 2013). Their overall efficiency is highly dependent on the parameters affecting the combustion process. Some of these parameters are the piston and the chamber geometry, the fuel injector type and the in–cylinder flow field. The flow field inside the combustion chamber is affected by the control valves and the aerodynamic forces arising from gas–liquid interactions. The combustion process and pollutant emissions are highly dependent upon the fuel-air mixing process, which is strongly influenced by fuel atomisation and evaporation. Various engine characteristics can be examined using numerical models and CFD simulations. Furthermore, early comprehensive information, parametric studies and initial conclusions can be determined and used in optimisation and development processes.

There are several computational approaches for solving turbulent dispersed multiphase flows including the Direct Numerical Simulations (DNS), the Discrete Particle Model (DPM), the Euler-Lagrangian (Particle Tracking) approach and the Euler-Eulerian (Two-Fluid) approach. The DNS and DPM approaches are extremely computationally intensive (Sommerfeld et al., 2008). The Euler-Lagrangian approach (Mikulčić et al., 2013) is commonly and widely used for calculating spray processes in diesel engines, but has several disadvantages (Abraham, 1997; Iyer and Abraham, 1997). However, it is suitable for solving diluted flows with low

Abbreviations: CFD, Computational Fluid Dynamics; DNS, Direct Numerical Simulation; DPM, Discrete Particle Model; PDF, Probability Density Function; IC, Internal Combustion; RT, Rayleigh-Taylor; KH, Kevin-Helmholtz; EGR, Exhaust Gas Residue; UPD, Upper Dead Point; DDP, Down Dead Point.

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concentration of the dispersed phase. To overcome the Euler-Lagrangian disadvantages the Euler-Eulerian multi-fluid approach can be employed. Using this approach, a stronger physical coupling of the gas and liquid phase is achieved making it suitable for computation of the dense area near the nozzle. In this research, the Euler-Lagrangian approach is applied. The gas phase is solved using the Eulerian formulation whilst the discrete phase is solved using the Lagrangian formulation. The phase coupling is performed by introducing the adequate source terms for mass, momentum and energy exchange. Several physical models are used for calculation of dispersed spray flow, combustion and pollutant formation. These models were integrated into the commercial CFD code FIRE (FIRE, 2011) using the user-defined functions capability. Linking the model equations with the code is performed with common FORTRAN routines (Baburić et al., 2005).

The spray is formed due to a high-pressure injection through a small nozzle hole into a cylinder. When the fuel jet enters the cylinder at high velocities, it disintegrates into ligaments and then into smaller droplets. The spray process is modelled as the primary break-up of the fuel jet and secondary break-up of the fuel droplets. There are several existing models for describing primary break-up process, such as WAVE, FIPA, KHRT and HuhGosman (Ashgriz, 2011; Bianchi and Pelloni, 1999; Huh and Gosman, 1991). The Diesel Core Injection (DCI) primary breakup model, based on the common WAVE model was applied in all performed calculations. The atomisation of the liquid fuel dictates the evaporation rate, and thus influences the combustion process. Since pollutants are measured at the exhaust pipe and not inside the combustion chamber, there is very little insight into their formation in the cylinder. For this reason, CFD simulation tools have proven to be an important addition to enhance the understanding of such processes. The focus of this paper is also to investigate the important thermo–chemical parameters and chemical kinetic mechanisms that describe the crucial features of the NO_x formation process. The NO_x can be formed through at least three reaction mechanisms: the thermal, the prompt and the fuel NO_x mechanism (Vujanović, 2010). Finite-rate kinetics play a role in determining the emission levels because NO_x pollutants are typically not emitted in equilibrium concentrations. NO_x emissions are limited because the reactions that produce NO are slower than the overall combustion and fuel oxidation processes. Detailed NO_x kinetic mechanisms have been proposed by many authors (Miller and Bowman, 1989; Baulch et al., 1994; Dagaut et al., 2000). However, the development of an effective NO_x model requires the simplification of such generalised reaction mechanisms. Sufficient details must be taken into account to adequately describe the NO_x reaction process and to allow coupling with the turbulent mixing process in a CFD simulation of practical combustion systems (Hill and Smoot, 2000; Zabetta and Kilpinen, 2001). In this paper the NO_x scheme is limited to few chemical reactions to allow effective coupling with the turbulent reacting multiphase flow. These homogeneous reactions contain sufficient information to appropriately predict the NO_x formation in combustion systems. Chemistry-turbulent interactions were modelled by the integration of the kinetic rates with respect to fluctuating temperature using a presumed Probability Density Function (PDF) approach (Vujanović et al., 2009). The NO_x reaction mechanism was implemented into the CFD code FIRE using the user-defined functions.

The pollutant emissions formed during diesel fuel combustion in Internal Combustion (IC) engines are highly dependent on the various combustion parameters and spray processes. The understanding of these processes can be used to influence overall engine energy efficiency and pollutant emissions. In this study numerical models for calculating fuel disintegration were used to predict fuel jet turbulent behaviour and droplet disintegration. Furthermore, numerical models for calculating pollutant emissions were developed and implemented within CFD code. The mentioned models were used to calculate the pollutant concentrations, pressure, temperature, the turbulent flow field and characteristic spray quantities. Calculations were performed on a 3D engine domain with moving boundaries. The calculation results are consistent with experimental pollutant emission trends. In addition, the calculated and experimental in–cylinder pressure and temperature results during the whole engine working cycle are found to be in a good agreement.

2. Available experimental data

The experimental research has been performed in the frame of DENSO bowl optimization project carried out by the AVL GmbH. A single cylinder engine with electro-hydraulic valve actuation and the ω shaped piston (LP7 EHVA) was examined using the AVL Single Cylinder Engine Test Bed. The pressure and temperature measurements have been carried out using the application-oriented automation system (PUMA Open) whilst pollutant emissions have been measured using the AVL emission measurement system. The main engine and injection system characteristics are presented in Table 1. For the research purposes, several combustion system parameters were varied as presented in Table 2. The NO_x and soot mass fractions, expressed in kilograms of species per kilogram of engine exhaust gas, have been measured in the exhaust pipe and are presented in Table 3. The experimental data were provided by AVL GmbH due to the long term collaboration project with the Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia. The project identification number is 05107-14/01 with the title: Implementation of combustion and radiation models into AVL's CFD codes SWIFT and FIRE.

3. Numerical model

In this research the Euler-Lagrangian approach was employed. The Lagrangian formulation was used for tracking droplet motion through the flow field and the Eulerian formulation was used for solving the gas phase (Mikulčić et al., 2012). In the Eulerian approach, the conservation equations for mass, momentum and enthalpy are solved. The liquid and gas phase coupling is achieved by introducing adequate source terms for mass, momentum and enthalpy exchange. This section describes the mathematical models based on empirical equations that are used within the CFD code.

3.1. The spray model

During the high-velocity fuel injection through the small diameter nozzle into the pressurized chamber, fuel is exposed to aerodynamic and turbulent forces. This leads to fuel disintegration into unstable ligaments and droplets of different shapes and sizes, also known as spray process. Spray influences fuel/air mixing, evaporation, combustion and thus affects the overall engine performance.

3.1.1. The WAVE model

Two types of surface instabilities can occur due to viscous forces, Kevin-Helmholtz (KH) and Rayleigh-Taylor (RT) instabilities. KH

Table 1
Experimental engine and BOSCH Piezo common rail injection system characteristics.

Bore (mm)	85	Spray Angle (deg)	158
Stroke (mm)	94	Displacement (mm^3)	533.4
Compression ratio (–)	16:1	Nozzle (–)	8-hole