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Research article

Modelling pollutant emissions in diesel engines, influence of biofuel on pollutant formation

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ABSTRACT

In order to reduce the harmful effect on the environment, European Union allowed using the biofuel blends as fuel for the internal combustion engines. Experimental studies have been carried on, dealing with the biodiesel influence on the emission concentrations, showing inconclusive results. In this paper numerical model for pollutant prediction in internal combustion engines is presented. It describes the processes leading towards the pollutant emissions, such as spray particles model, fuel disintegration and evaporation model, combustion and the chemical model for pollutant formation. Presented numerical model, implemented in proprietary software FIRE®, is able to capture chemical phenomena and to predict pollutant emission concentration trends. Using the presented model, numerical simulations of the diesel fuelled internal combustion engine have been performed, with the results validated against the experimental data. Additionally, biodiesel has been used as fuel and the levels of pollutant emissions have been compared to the diesel case. Results have shown that the biodiesel blends release lower nitrogen oxide emissions than the engines powered with the regular diesel.

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1. Introduction

During operation of Internal Combustion (IC) diesel engines a vast amount of fossil fuel is consumed, and therefore they represent a threat to the environment in terms of pollutant emissions. In theoretical conditions, when the complete fuel combustion is achieved, solely the CO_2 and H_2O species would be generated. However, such conditions are impossible to achieve due to the engine transient operating conditions. In 2013, 25% of the global CO_2 emissions originated from the transportation sector (Energy Agency, 2015). In addition, as a consequence of IC engine operating conditions, several other species, such as CO, HC, PM and NO_x, are produced. Relative to the total flue gases flow, 1% belong to these species, of which approximately 50% are the NO_x species (Khair and Majewski, 2006).

As a part of the tendency towards cleaner transport sector with lower impact on the environment, concentrations of the emitted pollutant emissions have been regulated in the past decade (Klemeš et al., 2012), and more stringent conditions are enforced by the governmental policies every year. Comparing to the spark ignition engines, the diesel engines are characterised by greater energy conversion and safety factor (Katrašnik, 2007). In order to remain the most used vehicle powering source on the European market, as well as to meet the higher efficiency standards, the IC engines efficiency must be constantly improved (Kozarac et al., 2014). In addition to the emission regulations, another obstacle for IC engine utilisation is the promotion of biofuels in the transportation sector (Niemisto et al., 2013). As a part of the European biofuels directive (2003/30/EC) in 2003, a minimum level of used biofuels was enforced to all EU member states. Recently, the European Standards Committee (CEN) allowed the maximum amount of bio − content up to 7%, and even a higher values are expected in the near future. Biodiesel is derived by transesterification, does not contain sulphur, degrades quickly, and is nontoxic (Tashtoush et al., 2007). In addition to the engine performance optimisation, NO emissions can be reduced by introducing various exhaust gas recirculation and engine boosting systems. A good review regarding exhaust particle filter technologies is shown in (Guan et al., 2015).

The combustion process within the IC diesel engine can be divided into two distinguished parts: the uncontrollable premixed combustion which takes place during the autoignition process, and mixing-controlled diffusion combustion. Most of the vaporised fuel is combusted in the diffusion regime and therefore the overall

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engine efficiency highly depends on the spray process. The spray is a highly transient and turbulent multiphase process, which consists of several distinguished processes, such as fuel jet disintegration, droplet atomization and collision, an evaporation process, air entrainment, etc.

Spray is a versatile process, apart from the internal combustion engines also used in removing pollutant emissions (Baleta et al., 2016), and the numerous experimental investigations have been performed. However, with the progress of computational power and development of Computational Fluid Dynamic (CFD) tools, combining experimental research with CFD analysis became the common approach. With such approach, an understanding of complex and transient turbulent flows that are hard to capture experimentally can be significantly improved. For the reliable use of CFD tools, each of the used submodels should be previously validated. Finally, combining the CFD tools with experimental research could result in a reduction of the overall expenses and investigation duration.

There are various approaches developed for the computational modelling of turbulent dispersed multiphase flows, such as Direct Numerical Simulation (DNS) for the particles, the Discrete Particle Model (DPM), the Euler-Lagrangian (EL), and the Euler Eulerian (EE) model, etc. (Martin Sommerfeld and Berend van Wachem, 2008). The EL approach is the most used approach for modelling the spray process. While it suffers from several disadvantages, such as mesh dependency, parallel calculation efficiency reduction, high particle loading (Petranović et al., 2015), the EL approach is sufficiently accurate and efficient for modelling the diluted spray region, as shown for the liquids by Faeth et al. (1995), as well as for solid particles (Mikulčić et al., 2016). In order to overcome its disadvantages, the EE approach can be used (Vujanović et al., 2016) (Petranović et al., 2017). Within EE approach both the liquid and the gas phases are treated as a continuum. For improved accuracy, the discrete phase is sorted into a finite number of classes, characterised by the mean droplet diameter (FIRE manual 2013, 2013). The phase interaction is achieved through source terms in the conservation equations accounting for the droplet dynamics. Despite the increased computational power requirements compared to the EL approach, the EE approach is suitable for modelling all spray regimes, including the dense spray region.

To overcome disadvantages inherent to the EL and the EE approaches, they can be coupled by using the AVL FIRE® Code Coupling Interface (ACCI) (von Berg et al., 2005) (Edelbauer, 2014) (Vujanović et al., 2016) or through the ELSA modelling concept (Vallet et al., 2001). The difference between these modelling concepts is that in the ACCI approach, the gas and the liquid phases in the vicinity of the nozzle are treated separately, and within the ELSA model they are treated as one mixture phase.

Available literature on usage of biodiesel blends as fuel in compression-ignition engines generally reports decrease in particulate matter (PM), hydrocarbon (HC) and carbon monoxide (CO) emissions as benefits, as well as increased levels of NO_x emissions as one of the main drawbacks of biodiesel implementation (Giakoumis et al., 2012). However, a deeper insight into reported experimental results questions this increasing trend and analyses its causes. For example, a comprehensive literature review (Lapuerta et al., 2008) examines differences in fuel injection and combustion due to disparities in physical and chemical properties of biodiesel, such as lower heating value, bulk modulus and viscosity etc. It is similarly (Sun et al., 2010) concluded that, although the increase in NO_x production exists, it is not inherent to the biofuel itself, but rather due to the usage of biodiesel in unmodified diesel engine setups. This way, the difference in biodiesel properties advances the start of injection process and increases the combustion temperatures, leading to the elevated NO_x emissions. In real-life experimental setups, it is often hard to ensure consistent operational parameters when comparing different fuels (e.g. the same start and the end of injection). In these situations, numerical simulations can be a great tool for analysis and comparison of performances of different fuels in the same working regimes.

It is one of this papers' aims to numerically investigate the NO_x pollutant emissions when using biodiesel blends, compared to the identical conditions with regular diesel fuel. Therefore, it is important to understand the thermochemical phenomena behind the formation of NO_x. Nitrogen-containing emissions from the combustion processes are commonly classified as thermal, prompt, and fuel NO_x, relative to the mechanism of their production (Vujanović, 2010). Thermal NO_x forms by dissociation of the molecular nitrogen from the air and is highly temperature-dependent, prompt NO_x occurs in nitrogen reactions with hydrocarbon radicals in the first stages of reactions, and the fuel NO_x is formed by complex reaction paths from nitrogen contained in the fuel. In modern CFD approaches, NO_x emissions are almost invariantly modelled as a post-processing step after calculation of the flow field and main combustion. This is justified by the, in absolute terms, small concentrations of NOx, which have a low impact on overall flow field, temperature and concentrations of major combustion products, as well as by different time scales of the fast combustion reactions and the relatively slower production of NO_x (Hill and Smoot, 2000). Although detailed kinetic mechanisms exist (Miller and Bowman, 1989), in order to obtain the computationally efficient model, some simplifications need to be made. Chemical model simplifications, such as omitting the species with negligible concentrations, removing reaction paths with minute influence on the overall NO_x production or the assumption of chemical equilibrium are a common approach to simplifying complex chemical phenomena for usage in CFD. Reduced number of chemical equations allows for an efficient coupling with the turbulent reacting flow. Chemistry-turbulence interaction was modelled by taking into the account temperature fluctuations, integrating the chemical reaction rates and applying the Probability Density Function (PDF) approach (Vujanović et al., 2009). Presented numerical model for modelling NO_x emissions has been implemented in the CFD code FIRE.

The paper is structured as follows: first, the description of the available experimental data is given. Later, the short introduction into the Euler-Lagrangian spray modelling is provided, together with the NO_x modelling equations. Afterwards, the numerical setup is described and the results are thoroughly discussed. Finally, the conclusions are drawn in section 'Conclusions'.

2. Available experimental data

To find the most suitable NO_x modelling approach, the single cylinder engine was computationally modelled. This engine is designed as a Single CYlinder ENgine (SCYLEN), with electro-hydraulic valve actuation, and the ω-shaped piston. The main SCYLEN engine and injector system characteristics are shown in Table 1.

Table 1
Engine specifications.

Bore (mm)	85	Spray Angle (°)	158
Stroke (mm)	94	Displacement (mm^3)	533.4
Compression ratio (−)	16:1	Nozzle (−)	8-hole
Nozzle location (mm)	2,0,−3.8	Inj. Pressure (bar)	1200−1600
Orifice diameter (mm)	0.1		

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