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Multi-zone model for reactivity controlled compression ignition engine based on CFD approach

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ABSTRACT

RCCI (Reactivity controlled compression ignition) combustion is a novel and promising strategy in reducing soot and NO_x emissions while obtaining diesel-like efficiencies. In this study, at first, a CFD (computational fluid dynamic) model is developed for RCCI engines simulation using semi-detailed chemical kinetics mechanism. N-heptane is injected directly into the combustion chamber as a high reactivity fuel while the low reactivity fuel, methane, is introduced as a premixed charge. The results of CFD investigations show significant differences between the injected and evaporated n-heptane. The CFD model is used to predict the evaporated n-heptane stratification. In the second part, a MMZM (modified multi zone model) is developed for RCCI engines simulation. The model contains both heat and mass transfer phenomena which are considered between all zones. The predicted n-heptane fuel stratification is introduced to the MZM (multi zone model). Semi detailed chemical kinetics mechanism is used for combustion simulation. A zero-dimensional single zone model, which is coupled to the MZM, is used to calculate the initial conditions and to model the gas exchange process. The simulation results are validated in a wide range of engine part loads operating conditions. The new way of introducing the evaporated fuel (direct injected) to each zone together with accurate heat and mass transfer models caused to accurate prediction of engine combustion and emission characteristics by MMZM. The MMZM can predict the SOC (start of combustion) and CA50 with sufficient accuracy. A maximum deviation of 1.5 CAD is observed comparing to the experimental results.

1. Introduction

Diesel engines are widely being used in transportation and energy production industries thanks to their high fuel efficiency. Despite the high-efficiency advantage of diesel fuels, however, they can contaminate environment due to their considerable NO_x and Soot emissions. Since these emissions have a negative impact on human health, attempts have been made to reduce them [1]. After treatment systems such as DPF (diesel particulate filter), LNT (lean NO_x trap) and SCR (selective catalytic reduction) generally increase fuel consumption rate. Therefore, the in-cylinder ignition techniques have attracted the attention of scientists. However, the need for such systems should be minimized in order to achieve a higher thermal efficiency [2]. Techniques for reducing NO_x and Soot emissions, formed inside the combustion chamber, have been studied by many researchers. The majority of such techniques could be categorized into the LTC (low temperature combustion) category. The LTC techniques reduce such emissions due to high activation energy required for NO_x emission reactions [3]. In addition, the high ignition delay and the availability of sufficient time for mixing reacting products, reduces the in-cylinder enriched zones. This, in turn, prevents soot formation [4].

Homogenous charge compression Ignition (HCCI) is one of the simplest techniques for reduction of NO_x and soot emissions in compression ignition engines, simultaneously. This technique was first studied by Najt and Foster in 1983 on a 4-stroke engine and it has been further developed up to now. In HCCI engines, ignition and combustion process are controlled by chemical kinetics [5]. Therefore, the ignition control seems to be difficult. However, establishing a relation between fuel injection and ignition seems necessary in order to control ignition process in the form of cycle-by-cycle control [6]. This has led to a new generation of LTC called premixed charge compression ignition (PCCI). In PCCI engines, there is a well-established relation between the start of injection

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and the start of ignition where at the initial stages of compression cycle, the fuel is directly injected inside combustion chamber. This improves air-fuel mixing process before ignition and in turn reduces NO_x and Soot emissions and improve fuel combustion efficiency [7]. However, HCCI and PCCI engines suffer from high contents of CO and unburnt hydrocarbons (UHC) [8]. Inagaki et al. studied the dual fuel PCCI engines (premixed isooctane and direct injection of diesel fuel) in order to reduce the required EGR in PCCI strategy [7]. Relying on the previous results of Inagaki, therefore, it can be concluded that a fit strategy is to inject a low reactive fuel at the inlet port and a high reactive fuel into the combustion chamber. Kokjohn et al. called this strategy as RCCI strategy [9]. In 2014, Benajes et al. published the results of their studies in order to further introduce the process of air-fuel mixing inside combustion chamber and to explain the auto ignition of air-fuel mixture in an RCCI engine using diesel and gasoline fuels with high and low reactivities, respectively [10]. They used a one cylinder four-stroke laboratory engine to conduct their tests. The obtained results were examined in a one-dimensional spray model, developed in Valencia University, abbreviated as DICOM. This code was used to evaluate that how the fuel injected inside the combustion chamber (high reactivity) is mixed with the inlet air-fuel mixture (low reactivity) at different ratios and in different injection times.

Investigations on RCCI engines are usually divided into two parts. The first part is related to the research carried out by experimental tests, and the second part is associated with the numerical simulations. Considering the second part, prediction of combustion, emission and performance characteristics of engine are normally carried out by CFD or thermodynamic methods. Regarding RCCI engines, most of the researches are done by experimental and/or CFD methods [11,12]. Powerful CFD tools can provide more insight to the combustion process than experimental tests alone.

Kokjohn et al. conducted a study to compare a typical diesel engine and an RCCI engine [13]. The results showed that NO_x and Soot emissions of RCCI engine can be reduced by the order of magnitude of 3 and 6, respectively, compared with the typical diesel engine. Considering experimental tests and numerical simulations, it can be argued that NO_x and Soot emissions are reduced inside the combustion chamber of RCCI engine due to the avoidance of high air-fuel equivalence ratio and the reduction of the number of high-temperature zones. These parameters were assessed in the model developed by Lim et al., in 2014 [14]. They adopted a genetic algorithm to optimize fuel injection specifications. The aim of their study was to derive injection timing and the fraction of fuel distributed between injectors in order to reduce some emissions such as NO_x, CO and UHC on the one hand and to optimize performance parameters such as fuel consumption rate on the other hand. They used a 2.4 l engine for experimental tests and KIVA3V for numerical studies. Nazemi et al. reported a CFD simulation base model which included two important analysis contributions. At first, a detailed 3D commercial CFD code (CONVEGE) was developed and the results were validated against the experimental data [12]. The in-cylinder pressure traces and combustion phasing parameters (such as CA50 and SOC) and emissions were calculated for different operating conditions. In the second part, the effects of fuel injection parameters (such as start of injection, injection pressure and injector nozzle spray angle) on the performance and emissions characteristics of an RCCI engine are discussed. The results were in good agreement with the corresponding experimental data.

Zhou et al. [15] numerically investigated a biodiesel/methanol RCCI engine with reduced chemical reaction mechanism coupled with 3D-CFD model to capture pressure and species concentration in 10 different zones. The model is developed to predict the knocking phenomenal inside the combustion chamber. Also the effect of cooled EGR, SOI and premixed methanol mass fraction on engine knocking were evaluated. The results showed that the cooled EGR and retarded SOI could significantly reduce the engine knocking because of low temperature rise rate and less premixed biodiesel in the combustion chamber.

Nowadays, the demands for natural gas as a reference fuel for un-road and stationary applications (such as gen-set applications) and as an alternative fuel for dual fuel applications are increased intensively [16]. The enormous resources of natural gas introduce this fuel an appropriate choice to use as an alternative fuel. Also it is promising path to explore efficiency increase and load range extension for the RCCI concept. As mentioned before, most of the investigations were done by CFD simulation. Due to high computational expenses, the scope of those studies are typically restricted to a few simulation cases. For the development of RCCI control strategies, developing a physical-based model for combustion phasing parameters prediction, and also increasing the insight into the combustion process, the authors have developed the fast and reliable thermochemical kinetics based, multi-zone model. The model can capture the most important phenomena in RCCI, such as zonal fuel and temperature stratification, start of combustion, CA50, burn duration, emissions and combustion chemistry. Its completeness and relatively fast computational times allow to cover wide range of part loads conditions for engine operating points, which is the main advantage over detailed CFD approaches and experimental procedures.

In 2013, Eguz et al. adopted a MZM (multi zone model) to simulate a dual fuel RCCI engine [17]. This study uses a 10-zone model and chemical kinetics mechanism including 137 species and 633 reactions where the fuel is a mixture of diesel and gasoline fuels in which iso-octane represents gasoline and N-Heptane represents diesel fuel. CFD (Computational Fluid Dynamic) was used to model fuel injection process to derive the distribution of fuel at each zone. The mass fraction of the injected diesel fuel was derived and normalized for each zone. The fuel distribution pattern obtained from CFD was applied to each zone of the adopted MZM. This study shows the high capacity of MZM in modeling start of ignition and heat release rate in the RCCI engine.

In 2016, Mikulski et al. modeled an RCCI engine was fueled with natural gas and diesel as high and low reactivity fuels using a thermochemistry MZM. The mixing phenomena caused by fuel stratification was investigated in this work. Results showed a slow rate of combustion in low load conditions [18]. Furthermore, all predicted emissions except for NOx emission (which was under-predicted), showed good agreement with the experimental results.

Mikulski et al., used a single point direct injection for low reactivity fuel (CH4) to characterize the fuel stratification inside the combustion chamber [19]. The results of a MZM with chemical kinetic reactions (Called XCCI) was validated with experimental data. The results indicate that methane fuel stratification increases thermal efficiency and decreases CO emission. Also, the stratification effects were more effective in the case of part load conditions.

Over the last few years, there has been limited investigation on the multi zone combustion modeling of RCCI engines. Therefore, the main purpose of this paper is to develop a kinetic-based MZM for RCCI engines as a fast and reliable tool to predict the engine