Applied Energy xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Development of a three-step hybrid simulation approach (THSA) for engine combustion investigation coupled with a multistep phenomenon soot model and energy balance analysis

Wenbin Yu, Wenming Yang *, Feiyang Zhao, Dezhi Zhou, Kunlin Tay, Balaji Mohan

Department of Mechanical Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117575, Singapore

HIGHLIGHTS

- A three-step hybrid simulation approach was proposed for engine combustion investigation.
- A multi-step phenomenon soot model was coupled into the three-step hybrid simulation approach.
- The energy balance analysis was coupled into the three-step hybrid simulation approach.
- KIVA4 and CHEMKIN II codes were coupled to solve the detailed chemical reactions for engine combustion.

ARTICLE INFO

Article history:
Received 7 June 2016
Received in revised form 17 October 2016
Accepted 25 October 2016
Available online xxxx

Keywords:
Internal nozzle flow
Cavitation
Spray characteristics
Combustion
Soot model
Energy balance

ABSTRACT

A comprehensive simulation approach is important in order to better replicate the complex combustion process over a wide range of engine operating conditions. This will allow a more accurate understanding of crucial factors that affect engine combustion. In this study, the entire engine combustion process was systematically considered and a three-step hybrid simulation approach (THSA) was proposed in order to achieve a more accurate engine combustion simulation. For this approach, a so-called "full cavitation" model was selected for 3-dimensional (3D) internal nozzle flow study and a Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) model was used for 3D spray prediction wherein the flow variables at the nozzle outlet obtained through internal nozzle flow simulations were used as the input information in the KIVA4 code. Besides, a compact and accurate primary reference fuel (PRF) mechanism with 46 species and 144 reactions, which is coupled with a multi-step phenomenon soot model and energy balance analysis, was used for engine combustion simulation. Based on it, a numerical study was conducted for a comparison between conventional direct injection combustion (CDIC) and partially premix combustion (PPC) fueled with diesel, gasoline and diesel/gasoline blend fuel (GD). The final result indicates that with PPC and gasoline fuel, an optimized and high thermal efficiency of 52.5% can be realized along with extremely low NOx and soot emissions.

1. Introduction

Improving economic performance and mitigating exhaust emissions are always the key motivations for researchers to pursue advanced internal combustion engine technologies. For this purpose, numerous engine technologies have been proposed and investigated. The technique of enhancing air-fuel mixing includes increasing injection pressure, reducing nozzle hole size, increasing boost pressure, organized air motion in the combustion chamber and multiple injections; the technique of inhibiting combustion temperature rising includes exhaust gas recirculation (EGR) and retarded intake valve closing timing (RIVCT).

It should be noted that, for all the technologies mentioned above, organizing air-fuel mixing is one of the most significant parts in the development of engines. Fuel injection and spray break-up process were proved to be complex in nature. The factors such as injection pressure, ambient pressure, nozzle geometry and fuel properties would affect the internal nozzle flow and the spray propagation [1–3]. Many researchers have indicated that cavitation inside the nozzle could influence liquid fuel break-up evidently [4,5]. According to [6], cavitation will appear wherever the local pressure drops below the vapor pressure of fuel. Bubbles caused by cavitation have been proved to contribute to the disintegration

* Corresponding author.
E-mail address: mpeywm@nus.edu.sg (W. Yang).

http://dx.doi.org/10.1016/j.apenergy.2016.10.137

Please cite this article in press as: Yu W et al. Development of a three-step hybrid simulation approach (THSA) for engine combustion investigation coupled with a multistep phenomenon soot model and energy balance analysis. Appl Energy (2016), http://dx.doi.org/10.1016/j.apenergy.2016.10.137

of spray. According to [7], once cavitation occurs, intense turbulence will be generated inside the nozzle hole. And according to the authors' group's previous study, the spray model which takes into account cavitation was more accurate for spray prediction [8]. In order to validate the spray model which takes into account cavitation against the engine combustion characteristics, experimental in-cylinder pressure data and heat release rate were compared with the simulation results in [8]: two different speeds (3600 and 2400 rpm) and two different loading conditions (100% and 50% load) were used for combustion validation. From the result, the predicted in-cylinder pressure and ignition delay time are consistent with the experimental results which indicates that the spray model taken into account cavitation captures the detail of the combustion process in the engine. Therefore, understanding internal nozzle flow is important for the investigation of spray characteristics.

In addition to the fuel injection and spray study, a series of combustion concepts were developed. Since 2003, an injection strategy of multi-pulse fuel injections starting from early compression stroke followed by a main-injection was put forward by Su et al. and realized very low NOx and soot emissions in a heavy duty diesel engine without EGR at IMEP of 0.78 MPa [9]. The strategy of early multi-pulse injection effectively prolonged the ignition delay period and improved the mixing process. After that, Su and Yu et al. [10–12] improved this multiple-injection-based partially premixed combustion (PPC): with the utilization of EGR and RIVCT, high thermal efficiency and near zero emissions were attained in a wide engine-operation range up to IMEPg of 1.1 MPa. In 2005, Wang et al. [13] proposed homogeneous charge induced ignition (HCII) combustion strategy to improve engine thermal efficiency and emissions, which is realized by gasoline port injection along with diesel direct injection. The results indicate that HCII engine owns smokeless combustion, and the thermal efficiency is higher than conventional gasoline engines. In 2009, Kokjohn and Reitz et al. [14,15] further proposed a concept of reactivity controlled compression ignition (RCCI). Factors including EGR rate and fuel injection strategies were optimized by simulation and experiment in a heavy duty diesel engine, and at the engine load of 0.9 MPa IMEP, ultra-low NOx and soot emissions were realized with 53% net indicated thermal efficiency. In 2013, Yu et al. [16] successfully applied this technology in a real vehicle. Besides, the coordination control of mixing rate and chemical rate by changing fuel properties including auto-ignition and volatility was also investigated. Simultaneous high efficiency and low emissions by mixing gasoline and diesel in a diesel engine were reported [17,18].

In the scope of engine research, numerical study was always considered as an effective approach to access to the entire engine combustion process. According to [19], modelling activities can make major contributions to engine engineering by identifying key controlling variables to provide guidelines for more rational and therefore less costly experimental development efforts. From [19], it can also be known that optimizing engine design and control could be conducted with sufficiently accurate model. [20] pointed out that the variable cost of an experiment, in terms of facility hire and/or man-hour costs, is proportional to the number of data points and the number of configurations tested. In contrast CFD codes can produce extremely large volumes of results at virtually no added expense and it is very cheap to perform parametric studies, for instance to optimize equipment performance. In the face of more advanced air-fuel mixing control technology and complex combustion process, any numerical study that only considers a single factor in the entire engine combustion process is not accurate enough. Also, so far, researchers rarely gave a comprehensive numerical study, including internal nozzle flow simulation, spray prediction, combustion simulation and even emissions and energy distribution prediction. Under this background, a comprehensive and accurate simulation approach for engine combustion investigation is needful to systematically investigate the combustion process over a wide range of engine operating conditions.

In this study, a three-step hybrid simulation approach, including 3D internal nozzle flow simulation, 3D spray propagation prediction and 3D engine combustion simulation, was proposed for engine combustion investigation. In the first two steps, a so-called "full cavitation" model was selected for internal nozzle flow study and a KH-RT model was used for spray prediction wherein the flow variables at the nozzle outlet obtained through internal nozzle flow simulations were used as the input information in the KIVA4 code. In the third step, a compact and accurate PRF mechanism with 46 species and 144 reactions was used for fuel chemical reaction. Fully understanding soot formation mechanism is always an on-going concern. In this study, a multi-step phenomenon soot model, which was developed by authors in previous research [21–24], was embedded into the fuel chemical reaction mechanism with KIVA4 code. This soot model, different from the widely used Hiroyasu two-step soot model [25], is capable of representing major phenomenon throughout soot formation, including precursor formation, soot particle inception and coagulation, soot surface growth and oxidation. And it will be competent for the forthcoming particle number regulations. Besides, in order to better understand the fuel energy distribution and to carry out detailed investigation on engine thermal efficiency, an energy balance analysis method based on the first law of thermal dynamics was also embedded into Step 3 of the hybrid simulation approach.

Finally, based on THSA, a numerical study was conducted for a comparison between conventional direct injection combustion (CDIC) and partially premix combustion (PPC) fueled with diesel, gasoline and diesel/gasoline blend fuel (GD). It can be found in the final results that, fueled with gasoline, an optimized high thermal efficiency of 52.5% can be obtained in PPC along with extremely low NOx and soot emissions. So far, due to relatively poor lubricating properties, gasoline fuel is rarely used in high-pressure supplied compression ignition engines. But it still can be inferred that, with the development of fuel supply system, gasoline may become a fuel with more advantages than diesel used in a high-pressure supplied compression ignition engine.

2. Simulation of internal nozzle flow and cavitation (Step 1)

2.1. Mathematical model

The commercial computational fluid dynamics (CFD) software ANSYS FLUENT 15 [26] was used for internal nozzle flow and cavitation simulation. The cavitation model implemented in this study is so-called "full cavitation" model proposed by Singhal et al. [27]. The two-phase model considers a mixture comprising of liquid and vapor fuel, which are modelled as incompressible. Also an assumption is that between the liquid and vapor phase there is no-slip. Then the mixture properties are computed by the Reynolds-averaged continuity and momentum equations

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1}$$

$$\rho \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_i} \tag{2}$$

where

$$\tau_{ij} = (\mu + \mu_t)\left\{\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right\} \tag{3}$$

and

Please cite this article in press as: Yu W et al. Development of a three-step hybrid simulation approach (THSA) for engine combustion investigation coupled with a multistep phenomenon soot model and energy balance analysis. Appl Energy (2016), http://dx.doi.org/10.1016/j.apenergy.2016.10.137