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A numerical investigation on the injection timing of boot injection rate-shapes in a kerosene-diesel engine with a clustered dynamic adaptive chemistry method☆

Dezhi Zhou[a], Kun Lin Tay[a], Yaojie Tu[a], Jing Li[b], Wenming Yang[a,*], Dan Zhao[c]

[a] Department of Mechanical Engineering, Faculty of Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117576, Singapore
[b] School of Mechanical and Power Engineering, Nanjing Tech University, Nanjing 211816, China
[c] Department of Mechanical Engineering, College of Engineering, University of Canterbury, Private Bag 4800, Christchurch 8140, New Zealand

HIGHLIGHTS

- A clustered dynamic adaptive chemistry (CDAC) method is proposed and validated for engine combustion simulations.
- Boot injection rate shapes in DICI engines are investigated fuelled with kerosene, diesel and their blending.
- The effect of start of injection of boot injection on the combustion and emission characteristics is investigated.
- CDAC is able to reduce the computational time by more than 60% while maintaining good accuracy.

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ABSTRACT

In this study, we conducted a numerical investigation on the effect of injection timing of boot injection rate shape on the combustion and emission characteristics in a direct injection compression ignition (DICI) engine fueled with kerosene/diesel blending. Considering the complex surrogate in kerosene chemical mechanisms and the huge computational workload in multi-dimensional engine simulations, we employed a clustered dynamic adaptive chemistry method (CDAC) to accelerate the chemistry integration process. This study firstly specified the user-defined parameters in this CDAC method by sensitivity analysis in a HCCI and DICI engine with different user-defined parameter combinations. With these specified parameters, CDAC is then validated by comparing its predicted in-cylinder pressure with the full chemistry ones. It is found that the current CDAC method could reduce the computational time by more than 60% compared with the full chemistry CPU time. CDAC, subsequently, is used to conduct the numerical investigation on the injection timing of boot injection rate shapes. Four different boot injection rate shapes are simulated and compared with the normal rectangular injection. The effect injection timing of the boot injection rate on the engine performance and combustion/emission characteristic is then analyzed in detail. It is found that the change of start of injection (SOI) in boot injection has little influence of the ignition delay in the DICI engine fuelled with diesel and kerosene blending due to the high cetane number of diesel and better volatility of kerosene. In addition, with kerosene addition into the diesel combustion, it is observed that the CO emission could be reduced at all the varied SOI.

1. Introduction

Kerosene has been normally used as the fuel for gas turbines, as well as for rocket engines. The research of kerosene in direct injection compression ignition (DICI) engines has recently drew much attention due to the introduction of Single Fuel Concept (SFC) by North Atlantic Treaty Organization (NATO) [1]. SFC suggested that using single fuel in aircrafts and ground vehicles could logistically facilitate the fuel supply worldwide. Another driving factor behind the application of kerosene in DICI engines is fuel adulteration, which inevitably lead to undesired emissions [2,3]. In this sense, a good understanding of the combustion in DICI engines is important to possibly achieve SFC as well as avoid the adverse effect of kerosene combustion in DICI engines.

In general, it is reported that due to the similar cetane number with

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

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diesel, the combustion characteristics in terms of in-cylinder pressure and heat-release rise is quite similar with diesel combustion in DICI engines [4,5]. It is also observed that owing to the higher volatility of kerosene and the slightly lower cetane number (CN) than diesel, more fuel burns in premixed phase, which leads to decreased soot emissions. Due to the same reason, more premixed combustion would lead to higher temperature and thus higher NO_x at high loads [6]. To directly apply kerosene into commercial diesel engines and test its combustion and emission characteristics, some researchers modified the diesel engines by improving turbo match, increasing compression ratio with revised piston bowl geometry to achieve low emissions with kerosene combustion without high exhaust gas recirculation (EGR) [7,8]. Some researchers tended to blend biodiesel and kerosene with diesel fuels to DICI engines without improving the commercial engines [9,10]. No matter which way to apply kerosene in engines, it is always desirable to manage the engine with different strategies to optimize its performance.

The engine management of EGR and the injection strategy [11,12] are typically employed to reduce emissions as well as maintain thermal efficiency under different operating conditions. Lee et al. [13] investigated the effects of EGR and injection strategy with two pilots on combustion and emission characteristics of JP-8 in a light duty diesel engines. They found that with multi-injection, more EGR rate could be introduced to reduce the NO_x and particulate matter (PM) by half without losing thermal efficiency. In the work of Park et al. [14], they observed that JP-8 could reduce the NO_x and PM emissions under low to medium loads due to the low cetane number, higher volatility and lower aromatic contents compared with diesel. It is also reported in [14] that EGR could be employed to suppress the higher NOx under high loads, but a trade-off between NO_x and soot is shown in this situation. In addition, our previous numerical study [15] investigated the boot injection rate shape strategy effect on engine performance and found that boot injection rate shape strategy is capable of reducing soot particle sizes and avoiding NO_x and CO trade-off.

No research has reported the boot injection timing effect on the engine performance, to the best knowledge of the authors. Hence, this study aims to provide a thorough numerical observation on the effect of boot injection timing. However, the realistic kerosene is complex mixtures of more than thousands of components which are impossible to emulate with its real components. The prevalent way to address this issue is the use of surrogate fuel to represent the combustion characteristics in gas phase as well as its other chemical and physical properties (e.g., cetane number, viscosity). Typically, kerosene could be represented by alkanes such as n-decane, cycloalkanes such as methylcyclohexane and aromatics such as toluene. The latest and significant detailed kerosene surrogates mechanisms could be found in [16–18]. It is seen that to emulate both the chemical and physical properties of kerosene, the typical detailed surrogate mechanisms contain more than one thousand species, which is computationally prohibitive when applied into multi-dimensional combustion simulations even in the context of Reynolds averaged Navier-Stokes (RANS). Hence, some researchers managed to reduce the size of kerosene mechanisms to around 200 species or even less [19,20], which, however, are still computational expensive for engine simulations. Tay et al. [15] developed a kerosene mechanism with 48 species and 153 reactions and showed good accuracy in predicting combustion characteristics in both ignition delays and engine simulations. Even with this mechanism, it is still desirable to further optimize the computation in terms of efficiency.

Thus besides reduced mechanism development, methods such as storage retrieval method (e.g., in situ adaptive tabulation (ISAT) [3]) which stores the chemical source terms in the process of computing and retrieves them when similar thermochemical conditions are found; parallel computing based on the hardware conditions (e.g., GPU-parallel [4,5], CPU-parallel); clustering methods where computational cells with same thermochemical conditions are clustered as one to reduce the number of cells (e.g., chemistry coordinate mapping (CCM) [6]); dynamic adaptive chemistry (DAC) method which dynamically reduces the chemical mechanism in the simulation within every time step, have been proposed to accelerate the chemistry integration. In this study, we innovatively proposed the clustered DAC (CDAC) method, which not only extended the DAC concept into multi-dimensional DICI engine simulations, but also couple the cell cluster method into DAC method to integrate the chemistry. This method bundles the spatial and temporal computational domain with similar thermodynamic conditions and utilizes the same reduced mechanism from DAC to consider the combustion chemistry in the bundled computational domain, thereby reducing the computational cost caused by the DAC and chemistry integration process.

To sum up, the objective of this study is to conduct numerical investigations on the injection timing of the boot injection strategy on the combustion characteristics and emissions of kerosene combustion in a DICI engine. To alleviate the computation workload, the newly-proposed CDAC scheme is firstly validated and then used to conduct these parametric simulations.

Table 1
Engine specifications.

Engine type	Toyota four-cylinder DI diesel engine
Bore & stroke	92 mm & 93.8 mm
Compression ratio	18.5
Charging	Turbocharged
Rated power	75 kW at 3600 rpm
Fuel injection system	Common rail, 6 holes

Table 2
Operating conditions of the simulations.

Parameters	Values
Engine speed	2400 rpm
Intake valve close timing	−149° ATDC
Exhaust valve open timing	150° ATDC
Swirl	0.3
Injection timing	−3.5° ATDC
Injection duration	15.5° crank angle

2. Methodology

2.1. CFD framework

The numerical CFD framework in this study is the ALE unstructured KIVA-4 codes [21]. Based on the previous version KIVA-3 V which uses a finite volume method for arbitrary hexahedrons, KIVA-4 is capable of treating with unconstructed meshes. The spatial discretization in KIVA family codes is based on the method of arbitrary Lagrangian Eulerian (ALE). The transport terms are differenced by a quasi-second-order upwinding scheme and a second-order central scheme respectively for the convection terms and the diffusion terms. The temporal integration is based on a first-order time-splitting scheme. Three phases are adopted sequentially to advance source, diffusion, and convection terms by splitting each time step. The combustion chemistry is originally in KIVA-4 calculated with generic species. In this study, we coupled CHEMKIN-II [22] into KIVA-4 for chemistry kinetics treatment and computation. The turbulence model and spray break-up model in the current KIVA-4 code are the modified RNG $k-\varepsilon$ model [23] and KH-RT break-up model [24], respectively.

2.2. Chemical reaction mechanism

The kerosene-diesel reaction mechanism used for engine simulations in this work consists of 48 species amongst 152 reactions and it