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Exploring the benefits of multiple injections in low temperature combustion using a diesel surrogate model

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HIGHLIGHTS

- Surrogate composition of diesel fuel arrived by modeling its distillation profile.
- Surrogate model captured well LTC trends with EGR in single and multiple injections.
- Locations of UHC and CO emissions are different in single and multiple injections.
- Ignition delay to be optimized for lower combustion noise and unburned emissions in LTC.

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ABSTRACT

Advanced low temperature combustion (LTC) strategies are promising to achieve high efficiency and low emissions of nitric oxides (NOx) and Particulate Matter (soot). The thermal efficiency advantages are obtained through lower temperatures with reduced heat losses. A lower charge temperature and the sufficiently longer time available for mixing help to avoid NOx and soot formation zones. However, important shortcomings of LTC strategies include higher unburned hydrocarbon emissions and higher combustion noise. The present work investigates the use of multiple injection strategies to combat the above shortcomings in low temperature diesel combustion. Numerical investigations were carried out using a three dimensional computational fluid dynamic (CFD) code KIVA-ERC-CHEMKIN to explore the benefits of multiple injections over a single injection. The physical and chemical properties of a typical American diesel fuel used in the present work were modeled using suitable surrogate components. The results show that significant benefits are possible with the use of multiple injections, including lower unburned emissions and lower combustion noise. The CFD investigations provide a better understanding of the mechanisms behind the benefits and are useful to suggest guidelines for further improvements.

1. Introduction

With the advent of highly efficient exhaust after-treatment systems, near zero emissions are achievable in internal combustion engines, and research focus is now intensified on improving thermal efficiency, both from the fuel economy standpoint and to mitigate carbon dioxide (CO_2) emissions. Higher thermal efficiency targets are being addressed with advanced low temperature combustion (LTC) strategies like Homogeneous Charge Compression Ignition (HCCI), whose lean overall fuel–air equivalence ratio results in lower wall heat and exhaust losses and a higher specific heat ratio [1]. However, an important limitation of this concept is that the fuel ignition and combustion phasing are kinetically controlled, and depend strongly on the molecular composition of the fuel. Hence precise combustion control is difficult to achieve [2]. Alternative LTC strategies like Partially Premixed Compression Ignition (PCCI) [3], High Efficiency Clean Combustion (HECC) [4] and Modulated Kinetics (MK) [5] have been proposed to provide better combustion control wherein the combustion phasing is closely coupled with the fuel injection event. Low temperature combustion is realized in these strategies by utilizing a large amount of cooled EGR (Exhaust Gas Recirculation). Although, the fuel ignition is closely coupled with the injection timing in the above strategies, additional control of the ignition timing and combustion rate is provided by varying the EGR rate [6]. Both NOx and soot are simultaneously reduced in LTC, by maintaining local combustion temperatures below 1700 K [7].

Currently, LTC operation is limited to a narrow load limit due to the potential for higher pressure rise rates and combustion noise at higher loads, and misfire and poor combustion efficiency at lower

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loads [8]. A major shortcoming identified with the low temperature PCCI strategy was higher combustion noise promoted by the long ignition delay [9,10]. A higher pressure rise rate after the ignition delay period produces vibrations of the engine block, which, in-turn, radiate air-borne combustion noise [11]. Combustion noise is a significant issue in passenger cars and the engine is the major source of noise in diesel-powered vehicles [9,11]. The lower cylinder gas temperatures and the lower oxygen availability also results in significantly higher unburned emissions in LTC [4,6,8,12–15]. The over-mixing of the charge promoted by the longer ignition delay and the partial oxidation of locally rich mixtures were found to be the major sources of unburned hydrocarbon (UHC) and carbon monoxide (CO) emissions, respectively, in LTC [16]. Further, low temperature operation poses challenges in exhaust after-treatment systems since the exhaust gas temperatures may be lower than catalytic converter light-off temperatures, especially at low loads [13,17,18].

Different strategies have been attempted to extend the operating load range and reduce unburned emissions and combustion noise in LTC. Ho et al. [19] proposed a novel methodology that uses direct EGR injection after the fuel injection event as a means of combustion control and of extending the operating load range under LTC conditions. From their experimental investigations, Han et al. [20] suggested that the limitations with high load operation under LTC were primarily due to the higher reactivity and lower volatility of the diesel fuel, and replacement of diesel with ethanol was found to be effective to enable high load operation. The effect of fuel oxygen content on the combustion efficiency and emissions under LTC conditions was investigated by Zhu et al. [21] using three different fuel blends viz. 80% Swedish diesel with 20% gasoline to represent a 0% oxygen fuel, 70% Soybean biodiesel with 10% Swedish diesel and 20% gasoline to represent a 7% oxygen fuel and 80% biodiesel with 20% ethanol to represent a 15% oxygen fuel. Among these fuel blends a maximum combustion efficiency of above 98% is reported with 15% oxygen fuel at 14% intake oxygen concentration. Investigations by Kimura et al. [5] and Kook et al. [22] highlighted that a higher unburned emissions in LTC could be reduced by optimizing the swirl and the combustion chamber geometry. A double injection strategy with an equally split fuel injection quantity was found to be effective to reduce the unburned emissions compared to a single injection event [23]. In PCCI operation it was found that the combustion noise was highly sensitive to the start of injection timing and the intake oxygen concentrations, and the use of multiple injections or a higher EGR rate was most promising to reduce combustion noise [10].

Although significant research efforts have been made in terms of experimental investigations to understand and improve diesel LTC, corresponding modeling studies are very limited. Considering the complexity of diesel fuel in terms of the presence of a broad range and large number of hydrocarbon species, most practical modeling approaches adopt a few representative surrogate components to attempt to capture the overall combustion and emission characteristics of diesel fuel. A review of available diesel surrogates for different application targets, viz., spray, ignition and emissions is provided in [24]. However, these surrogates were tested under conventional diesel combustion conditions where fuel effects are not as significant as in LTC [25]. Recently, Luo et al. [26] proposed a TRF20 (80% n-heptane + 20% toluene) and 1-hexene mixture (95/5 vv) as a surrogate for diesel fuel. Better agreements in auto-ignition delay and emissions were obtained using this surrogate both under conventional and LTC conditions. However, since diesel fuel composition is highly variable depending on the crude oil source, the applicability of the above surrogate mixture for a diesel fuel with a higher proportion of naphthene is questionable. More recently, Anand et al. [25] proposed multi-component surrogate models to capture the composition and property variations of European and American diesel fuels. The applicability of these models to capture fuel effects was demonstrated over a broad range of LTC conditions.

The present work investigates the use of multiple injection strategies to combat the major shortcomings seen in low temperature diesel combustion in terms of the observed higher unburned hydrocarbon emissions and higher combustion noise. Low temperature combustion was realized by maintaining high levels of EGR. The surrogate model developed by Anand et al. [25] for a typical American diesel fuel was used in the present work to explore the benefits of multiple injections over single injections. Numerical investigations were carried out using the 3D CFD code, KIVA-ERC, incorporated with a reduced chemistry mechanism for the diesel surrogate components.

2. Methodology

The measured hydrocarbon class composition and the important properties of the diesel fuel used in the present work are provided in Table 1. The composition and properties of this fuel are within the ASTM specifications for a typical North American diesel fuel (>40 cetane, <35% vol. aromatics [27]). The overall methodology adopted in the present work to develop the surrogate fuel model and to predict engine combustion and emission characteristics is summarized in Fig. 1.

2.1. Diesel surrogate models

Since the distillation of a fuel is a preferential vaporization process which solely depends upon the molecular composition of its components, the measured distillation profile of the diesel fuel was modeled to arrive at suitable surrogate compositions. The detailed description of the distillation model formulation is discussed in detail in Ref. [24], and a brief summary of the methodology is provided next.

From the measured hydrocarbon class composition and the distillation temperatures of the diesel fuel given in Table 1, an initial list of surrogate species were chosen covering the hydrocarbon classes (paraffins, aromatics, etc.) and the initial and final boiling range of the fuel. The customized version of the KIVA3V release 2 code [28], viz., KIVA-ERC-CHEMKIN with improved sub-models [29,30] including a discrete multi-component model to capture the preferential vaporization of the multi-component fuel was used to simulate the distillation profile of the diesel fuel. The optimum surrogate composition was arrived at based on a manual

Table 1
Measured hydrocarbon class composition and properties of diesel fuel.

Diesel fuel composition/ properties	Measured	Surrogate model
Saturates (vol.%)	70.1	70.1
Total aromatics (vol.%)	28.6	28.6
Polycyclic (vol.%)	6.6	6.6
Olefins (vol.%)	1.3	1.3
Cetane number	43	52
Density @ 15 °C (g/cc)	0.848	0.811
Viscosity @ 40 °C (cSt)	2.4	–
Lower heating value (MJ/kg)	42.86	42.81
Hydrogen to carbon (H/C) ratio	1.83	1.86
Flash point (°C)	67	–
Cloud point (°C)	−7.4	–
Distillation temperatures (K) IBP, T5, T10, T20, T30, T40, T50, T60, T70, T80, T90, T95, FBP	451, 471, 482, 498, 510, 521, 530, 540, 551, 564,584,606, 623	470, 475, 481, 493, 507, 521, 536, 548, 559, 571, 585, 593, 608