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Experimental and modelling investigations of the diesel surrogate fuels in direct injection compression ignition combustion

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HIGHLIGHTS

- The engine combustion of three diesel surrogate fuels were investigated.
- A reduced *n*-dodecane-TRF-*c*-hexane-PAH mechanism was developed and validated.
- 3-D modelling investigations were performed.
- The physical and chemical effects on the soot formation were clarified.

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ABSTRACT

Experimental investigations on the combustion and emission characteristics of diesel and three potential diesel surrogate fuels have been performed, including the 85% (vol.) *n*-heptane blended with 15% toluene (T15), 81% *n*-heptane blended with 14% toluene and 5% *c*-hexane (T15 + CH5), and 80% (vol.) *n*-heptane blended with 20% toluene (T20). The experimental results showed that due to the lower reactivity of the three diesel surrogate fuels, the combustion phases were more retarded and the indicated thermal efficiencies were lower compared to diesel. For the diesel surrogate fuels with higher volatility, the soot emissions were lower than those of diesel due to more premixed combustion. Moreover, a reduced *n*-dodecane-toluene reference fuel-*c*-hexane-polycyclic aromatic hydrocarbon (PAH) mechanism composed of 167 species and 671 reactions was formulated and was extensively validated against the experimental results. To clarify the experimental results, the reduced mechanism was then used for the three-dimensional (3-D) modelling investigations. The modelling results showed that the reduced mechanism can reasonably capture the combustion characteristics of T15 + CH5 in the direct injection compression ignition combustion. The NOx and soot emissions were both reasonably predicted. From the modelling investigations, it was inferred that the physical effects on the soot emission were larger than the chemical effects of the different fuel carbon-chain structures. According to the 0-D modelling investigations, the soot tendency of the four pure diesel surrogate constituents can be sequenced as toluene > *c*-hexane > *n*-dodecane > *n*-heptane. Given that toluene is the dominant factor affecting the soot formation than the other three components, the soot tendency of the four diesel surrogate fuels can be sequenced as T20 > T15 + CH5 (*n*-dodecane) > T15 + CH5 (*n*-heptane) ≈ T15.

1. Introduction

Due to the higher thermal efficiency compared to the spark ignition (SI) engines fueled with gasoline, compression ignition (CI) engines fueled with diesel have been widely used in transportation, power plant, engineering, and agriculture [1–3]. However, owing to the diffusion-controlled combustion, it is difficult for the conventional diesel engines to meet the more and more stringent fuel consumption and emission regulations. Advanced engine combustion concepts like homogeneous charge compression ignition (HCCI) combustion and low temperature combustion (LTC) have been put forward, which may help relieve the concerns on the trade-off between fuel consumption and emission control [4]. HCCI combustion is characterized by the homogeneous fuel-air mixture distribution ahead of the main combustion [5]. Owing to the lean mixture and low temperature during combustion, the soot and NOx emissions are extremely lower. However, as a consequence of the kinetically controlled heat release, the combustion is difficult to be controlled and the pressure rise rate (PRR) is too high

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Nomenclature

A_1	benzene
A_1-	phenyl
A_1C_2H	phenylacetylene
A_2R_5	acenaphthylene
A_3	phenanthrene
A_4	pyrene
ATDC	after top dead center
CA	crank angle
CA10	crank angle corresponding to the 10% of the total heat release
CA50	crank angle corresponding to the 50% of the total heat release
CA90	crank angle corresponding to the 90% of the total heat release
CI	compression ignition
CFD	computational fluid dynamic
CN	cetane number
CO	carbon oxide
C_2H_2	acetylene
C_4H_2	biacetylene
C_5H_5	cyclopentadienyl
$C_6H_5CH_2$	benzyl
$C_6H_5CH_3$	toluene
DI	direct injection
EGR	exhaust gas recirculation
ϕ	equivalence ratio
HACA	H-abstraction C_2H_2-addition
HCCI	homogeneous charge compression ignition
ICE	internal combustion engine
IMEP	indicated mean effective pressure
ISFC	indicated specific fuel consumption
ITE	indicated thermal efficiency
JSR	jet stirred reactor
LTC	low temperature combustion
Mol.	mole fraction
MPRR	maximum pressure rise rate
n-c7h16	*n*-heptane
n-c12h26	*n*-dodecane
PAH	polycyclic aromatic hydrocarbon
PRF	primary reference fuel
PRR	pressure rise rate
RCM	rapid compression machine
ROP	rate of production
SI	spark ignition
SOI	start of injection
ST	shock tube
THC	total hydrocarbon
TRF	toluene reference fuel
T15	85% *n*-heptane blended with 15% toluene
T15 + CH5	81% *n*-heptane blended with 14% toluene and 5% *c*-hexane
T15 + CH5 (*n*-dodecane)	81% *n*-dodecane blended with 14% toluene and 5% *c*-hexane
T20	80% *n*-heptane blended with 20% toluene
Vol.	volume fraction
3-D	three-dimensional

for practical application under high load conditions. LTC has gained much attention for the partially premixed combustion characteristic. By using exhaust gas recirculation (EGR) dilution, the combustion can be partially decoupled from the injection event. The ignition delay time is longer while the mixture is leaner, result in lower combustion temperature. Thus, the NOx and soot emissions can be reduced simultaneously. For the superiority and the complexity of LTC, it is necessary to further investigate the combustion and emission characteristics experimentally and theoretically.

Three-dimensional computational fluid dynamics (3-D CFD) simulations have been widely used for the engine design and combustion optimization at a comparatively lower cost [6,7]. To better describe the fuel combustion and emission characteristics, the CFD code should be coupled with the corresponding detailed chemical kinetic mechanisms for combustion and emission predictions. In the simulations, the corresponding physical properties, such as density, viscosity, vapor pressure, specific heat capacity, latent heat of vaporization, and thermal conductivity, should also be considered to describe the multi-phase interaction processes, i.e. in the injection and spray processes [8,9]. While diesel comprises of hundreds of compositions, and the compositions vary for the different origins and refinery methods, making it quite hard to develop the full-scale detailed combustion kinetic mechanism and measure all the relevant physical properties [10–12]. Thus, some main surrogate fuels of diesel were often used to simulate the combustion characteristics. Farrell et al. [13] summarized the database and kinetic models for the diesel surrogate fuels, and they proposed the main criterion in the selection of the surrogate fuels. Mati et al. [14] proposed a detailed surrogate model fuel consisted of *n*-hexadecane, *n*-propylcyclohexane, *n*-propylbenzene, *iso*-octane, and 1-methylnaphthalene. They used this model to simulate the experimental species mole fraction profiles measured in a jet stirred reactor (JSR), and general good agreement was achieved. Lemaire et al. [15] compared the soot formation in turbulent flames of diesel and the diesel surrogate fuels of *n*-decane and 1-methylnaphthalene. Experimental results showed that the fraction of 20% 1-methylnaphthalene of the diesel surrogate fuels exhibited the similar soot formation region with that of diesel.

However, the detailed combustion mechanism of the diesel surrogate fuels usually includes hundreds of species. Due to the limit of the computational resources and expenses, in the short-term, direct coupled with the detailed mechanism for the 3-D CFD modelling studies cost a lot of CPU time, which is unbearable for the practical application. Thus, reduction of the detailed combustion kinetic mechanism is necessary.

n-Heptane is the most widely used single diesel surrogate to describe the diesel combustion for its close cetane number (CN ≈ 56) to that of diesel (CN ≈ 40–55). Halstead et al. [16] developed a reduced *n*-heptane kinetic model to simulate the autoignition measured in a rapid compression machine. Known as the Shell model, this model has been incorporated in many commercial CFD codes. However, the Shell model was based on empirical fit, and the operating condition was confined to the lower temperature region (650–805 K). Curran et al. [17] developed a comprehensive detailed combustion mechanism of *n*-heptane, which has been extensively validated against the experimental ignition delays and species concentrations. This detailed *n*-heptane combustion mechanism has been used as the basis to obtain the reduced mechanism in many investigations [18–20]. However, *n*-heptane produces lower soot emission compared with diesel, given that diesel comprised of a certain amount of aromatics, which contribute to the soot emission tremendously [21]. Luo et al. [22] developed a reduced *n*-heptane-toluene-1-hexene mechanism to describe the combustion of diesel in LTC combustion. Although the addition of