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Development of a new reduced diesel/natural gas mechanism for dual-fuel engine combustion and emission prediction

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ABSTRACT

A diesel/natural gas (NG) dual-fuel engine is regarded as an appealing option to reduce emissions while maintaining high thermal efficiency. In this study, a reduced *n*-heptane–*n*-butylbenzene–NG–polycyclic aromatic hydrocarbon (PAH) mechanism with 746 reactions and 143 species was developed for predicting the combustion characteristics and emission in dual-fuel engines. A mixture of methane, ethane, and propane was used to model the NG, and a mixture of *n*-heptane and *n*-butylbenzene was used to model the diesel. This mechanism was based on a reduced *n*-heptane–PAH mechanism, and the detailed mechanisms of *n*-butylbenzene and NG were reduced using the methods of directed relation graph with error propagation (DRGEP), rate of production (ROP), and sensitivity analysis. The key kinetic parameters of the model were optimized and adjusted according to the results of sensitivity analysis. The final optimized dual-fuel mechanism was verified against ignition delay, laminar flame speed, and homogenous charge compression ignition (HCCI) engine combustion, and a good prediction was obtained. Finally, the present mechanism was coupled into the CFD software to simulate the combustion characteristics and emission of a dual-fuel engine under four different NG substitution rates. The simulation results are consistent with the experimental data of emissions and combustion characteristics, indicating that the current mechanism can be applied to simulate practical diesel/NG dual-fuel engines.

1. Introduction

With the rapid development of automobile industry, increasing demand for energy and decreasing rate of petroleum production, and pollution problems caused by using fossil fuels, it is becoming increasingly essential to explore alternative fuels that are renewable, clean, and cost-effective [1,2]. Among various alternative fuels, natural gas (NG) is a promising suitable alternative fuel to satisfy increasingly stringent emission standards owing to its high fuel economy [3], clean combustion characteristics [4], abundance, and relatively low cost [5].

In a diesel/NG dual-fuel engine, the main method of fuel delivery is that a small amount of diesel is used as the ignition source and directly injected into the cylinder, while NG is injected into the intake passage to form a good premixed fuel-air. A diesel/NG dual-fuel engine can produce a reliable output power and efficiency under different engine loads. A diesel/NG dual-fuel engine not only has most of the advantages of traditional diesel engines, but also has more advantages than traditional diesel engines [6–8]. In a diesel/NG dual-fuel engine, the NG combustion mode is lean premixed combustion, refraining from the oil-rich area produced by diesel spray producing soot. In addition, diesel/NG dual-fuel engines have also attracted much interest because of other advantages; for example, it is easy and inexpensive to convert traditional diesel engines to dual-fuel engines in a flexible manner [4]. Dual-fuel engines emit a low amount of CO_2 emission because of the low C/H ratio of NG [9,10] and produce a low amount of particulate matter (PM) and NO_X emissions compared with traditional diesel/gasoline engines [6,11,12]. Further, an increase in the NG substitution rate can effectively reduce the PM and NO_X emissions of dual-fuel engines. However, if the NG in the cylinder incompletely burns, the methane emission will increase, thus increasing greenhouse gas emissions. This is because the global warming potential of methane is 25 times higher than that of total CO_2 during a hundred year period [13]. If the emission of unburned hydrocarbon (UHC) can be minimized in dual-fuel engines, a new method can be provided for implementing new greenhouse gas emission regulations, thereby saving a lot of fuel cost. Therefore, for researchers and engine producers, dual-fuel engine has become an important research topic.

Extensive studies have been carried out to evaluate the emission and combustion characteristics of dual-fuel engines. Zhang et al. [14] investigated the impact of injection timing on the emission and combustion performance of dual-fuel engines, and found that the emissions of carbon oxide (CO) and total hydrocarbon (THC) decreased while the

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Nomenclature

A_1	benzene
A_2	naphthalene
A_3	phenanthrene
A_4	pyrene
CA50	crank angle corresponding to 50% of the total heat release
3D CFD	three-dimensional computational fluid dynamic
HCCI	homogeneous charge compression ignition
PRF	primary reference fuel
TRF	toluene reference fuel
THC	total hydrocarbon
DICI	direct injection compression ignition
NTC	negative temperature coefficient
P_{in}	initial pressure
PM	particular matter
C_n	the number of carbon atoms in a fuel molecule
ATDC	after top dead center
CA	crank angle
CO	carbon oxide
C_2H_2	acetylene
CA90	crank angle corresponding to 90% of the total heat release
HACA	hydrogen abstraction acetylene addition
PAH	polycyclic aromatic hydrocarbon
SOI	start of injection
EGR	exhaust gas recirculation
HRR	heat release rate
NG	natural gas
T_{in}	initial temperature
HC	hydrocarbon
UHC	unburned hydrocarbon
C_4H_4	tetrahedrane
C_4H_2	Diacetylene

NO_X emission increased with increasing injection timing. Zhou et al. [15] evaluated the impact of injection timing and quantity of pilot diesel fuel on the combustion performance of a dual-fuel engine. The results of the study show that the ignition delay increased with increasing injection timing and decreased with increasing amount of pilot diesel fuel. Imran et al. [16] carried out related experiments for examining the impact of pilot diesel fuel on the combustion performance of a dual-fuel engine. It was found that the maximum cylinder pressure increased, and the ignition delay decreased with the increase in pilot diesel amount. At high loads, the thermal efficiency was the same or slightly higher than conventional diesel engines; however, at low loads, the thermal efficiency was slightly lower than conventional diesel engines. Mittal et al. [17] carried out the experiments to study the characteristics of emissions such as soot, PM, HC, CO, NO_X and CO_2 on a six-cylinder conventional diesel engine and dual-fuel engine under different conditions. Karim et al. [18,19] evaluated the effect of methane fraction, engine load, and quantity of pilot diesel fuel on methane and CO emissions on a single-cylinder diesel/NG dual-fuel engine.

However, it is time-consuming and expensive to gain in-depth knowledge and optimize the emission and combustion characteristics of dual-fuel engines by experiments only. Numerical simulation is a fast and economical way to better understand the complex combustion, spray, pollutant formation processes, and evaporation in dual-fuel engines in detail, for which it is difficult to obtain these information through experimental studies. Singh et al. [20] proposed a dual-fuel chemical kinetic mechanism and coupled it into KIVA3V software to model the emission and combustion characteristics of a dual-fuel engine, and found the limitations of this kinetic mechanism for simulating premixed combustion of NG and air. Aggarwal et al. [21], Maghbouli et al. [22], and Zhao et al. [23] developed a reduced chemical mechanism for dual-fuel engines respectively, where *n*-heptane was used as the representative of diesel and methane was used as the representative of NG. These reduced mechanisms were coupled into CFD software for multidimensional numerical simulation of engine performance [22–24]. Yousefi et al. [24] and Maghbouli et al. [22] only validated the modeled results of in-cylinder heat release rate (HRR) and pressure but neglected the laminar flame speed and ignition delay. In contrast, Zhao et al. [23] simulated the in-cylinder pressure, ignition delay, HRR, NO_X and CO emissions for validation while neglecting the laminar flame speed, soot and methane emissions. NG is a mixture of fuel, mainly consisting of methane, ethane, and propane; the related chemical kinetic mechanisms should include these three substances as much as possible. Hocktt et al. [25] proposed a reduced chemical mechanism for a dual-fuel engine, where *n*-heptane was used as the representative of diesel and methane, ethane and propane were used as the representatives of NG. Moreover, they coupled the mechanism into CFD software for multidimensional numerical simulation engine and calculated the ignition delay, in-cylinder pressure, HRR, and laminar flame speed. Based on the numerical simulation results, the developed reduced mechanism well reproduces the characteristics of detailed mechanism; however, the emission properties including methane, NO_X, soot and CO emissions were not validated.

In summary, in the simplified dual-fuel kinetic models mentioned above, most of the kinetic models used a single component of *n*-heptane as the representative of diesel and a single component of methane as the representative of NG. However, diesel is a mixture of more than 200 components. The main components of diesel include alkanes (straight-chain and branched-chain alkanes), naphthenes, and aromatic hydrocarbons [26,27]. NG is also a mixed fuel mainly containing methane, ethane, and propane. It is difficult to establish a dual-fuel chemical kinetic model containing all the components of diesel and NG. Therefore, the established dual-fuel engine model should include important components of diesel and NG as much as possible. Qian et al. [28] performed engine bench tests on toluene/diesel and *n*-butylbenzene/diesel mixtures with the same ratios. The results showed that *n*-butylbenzene was more appropriate as the representative of aromatic hydrocarbons. In the existing reduced chemical kinetic mechanisms of dual fuels, two or more components have been rarely used as the representative of diesel (*n*-butylbenzene was used as the representative of aromatic hydrocarbons), and a mixture of methane, ethane and propane has been rarely used as the representative of NG.

Based on the abovementioned reasons, the objective of this study was to develop a reduced chemical kinetic mechanism of *n*-heptane–*n*-butylbenzene–NG–polycyclic aromatic hydrocarbon (PAH) (denoted as GXU mechanism) for simulating the combustion characteristics and emission of a dual-fuel engine. First, the detailed mechanisms for *n*-butylbenzene and NG developed by Nakamura et al. [29] and Healy et al. [30], respectively, were reduced. The reduced mechanisms for NG and *n*-butylbenzene were then coupled into the *n*-heptane–PAH mechanism developed by Wang et al. [31,32], thus developing the GXU mechanism. The GXU mechanism was adjusted by sensitivity analysis combined with the optimization method proposed by Ra and Reitz [33,34]; the mechanism was extensively verified by evaluating laminar flame speeds, ignition delays, and homogenous charge compression ignition (HCCI) engine combustion. Finally, the GXU mechanism was coupled into CFD software to verify the emission and combustion characteristics of a six-cylinder dual-fuel engine against experimental results under four different NG substitution rates (0, 25%, 50%, and 75%) through numerical simulations.