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Full Length Article

A multi-component wide distillation fuel (covering gasoline, jet fuel and diesel fuel) mechanism for combustion and PAH prediction

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HIGHLIGHTS

- A reduced 11-component chemical mechanism is proposed for wide distillation fuel.
- The mechanism includes six classes of hydrocarbons and PAH pathways up to pyrene.
- The mechanism is validated for pure components, mixtures, surrogate and real fuels.
- A detailed soot model is coupled with the mechanism to predict the soot formation.
- The CFD simulations capture the engine combustion process and the soot formation.

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ABSTRACT

A reduced 11-component (*n*-heptane, *iso*-octane, toluene, ethanol, methanol, *n*-decane, *n*-dodecane, *n*-hexadecane, diisobutylene, cyclohexane and methyl-cyclohexane) chemical mechanism consisting of 178 species and 758 reactions is proposed for combustion and soot formation predictions of wide distillation fuel (WDF) covering gasoline, jet and diesel fuels. Six different classes of hydrocarbons (straight alkanes, branched alkanes, cycloalkanes, alkenes, aromatics and alcohols) are included in the present mechanism, which is constructed with a hierarchical structure. Optimizations based on sensitivity analyses are conducted for each sub-mechanism and the base mechanism. This reduced multi-component mechanism has been extensively validated against experimental data including ignition delay times, laminar flame speeds, species concentration profiles and new direct injection compression ignition (DICI) engine combustion data. The present mechanism is not only validated for each pure component, but also for different surrogate fuels for gasoline, jet fuel and diesel fuel. Measured ignition delay and laminar flame speed data for real fuels are also used to validate the present mechanism. The good agreement suggests the present mechanism can be used for simulation of multi-component surrogates of conventional transportation fuels. Furthermore, the present mechanism is used for multidimensional modeling studies to investigate the DICI combustion fueled with gasoline, diesel fuel and WDF. The experimental combustion characteristics as well as the soot and NOx emissions are all reasonably predicted, indicating the proposed mechanism can be applied for modeling in practical engine applications.

1. Introduction

Internal combustion engines (ICEs) remain one of the most significant power sources in modern society. Improving energy utilization while minimizing pollutants has become a key scientific target in the field of ICEs, driven by the global concern about energy saving and emission reduction. Fuel design has recently received substantial attention as a pathway to achieve high efficiency and clean combustion [1], highlighting the importance of chemical reaction kinetics [2–4].

Recently, wide distillation fuel (WDF) was utilized to combine the advantages of spark ignition (SI) engines and compression ignition (CI) engines, namely to maintain the high thermal efficiency of CI engines while achieving the low emissions of SI engines. WDF refers to the fuels with a distillation ranging from the initial boiling point of gasoline (about 40 °C) to the final boiling point of diesel fuel (about 360 °C). Highly volatile components contained in

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Nomenclature

AMR	adaptive mesh refinement
ATDC	after top dead center
CA	crank angle
CFD	computational fluid dynamics
CHX	cyclohexane
CI	compression ignition
CN	cetane number
DIB	diisobutylene
DICI	direct injection compression ignition
EGR	exhaust gas recirculation
EVO	exhaust valve open
FDF	full distillation fuel
FE	fixed embedding
HACA	hydrogen abstraction acetylene addition
HCCI	homogeneous charge compression ignition
HRR	heat release rate
ICE	internal combustion engine
IVC	intake valve closure
JSR	jet-stirred reactor
LTC	low-temperature combustion
MCH	methyl-cyclohexane
NTC	negative temperature coefficient
PAH	polycyclic-aromatic hydrocarbon
PFB	premixed flame burner
Phi	equivalence ratio
P_{in}	initial pressure
PRF	primary reference fuel
RON	research octane number
SI	spark ignition
SOI	start of injection
T_{in}	initial temperature
TRF	toluene reference fuel
WDF	wide distillation fuel

WDF benefit the fuel atomization and evaporation, while highly ignitable components ensure the combustion stability. The most convenient way to produce WDF is to blend commercial gasoline and diesel fuel directly. Xu et al. [5] named gasoline–diesel fuel blend fuel as 'dieseline' and found that dieseline increased the combustion stability and extended the operating range of homogeneous charge compression ignition (HCCI) combustion compared with pure gasoline. Liu et al. [6] studied the effects of gasoline octane number on premixed low-temperature combustion (LTC) of WDF and found that WDF could significantly reduce soot emissions at both medium and high engine load in LTC compared with diesel fuel. Furthermore, Wang et al. [7,8] proposed a novel concept of full distillation fuel (FDF), a liquid fuel whose distillation temperature range covers gasoline, kerosene and diesel fuel. This may simplify the petroleum refining process and yield a design revolution for unified ICEs. It was found that the common rail diesel engine could work normally with FDF without any modifications to the fuel supply system and FDF significantly increased energy efficiency compared to the conventional approaches of using gasoline and diesel fuel separately. In addition, numerous studies have focused on the combustion and emission characteristics of WDF with applications in ICEs [9–13].

Computational fluid dynamics (CFD) coupled with chemical kinetics has been playing an increasingly significant role in the development in ICEs. A reliable kinetic model is one of the keys to simulate the combustion process. Since real fuels such as gasoline and diesel fuel consist of hundreds of components, studies focusing on developing a molecular-level understanding of transportation fuel combustion usually utilize surrogate fuels, which are a blend of selected species of known concentrations and exhibit similar combustion characteristics to those of the real fuels [14–16].

Numerous studies have focused on developing kinetic mechanisms for gasoline primary reference fuels (PRF) (i.e., iso-octane, PRF = 100, and n-heptane, PRF = 0) [17–20]. The comprehensive PRF mechanism proposed by Curran et al. [17] is the most detailed PRF model. A reduced mechanism by Ra et al. [18] has been shown to capture the ignition delays of PRF accurately and is widely used in engine CFD simulations. However, practical transportation fuels are very different from gasoline PRFs because they are complex mixtures of aromatics, olefins, paraffins, oxygenates, etc. Therefore, the PRF mixture has limitations in engine combustion modeling, since its ignition chemistry fails to reproduce the real fuel behavior over the wide range of conditions needed in application [21]. Recent research has shown that a mixture with more components is required to reproduce the target fuels of interest [22,23].

Different classes of compounds need to be considered in surrogate chemical mechanisms [14–16]. Aromatics constitute a non-negligible concentration in real fuels affecting soot formation in the engine combustion process. Andrae et al. [24,25] proposed a toluene reference fuel (TRF) model with toluene representing aromatic components in the fuel and the model successfully predicted the measured ignition delays. Wang et al. [26] developed a reduced TRF mechanism, which was well validated for combustion and polycyclic-aromatic hydrocarbon (PAH) predictions. Much research has also focused on the TRF surrogate [27,28]. Moreover, alcohols and olefins are also important components in real fuels, which can obviously influence the fuel oxidation and combustion characteristics. Much of the chemistry for alcohol compounds is suggested to be relevant to ethanol [29], where reaction pathways include most of the important characteristic oxidation processes of alcohols. Diisobutylene (DIB) has a similar molecular structure to *iso*-octane so that its chemistry offers an insight into the effect of including a double bond in the carbon skeletal structure of *iso*-octane. Metcalfe et al. [30] developed a detailed DIB mechanism aiming to represent alkenes in practical fuels. Furthermore, medium and long-chain straight-alkanes such as *n*-decane, *n*-dodecane and *n*-hexadecane are necessary components because their boiling range is comparable to those of jet or diesel fuels [31]. In addition, naphthenes (cycloalkanes) are also an important chemical class of hydrocarbons since they make up a significant portion of diesel fuel (up to 35%), jet fuel (up to ~20%) and gasoline (up to ~10%) [14–16]. Because of their propensity to produce PAH, cycloalkanes are also essential components for soot emission prediction. Typically, cyclohexane (CHX) and methyl-cyclohexane (MCH) are suggested to represent the hydrocarbon class of naphthenes [14–16].

Multi-component chemical kinetic mechanisms are widely used for different real fuels. For gasoline, Andrae et al. developed a detailed five-component (*n*-heptane, *iso*-octane, toluene, ethanol and DIB) gasoline surrogate fuel mechanism [32] and its reduced mechanism [33] based on their TRF mechanism. Cancino et al. [34] developed a detailed multi-component gasoline surrogate mechanism with the same components as Andrae's model. Another reduced multi-component mechanism for a gasoline surrogate containing the same components was proposed by Zhong et al. [35] and widely validated with experimental data. Jet fuel is also contained in the WDF distillation range. A widely accepted jet fuel