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Heating and evaporation of a new gasoline surrogate fuel: A discrete multicomponent modeling study

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HIGHLIGHTS

- Gasoline is modeled by a six-component surrogate fuel covering three major hydrocarbon groups.
- The new surrogate emulates real gasoline distillation curve and contains the toluene reference fuel components.
- Discrete multicomponent model is used to investigate heating and evaporation of gasoline fuel droplets.

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ABSTRACT

In Gasoline Direct Injection (GDI) engines, a fuel spray is injected directly into the cylinder during the compression stroke, creating a fuel–air mixture with an ignitable composition at the spark gap at the time of ignition. Spraying droplet breakup, heating and evaporation is essential for the mixture preparation and the ignition/combustion. For numerical modeling of spray evaporation and combustion, it is impractical to include all real components. In this study, a new 6-component surrogate mixture composed of i-pentane/n-heptane/toluene/iso-octane/n-propyl cyclohexane/iso-undecane is developed to match the targeted gasoline in terms of thermo-physical properties and experimental distillation curve. This new surrogate also covers TRF (toluene reference fuel) components, which are the three basic components for ignition modeling. This allows both physical and chemical modeling of gasoline using only one surrogate. This new surrogate fuel is implemented into an existing modeling methodology which simultaneously accounts for finite conductivity, finite mass diffusivity and turbulence effects within atomizing multicomponent liquid fuel sprays. The main purpose of this study is to perform analysis of heating and evaporation of the new surrogate gasoline. Both normal evaporation and flash boiling evaporating processes are investigated.

1. Introduction

Real transportation fuels are complex mixtures of thousands of hydrocarbon species and the use of which for multi-dimensional spray combustion simulations is not computationally feasible. In the past, surrogate fuels with a limited number of components have been developed to represent various aspects of real fuels. Multi-component fuel models are generally classified into two types: Discrete Multi-Component models (DMC) [1–3] and Continuous Multi-Component models (CMC) [4]. The DMC approach models a fuel with a limited number of real components to match the actual fuel distillation curve. Other fuel surrogate properties such as thermal conductivity, density and heat capacity are not necessarily close to that for the real fuel [1]. Recently, quasi-discrete model approach [5] has been developed in which the components of the real fuel with close thermodynamic and transport properties, including alkanes and other various groups of hydrocarbons are grouped together to form quasi-components. Using combination of quasi-components and real components, the physical properties of the real fuel can be accurately modeled [5]. The present fuel model development is based on the DMC framework. Components selection for surrogate fuels depends on the targeted applications. Surrogate fuels developed to mimic thermo-physical properties and evaporation processes can be viewed as "physical" surrogate models [1,2]. On the other hand, components selected to match real fuel chemical kinetics (for example, ignition delay) are "chemical" surrogate models. It has been shown that the commonly used chemical surrogates are not suitable for analyzing the complex behavior of droplet heating and evaporation [6]. The

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Nomenclature

A	droplet surface area
C_μ	constant (=0.09)
c_p	specific heat at constant pressure
D	molecular mass diffusivity
h	heat transfer coefficient
J	mass transfer coefficient
k	thermal conductivity; liquid turbulent kinetic energy
L	latent heat of evaporation
$\dot{m}$	mass transfer rate
P	pressure
Pr	Prandtl number
Q	heat transfer rate
r	instantaneous drop radius
R	universal gas constant
Re	Reynolds number
Sc	Schmidt number
t	time
T	temperature
v	velocity
X	mole fraction
Y	mass fraction

Greek letters

α	thermal diffusivity/heat transfer enhancement
ε	dissipation rate of kinetic energy in $k-\varepsilon$ model
μ	viscosity
ρ	density
τ	time associated with surface wave motion
τ_t	characteristic time scale associated with liquid turbulence time scale

Superscripts

d	associated with droplet
eff	associated with effective coefficient
g	gas phase
i	surrogate component
l	liquid phase
o	initial condition
p	at the constant pressure
r	radiative heat transfer
s	at the droplet surface
sh	associated with superheated heating
t	parameter associated with turbulence
∞	free stream condition

preferential evaporation of the light-end components greatly influences the fuel distribution near the spray and cannot be predicted by the chemical surrogates containing n-heptane, iso-octane and toluene (TRF model) only. Such that, the European gasoline TRF surrogate from [7] can only be applied to port fuel injection operating points because only the gas phase properties of gasoline were emulated with the selected mixture. At the same time, more complex surrogates with additional chemical family groups have been proposed to simulate the kinetic mechanism to extend the current TRF model [8–10]. Most of the current surrogate models focus on predicting and simulating the distillation curve, evaporation behavior and kinetic mechanism separately. To effectively model the spray combustion process, a surrogate must be capable of describing or predicting both the physical and chemical properties of gasoline [11]. The originality of this current work is to propose a surrogate that can mimic both the physical and chemical properties to be used in modeling spray combustion processes involving gasoline.

Recent studies [11,12] have indicated that a gasoline surrogate should cover different hydrocarbon groups including linear and branched paraffin, naphthene, olefin and aromatic in order to match gasoline thermo-physical/distillation behavior. It is widely believed that a simpler surrogate with a limited number of components could effectively reproduce the real fuel's heating and evaporation behavior. For physical surrogates, the FACE (Fuel for Advanced Combustion Engines) working group has identified that 90% distillation curve matching is one of the three properties which are of primary importance in deciding the performance of advanced combustion engines [12]. The vaporization of droplets and spray also has significant meaning in engineering application and substantial effort has been made to predict its behavior numerically. Most of the evaporation models concentrate on the cases under normal boiling where Spalding's transfer number approach is valid [13]. In general, gasoline has high volatility and flash boiling takes place easily in the fuel spray when injected into the combustion chamber at high temperature [6]. Therefore, it is also important to investigate flash-boiling processes in fuel spray.

In this study, a new surrogate was developed, which could be regrouped and used in further investigation for chemical kinetic modeling. The novelty of the proposed surrogate, which is different from most existing surrogate fuel models assuming that the gasoline is only made of alkanes [e.g. 1, 6], is that the contributions from different hydrocarbon groups apart from alkanes are taken into account in this new surrogate. This new surrogate also covers n-heptane, toluene and iso-octane, which are the three basic components for kinetic modeling in the current literatures. This allows the possibility of physical and chemical modeling of gasoline with only one surrogate for further study. Recently, several surrogates for gasoline have also been developed to include various hydrocarbon groups [14,15]. In addition to distillation behavior validation, this new surrogate fuel is implemented into a recently developed discrete multicomponent modeling methodology which simultaneously accounts for finite conductivity, finite mass diffusivity and liquid turbulence effects within spraying liquid fuel droplets. The main purpose of this study is to perform analyses of heating and evaporation of the new surrogate gasoline. The distillation curve was predicted under ambient pressure of one bar and different ambient pressures and initial droplet temperatures were tested under both normal and flash boiling conditions for droplet heating and evaporation.

2. Theoretical formulations

2.1. The new gasoline surrogate

Depending on the oil refinery process, gasoline fuel consists of hydrocarbons ranging from four to twelve carbon atoms per molecule (C4–C12) [16]. Even though real gasoline is a complex mixture of thousands of hydrocarbon species, a typical gasoline is predominantly a mixture of three groups including alkanes (linear and branched paraffin), naphthene (cycloalkanes) and alkenes (olefin and aromatic). From these groups, six components composed of i -pentane/n-heptane/toluene/iso-octane/n-propyl cyclohexane/iso-undecane were chosen to match the targeted gasoline in terms of thermo-physical properties and experimental distillation curve [17]. The choice of the six components is somewhat arbitrary; however, this surrogate has been proved to produce excellent dis-