Fuel 182 (2016) 284–291

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Full Length Article

A unified jet fuel surrogate for droplet evaporation and ignition

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HIGHLIGHTS

- Jet fuel is modeled by a four-component surrogate fuel covering four major hydrocarbon groups.
- The new unified surrogate emulates real jet-A fuel distillation curve and combustion characteristics.
- Discrete multicomponent model is used to investigate heating, evaporation and ignition of jet-A fuel droplets.

ARTICLE INFO

Article history:
Received 15 March 2016
Received in revised form 3 May 2016
Accepted 24 May 2016

Keywords:
Jet-A
Surrogate
Droplet heating
Evaporation
Ignition

ABSTRACT

Kerosene fuels such as Jet-A and JP-8 have been considered for dual-purposed utilizations by both jet engines and ground transportation diesel engines. These complex fuels are composed of thousands of different kinds of hydrocarbon species. The spray combustion process in diesel engines requires detailed characterization of the ignition delay of the fuels used for the preparation of stratified fuel-air charge. Ignition delay phenomenon is dominated by the fuel heating and evaporating spray processes. For computational modeling of the spray combustion processes, it is essential to have accurate characteristics of fuel thermo-physical and chemical kinetics properties. Real kerosene fuels with such a large number of components are not feasible to be used in multicomponent spray combustion calculations. The object of this study is to develop a surrogate fuel, composed of a few components, to mimic the heating, evaporating, and ignition behaviors of the real fuel. To this end, we have utilized a recently developed inversed batch distillation methodology, to select a group of hydrocarbon species that can closely match the experimental distillation curve of a Jet-A (POST-4658) blend. For chemical kinetics target, a multicomponent skeleton reaction mechanism of 231 species and 5591 reactions was used to predict ignition delay times and laminar flame speeds with satisfactory results. From the hydrocarbon groups of typical kerosene fuels of linear paraffins, cycloparaffins and aromatics, we have identified the 4-component surrogate fuel as: n-dodecane/isocetane/transdecalin/toluene (mole fraction: 0.3/0.36/0.246/0.094). Droplet heating, evaporation, and ignition processes using the current unified surrogate are presented and discussed in this study.

1. Introduction

For advanced combustion engine technologies, it is essential to understand the effect of fuel properties on spray combustion behaviors in order to achieve projected engine operation and emission improvements. Liquid-fueled combustion engines running on petroleum-derived fuels will remain the prime power sources for air, ground, and ocean transportation within the foreseeable future. Recently, bio-derived and related alternative fuels offer exciting opportunities for renewable power generation and transportation with zero or minimal carbon and/or NOx emissions. However, it is important to recognize the full range of requirements for spray-combustion-based energy conversion devices and to ensure that their deployments do not cause adverse effects on such issues as combustion efficiency, particulate formation and emissions, and power system reliability. To obtain the benefits provided by emerging engine technologies (for example, the Low Temperature Lean Premixed Pre-vaporized combustor, Reactivity Controlled Compression Ignition Engine (RCCI) [1]), the properties of liquid fuels will be modified continuously considering market need and new engine technologies. In fact, the recent FACE (Fuel for Advanced Combustion Engines) project [2] seeks to design tailored-made fuels, by combining petroleum and alternative-based advanced fuels, to meet next generation engine performance in terms of combustion efficiency and emission reduction. But the

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http://dx.doi.org/10.1016/j.fuel.2016.05.114
0016-2361/

Nomenclature

A	droplet surface area
C_μ	constant (=0.09)
C_p	specific heat at constant pressure
D	molecular mass diffusivity
J	mass transfer coefficient
k	thermal conductivity; liquid turbulent kinetic energy
L	latent heat of evaporation
m	mass
$\dot{m}$	mass transfer rate
Nu	Nusselt number
P	pressure
Pr	Prandtl number
r	instantaneous drop radius
t	time
T	temperature
X	mole fraction
Y	mass fraction

Greek letters

α	thermal diffusivity
δ	thermal layer or mass transfer layer thickness
ε	dissipation rate of kinetic energy in $k-\varepsilon$ model
μ	viscosity
ϕ	fugacity coefficient
Φ	equivalence ratio
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
g	gas phase
l	liquid phase
r	radiative heat transfer
s	at the droplet surface
t	parameter associated with turbulence
∞	free stream condition

Subscripts

d	associated with droplet
eff	associated with effective coefficient
i	surrogate component
o	initial condition
$thermal$	associated with thermal coefficient

impacts of mixing alternative fuels with these traditional fuels on spray combustion phenomena should also be known. Forecasting the coupled physical (fuel spray and evaporation) and chemical (combustion) property impacts of real liquid fuels on energy efficiency and emissions while utilizing multi-dimensional spray combustion simulations, are computationally challenging. Fuels used in liquid-fuels engines, such as gas turbine and IC engines, are complex mixtures of different kinds of hydrocarbon species. Running numerical simulations of spray combustion of real fuels, including the entire hydrocarbon species, is not possible, even with rapid advances in high performance computers in the near future.

For spray combustion simulations, the well-considered modeling approach starts with designing a multi-component surrogate fuel to emulate the real fuel. This surrogate can then be incorporated into a phenomenological-based atomization spray of the liquid fuel, evaporation, combustion, and turbulence/chemistry interaction models within fully coupled numerical simulation tools. Years of fuel research and extensive chemical analyses have indicated that using mixtures of limited components, known as surrogate fuels, to study spray and combustion properties of real liquid fuels is obtainable [3]. Strategies of screening components to form surrogate fuels depends on the targeted applications. Developed surrogates, to characterize multi-phase, thermophysical properties and the resulting fuel evaporation processes, are viewed as "physical" surrogates [2]. On the other hand, components selected to mimic fuel chemical kinetics (for example, ignition delay and laminar flame speed) are "chemical" surrogate models [3]. Previous research activities have put emphasis on the vaporized chemical kinetics aspects, thus the suggested surrogates have been used for single phase gas combustion research extensively [3]. However, some commonly used chemical surrogates cannot match the physical properties, such as the distillation curve, and are not suitable for analyzing the complex behavior of droplet heating and evaporation [4,5]. The majority of current surrogate models focus on predicting and simulating the distillation curve, evaporation behavior, and kinetics mechanism separately. To meet the fuel evaporation process target, the FACE [2] working group has emphasized the importance of matching 90% distillation curve which is one of the three properties displaying dominant roles for the advanced combustion engine's performance. These selected surrogates were able to represent real liquid fuel properties including, H/C (hydrogen carbon) ratio, lower heating value (LHV), and distillation characteristics. For the purpose of modeling a multiphase spray combustion process, a "unified" surrogate, that is capable of emulating the physical and chemical (kinetics) properties of the real liquid fuel at the same time, is highly desirable. Such a unified surrogate has been developed for Jet-A [4] and for gasoline [6]. Optimization procedures were used in [4,6] to match various physical properties for the selection of pure components to form the surrogate fuels. Properties such as ignition delay time and flame propagation speed predictions were then used to validate surrogate fuels' chemical characteristics. In order to properly address the dependency of diesel ignition processes on various liquid fuel properties, Kim et al. [4] chose eight properties as target properties for the surrogate. Four properties including cetane number (CN), lower heating value (LHV), H/C ratio, and mixture molecular weight (MW) are temperature-independent. In addition, three temperature dependent physical property targets were selected, including liquid density, kinematic viscosity, and surface tension. At the end, the distillation curve was used to represent the volatility of the fuel. Density and distillation curves for liquid fuels are two important properties which are known in spray prediction under engine relevant conditions. The surrogates were developed with only those species readily available in existing reaction kinetic mechanisms. In [4], the chemical target of the proposed surrogate was validated by comparing ignition delay time predictions and utilizing a detailed multicomponent reaction mechanism (Diesel surrogate mechanism ID161) of 4014 species and 16936 reactions with experimental data. As recently indicated by [7], this level of large-size detailed reaction mechanisms could pose problems for multi-dimensional simulations. Using reduced mechanisms are highly desirable to achieve the goal of large-scale computational simulations for engine configurations.

The objective of this study is to develop a surrogate fuel, composed of a few components, to mimic the heating, evaporating and, ignition behaviors of the conventional jet fuels. The