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Full Length Article

Surrogate formulation for a coal-based jet fuel using a mixing model based on explicit equations and artificial neural network

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ABSTRACT

Coal-based jet fuel is an important alternative energy source for aviation sector. To formulate the surrogate of a coal-based jet fuel, a hybrid mixing model based on explicit equations and artificial neural network (ANN) is developed to emulate fuel atomization characteristics and pollutant emissions in aero-engine combustor. Hydrogen–carbon ratio, molecular weight, and lower heating value are calculated by explicit equations, and the ANN mixing model is used to predict the density, viscosity, surface tension, and distillation curve for the surrogate mixture at various temperatures. In the ANN model, the learning task is completed through tan-sigmoidal and linear functions, and the Levenberg–Marquardt algorithm is employed for the optimization process. The resulting surrogate of the coal-based jet fuel obtained by the hybrid mixing model is composed of *n*-decane/*n*-dodecane/*n*-tetradecane/iso-octane/methylcyclohexane (0.026/0.603/0.229/0.117/0.025 by mole). The proposed surrogate can match the physicochemical properties of the target fuel, and also shows good agreement with the target fuel in terms of atomization characteristics and CO emissions, while the NOx emissions of the surrogate is higher than those of the target fuel for most test conditions.

1. Introduction

In recent years, alternative jet fuels including Fischer-Tropsch (FT) synthetic fuels and bio-jet fuels have been increasingly used in the aviation sector due to the fluctuation in oil prices and environmental concerns stemmed from conventional petroleum-derived jet fuels. Coal-based FT fuel contains no sulfur, no nitrogen, and little aromatics, thereby emitting less pollutant emissions than conventional jet fuels. However, coal-based jet fuel has complex composition containing hundreds of hydrocarbon components, making it impossible for direct simulation. To overcome this problem, a surrogate fuel containing limited number of species needs to be designed and formed to emulate the combustion process of the target real fuel.

Edwards and Maurice [1] defined two types of surrogates: physical surrogate and chemical surrogate. Physical surrogates are constructed to reproduce the physical properties of practical fuels, such as density, viscosity, etc. Chemical surrogates generally have the same chemical-class composition of real fuels, focusing on hydrogen–carbon ratio (H/C), low heating values (LHV), etc. They are constructed to reproduce selected aspects of combustion characteristic of target real fuels.

To be useful for combustion within practical devices, surrogates must successfully emulate the properties and combustion behaviors of the target real fuel. Equations are used to calculate properties, including H/C, molecular weight (MW), density, etc., then an optimizer is utilized to formulate the surrogate composition. For example, Kim et al. [2] formulated two jet fuel surrogates using five hydrocarbon species by several explicit equations to calculate density, cetane number, etc.; the surrogates show close agreement of physicochemical properties and ignition delay times with target real fuel. Huber et al. [3] developed surrogate mixture models to represent the thermophysical properties of two jet fuels, and two surrogates with eight and fewer compounds respectively are in good agreement with the real fuels in terms of their thermophysical properties.

Accurate results are estimated by equations, such as H/C and MW, which are linearly associated with the component fraction, while other properties, such as surface tension [4,5], viscosity [6,7], and distillation curve [8], cannot be accurately predicted by a linear mixing rule. To overcome such problem, the artificial neural network (ANN) can be used to solve nonlinear and multivariable problems associated with complex physical and chemical phenomena [9]. The ANN composed of interconnected processing units named neurons is an algorithm of distributed parallel information processing. Balabin et al. [10] showed that advanced artificial neural network has a small mean squared error with respect to other models. Rocabruno-Valdés et al. [11] predicted

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Table 1
Surrogate component candidates considered in the surrogate mixing model.

HC class	*n*-Alkane			Iso-alkane	Cycloalkane	Aromatic
Name	*n*-Decane	*n*-Dodecane	*n*-Tetradecane	Iso-octane	MCH[a]	Mesitylene
Formula	$C_{10}H_{22}$	$C_{12}H_{26}$	$C_{14}H_{30}$	C_8H_{18}	C_7H_{14}	C_9H_{12}
H/C	2.200	2.167	2.143	2.250	2.000	1.333
MW[b]	142.28	170.33	198.39	114.23	98.19	120.19
LHV[c]	44.24	44.11	44.02	44.34	43.36	41.01
DT[d]	444.78	485.24	520.83	372.29	373.94	435.71

[a] Methylcyclohexane.
[b] Molecular weight, g/mol.
[c] Lower heating value, MJ/kg.
[d] Distillation temperature, Kelvin.

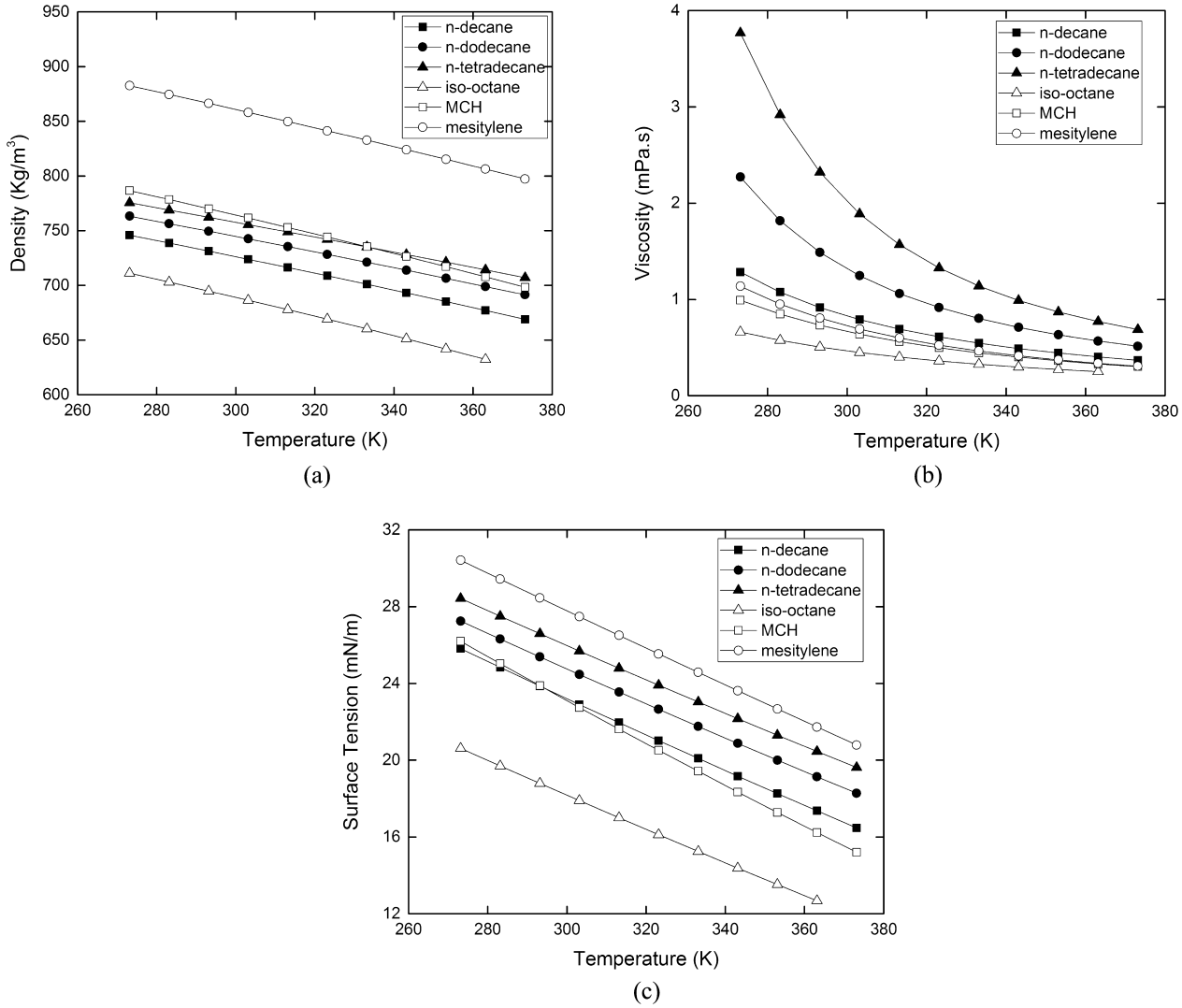

Fig. 1. Physical properties of the neat surrogate candidates as a function of temperature; (a) density, (b) dynamic viscosity, and (c) surface tension.

Table 2
Equations used for calculating the mixture properties.

Target property	Estimation equation
H/C	$H/C_{mix} = (\sum_{i=1}^{k} x_i N_{Hi})/(\sum_{i=1}^{k} x_i N_{Ci})$
MW	$MW_{mix} = \sum_{i=1}^{k} x_i MW_i$
LHV	$LHV_{mix} = \sum_{i=1}^{k} y_i LHV_i$

x_i is the mole fraction of component i, y_i is mass fraction of component i.

density, dynamic viscosity, and cetane number of biodiesel using artificial neural networks with correlation coefficient between 0.91946 and 0.99401. Filho et al. [12] predicted viscosity, iodine value, and induction period using artificial neural networks within two hidden layers. Estiati et al. [13] compared ANN with empirical correlations to estimate the higher heating values of biomass, and twelve values of biomass were used to verify the validity of the fittings.

In order to facilitate the surrogate formation for jet fuels in aero-engine combustion modeling, this paper presents the development of a surrogate that can emulate the physical and chemical properties of jet