Full Length Article

Development of correlations for combustion modelling with supercritical surrogate jet fuels

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ABSTRACT

Supercritical fluid technology finds its application in almost all engineering aspects in one or other way. Technology of clean jet fuel combustion is also seeing supercritical fluids as one of their contender in order to mitigate the challenges related to global warming and health issues occurred due to unwanted emissions which are found to be the by-products in conventional jet engine combustion. As jet fuel is a blend of hundred of hydrocarbons, thus estimation of chemical kinetics and emission characteristics while simulation become much complex. Advancement in supercritical jet fuel combustion technology demands reliable property statistics of jet fuel as a function temperature and pressure. Therefore, in the present work one jet fuel surrogate (n-dodecane) which has been recognized as the constituent of real jet fuel is studied and thermophysical properties of each is evaluated in the supercritical regime. Correlation has been developed for two transport properties namely density and viscosity at the critical pressure and over a wide range of temperatures (T_C + 100 K). Further, to endorse the reliability of the developed correlation, two arithmetical parameters have been evaluated which illustrates an outstanding agreement between the data obtained from online NIST Web-Book and the developed correlation.

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1. Introduction

Minimizing the pollutant emissions contributed by the transport sector (gasoline and jet engines) causing environmental and health issues due to the increase in utilization of conventional fossil fuels has become one of the major challenges. In order to conquer these challenges, enormous effort is needed not only in discovering the new energy sources but also in exploring the scientific innovations in clean fuel utilization. Pre-combustion treatment has been employed with surrogate fuels [1–2] with the generation of relevant data along with studies on the flames [3]. Further, the properties of such jet fuels were studied in literature [4–6]. In addition, the effect of temperature and pressure on the delays in combustion kinetics were also studied [7–12] in order to enhance combustion efficiency and to minimize the emissions. Near the supercritical (SC) region, the system properties are found to be highly sensitive to pressure and temperature which results in instant variation in physical properties [13–16]. Thus, supercritical fluids bring new directions to jet fuel combustion research communities because of their peculiar variation in their thermophysical properties [17]. Recent studies on supercritical fluids reveal that these fluids can also be used in cooling of nozzles [18] and superconducting magnets and cables also [19,20]. Hence, it is important to investigate the feasibility of diesel fuel surrogates under supercritical conditions to be used for combustion applications.

In the present work, one jet fuel surrogate (n-dodecane) which has been recognized as the constituent of real jet fuel is studied and thermophysical properties of each is evaluated in the supercritical regime. Correlation has been developed for two transport properties namely density and viscosity at the critical pressure and a range of temperatures (T_C + 100 K). Further, to confirm the reliability of the developed correlations, two statistical parameters have been evaluated and which explains an outstanding accord among the data obtained from NIST software program [18] and the correlated property values. It has been concluded from the study that while using supercritical fluids in jet engines, there is no need to maintain such high pressures while injection of fuel as they are held in conventional jet engine design. Due to exclusion of fuel vaporization process, the augmentation in mixing of fuel-air mixture, momentous enhance in engine efficiency and concurrent

decline in harmful emissions like CO, CO_2, NO_x, PM, aldehydes and Polycyclic Aromatic Hydrocarbons (PAHs) are expected.

2. Estimation of thermophysical properties of diesel fuel surrogates (DFS)

Vapour-liquid critical temperature (658.25 K) and pressure (1.806 MPa) for n-Dodecane (C12H26) is available in the literature. The property data at critical point of n-Dodecane is exported from the NIST software program SUPERTRAPP [21] which was used to calculate the transport properties such as density and viscosity of the Diesel Fuel Surrogates (DFS). This program is based on the most consistent pure fluid and mixture models currently available. Fig. 1 (a) shows density variation of n-dodecane with temperature at various pressures in the supercritical regime. It can be noticed that as temperature increases a drastic decrease in density is experienced by n-dodecane. It is also to be observed that as pressure increases, the density of the surrogate fuel increases which will affect the flame speed. The decrease in density is due to the fact that with respect to temperature increase the molecular kinetic energy is found to increase which leads to increase in specific volume of the fluid in supercritical regime. Fig. 1(b) shows the viscosity variation of the n-dodecane as a function of temperature at various pressures in the supercritical regime. It can be observed that there is a reduction in the viscosity of DFS with the increase in temperature under the constant pressure condition. From the plots it can be noticed that both the properties suffer from abrupt changes with respect to temperature at critical pressure. A significant drop in viscosity has been observed up to 20 K temperature above the critical point for all the pressures. It is also to be noted that with an increase in pressure the viscosity of DFS increases resulting in higher frictional losses while flowing through the channels and it can also affect the shear boundary layer which in turn the mixing

process before actual combustion. Such trends are also observed in case of DFSs investigated in the past [13,16]. However, the range of the pressures considered by Ronghong Lin [8] is 10–100 MPa whereas in the present work the same ranges from 1.806 MPa to 2.806 MPa just above the supercritical region which is comparatively in accordance with the studies done in the past [16].

3. Development of correlations

Initially, at critical pressure variation of properties as a function of temperature, for DFS (n-dodecane) has been plotted. After visualizing the plots, a severe variation in both transport properties has been observed. Therefore it becomes moreover complex to fit the curve through a single correlation, in results piecewise modelling is done to estimate the properties with highest accuracy and least standard errors. Basically, in this study Dose Response (DoseResp) (Eq. (1)) model has been employed in order to estimate the thermophysical properties.

$$transport\,property\,(\rho,\,\mu) = a_1 + \frac{(a_2 - a_1)}{1 + 10^{(T_0 - T)p}} \qquad (1)$$

Where T is temperature measured in K and all others are constants. Values of constants are tabulated in Table 1. The correlations have been developed for n-dodecane (C12H26) at critical pressure (1.806 MPa) and for a temperature range of (658.25–

Table 2
AARE (%) and SAR Values.

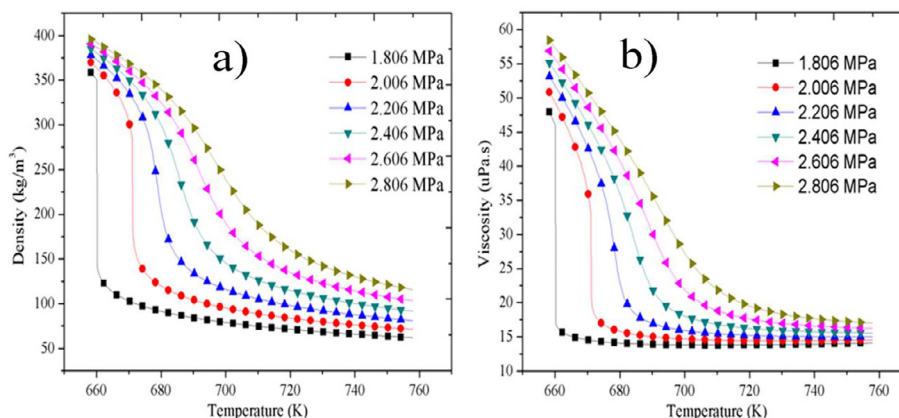| DFSs	n-Dodecane	
Data Points (1996)	AARE	SAR
Density	0.47	761.24
Viscosity	0.031	9.15

Fig. 1. (a) and (b) Variation of density and viscosity of n-dodecane as a function of temperature at various pressures.

Table 1
Correlation coefficients for density of n-dodecane for curve fit.

n-dodecane	Correlation Coefficients			
Temperature Range	a_1	a_2	T_0	p
Density (kg/m^3)				
658.25–660.1 K	125.967	397.337	672.261	−0.05566
660.15–670.15 K	100.4163	122387.4	626.8139	−0.10497
670.2–758 K	56.86815	46266.59	367.8166	−0.01
Viscosity (µPa-s)				
658.25–660.1 K	16.21199	58.11392	666.6822	−0.05866
660.15–665.15 K	14.98101	9751.912	643.5134	−0.22169
665.2–705.2 K	13.77528	1916.819	586.5604	−0.04043
705.25–758 K	13.77594	14.28758	748.4478	0.03141