ANALYTICAL ESTIMATION FOR TEMPERATURE DEPENDENT TRANSPORT PROPERTIES OF SUPERCRITICAL JET FUEL SURROGATE

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ABSTRACT

Supercritical fluid technology finds its application in almost all engineering aspects in some 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 (JFS) i.e. n-dodecane which has been recognized as the constituent of real jet fuel is studied and transport 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 (Tc+100K). Further, to endorse the reliability of the developed association, two arithmetical parameters have been evaluated and which illustrates an...
outstanding agreement between the data obtained from online NIST Web-Book and the correlated property values.

**Key words:** Combustion modeling, jet fuels, jet fuel surrogates, transport properties, supercritical jet fuel.


http://www.iaeme.com/IJMET/issues.asp?JType=IJMET&VType=8&IType=7

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 in literature [1]–[11] till now in order to enhance combustion efficiency and to minimize the emissions. Near the supercritical (SC) region, the system properties are highly sensitive to that of pressure and temperature which results in instant variation in physical properties [12]–[15]. Thus, supercritical fluids bring new directions to jet fuel combustion research communities because of their unique property behavior. These fluids have been actively used in various engineering applications[16]–[21] and they have been positively accepted by the research communities due to their excellent properties.

In the present work, one JFS (n-dodecane) which has been recognized as the constituent of real jet fuel is studied and transport 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 +100K). 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 [22] 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, CO₂, NOₓ, PM, aldehydes and Polycyclic Aromatic Hydrocarbons (PAHs) are expected.

2. RESEARCH METHODOLOGY

Vapour-liquid critical temperature (658.25K) and pressure (1.806MPa) for n-Dodecane (C₁₂H₂₆) is available in the literature. The property data at critical point of n-Dodecane is extorted from the NIST software program SUPERTRAPP [22]. NIST software program, SUPERTRAPP was used to calculate the transport properties such as density and viscosity of the JFS. The program SUPERTRAPP is based on the most consistent pure fluid and mixture models currently available

2.1. Variation of Transport Properties

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.

**Figure 1.** Variation of density and viscosity of n-dodecane as a function of temperature at various pressures.

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 JFS with the increase in temperature under the constant pressure condition. A significant drop in viscosity has been observed up to 20K temperature above the critical point for all the pressures. It is also to be noted that with an increase in pressure the viscosity of JFS 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 JFSs investigated by Ronghong Lin [12] and Abhinav and Raja Sekhar [15]. However, the range of the pressures considered by Ronghong Lin [12] is 10-100MPa 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 study done by Abhinav and Raja Sekhar [15].

Fig. 2 shows the property variation in 3D (temperature along x-axis, pressure along y-axis and property along z-axis) for n-dodecane. From the plots it can be noticed that both the properties suffers abrupt change with respect to temperature at critical pressure.
3. RESULTS AND DISCUSSION

3.1. Development of Correlations

Initially, at critical pressure variation of properties as a function of temperature, for JFS (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 transport properties.

\[
\text{transport property } (\rho, \mu) = a_i + \frac{(a_2 - a_1)}{1 + 10^{(T_i - T)_p}}
\]  

Where T is temperature measured in K and all others are constants. Values of constants are tabulated in Table I. The correlations have been developed for n-dodecane (C12H26) at critical pressure (1.806MPa) and for a temperature range of (658.25-758K). Total 1996 data points are plotted for each transport property to fit the curve with higher accuracy.

Fundamentally, along mantissa temperature values are considered and the JFS property is drawn along y-axis at critical pressure in order to fit the curve through piecewise modeling.

3.2. Error Analysis

To appraise the developed correlation, two statistical parameters are used namely Arithmetic Average of the Absolute values of the Relative Errors (AARE %) and Sum of Absolute of Residual (SAR). First parameter defines the accuracy of developed correlations and second shows the reliability of correlations for more dense data points.

\[
AARE\% = \frac{100}{N} \sum_{i=1}^{N} \left| \frac{f_i^{act} - f_i^{cal}}{f_i^{act}} \right|
\]  

\[
SAR = \sum_{i=1}^{N} \left| f_i^{act} - f_i^{cal} \right|
\]
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Here ‘f’ indicates the transport property of the JFS. Table II reports the AARE (%) and SAR of the developed correlation.

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

<table>
<thead>
<tr>
<th>n-dodecane</th>
<th>Correlation Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature Range</td>
<td>$a_1$</td>
</tr>
<tr>
<td>Density (kg/m$^3$)</td>
<td></td>
</tr>
<tr>
<td>658.25-660.1K</td>
<td>125.967</td>
</tr>
<tr>
<td>660.15-670.15K</td>
<td>100.4163</td>
</tr>
<tr>
<td>670.2-758K</td>
<td>56.86815</td>
</tr>
<tr>
<td>Viscosity (μPa-s)</td>
<td></td>
</tr>
<tr>
<td>658.25-660.1K</td>
<td>16.21199</td>
</tr>
<tr>
<td>660.15-665.15K</td>
<td>14.98101</td>
</tr>
<tr>
<td>665.2-705.2K</td>
<td>13.77528</td>
</tr>
<tr>
<td>705.25-758K</td>
<td>13.77594</td>
</tr>
</tbody>
</table>

**Table 2** AARE (%) and SAR Values.

<table>
<thead>
<tr>
<th>JFSs</th>
<th>n-Dodecane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data Points (1996)</td>
<td>AARE</td>
</tr>
<tr>
<td>Density</td>
<td>0.47</td>
</tr>
<tr>
<td>Viscosity</td>
<td>0.031</td>
</tr>
</tbody>
</table>

Percent Relative Error (PRE) is a factor that describes the relative error among the calculated properties by fit for all the JFSs. Fig. 3 shows the variation of Percent Relative Error (RE%) of curve fit for JFS as a function of temperature which is defined in Eq. (4).

$$RE\% = \frac{f_{i}^{act} - f_{i}^{cal}}{f_{i}^{act}} \times 100$$  \hspace{1cm} (4)

Fig. 3 (a) shows that near to critical temperature, error is found to be large (up to 4%) comparatively to the higher temperatures. From Fig. 3 (b), it can be found that the error is very less thus developed correlation estimate viscosity in precisely.
4. CONCLUSIONS

It has been concluded from the present study that there is not much need to maintain high pressures in the common rail while injecting the fuel in supercritical state as they are maintained in conventional engine design. Due to exclusion of fuel vaporization process, the enhancement in fuel-air mixing, momentous increase in engine efficiency and concurrent reduction in harmful emissions like CO, CO₂, NOₓ, SOₓ, PM, aldehydes and Polycyclic Aromatic Hydrocarbons (PAHs) are expected.

REFERENCES


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