Vaporization Performance Study of Pre-atomized Liquid Fuel Sprays in a Crossflow Pre-mixer

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Abstract
Pre-vaporization and pre-mixing are the two main features of LPP type of combustor that operate on liquid fuels. The pre-vaporization length scale is one of its most important design parameters. In this study, the goal is to put forward a simulation based correlation for fuel vaporization performance as a function of dimensionless parameters for crossflow type of injections. Two types of fuels are studied here: jet-A and one of its potential biofuel substitutes, RME. Different sets of spray simulations are considered for crossflow type of injections. Correlations are provided for both Jet-A and RME’s vaporization performance as a function of non-dimensional inlet air temperature, fuel/air momentum flux ratio and normalized spray traverse distance.

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1. Introduction

Lean Premixed and Pre-vaporized (LPP) combustion is well-known for its high efficiency and performance while producing less pollutant. For LPP combustors that operate on liquid fuels, a pre-vaporization duct, called premixer where the liquid fuels are sprayed into hot air-stream is necessary prior to combustion. Homogeneous lean fuel vapor and air mixture is then delivered to the primary reaction zone. Therefore, it is very important to understand the spray dispersion and vaporization dynamics for better premixer designs.

Different liquid fuels normally have very different transport properties (such as density, viscosity, latent heat of vaporization and vapor pressure), which will result in different vaporization characteristics. This could lead to different designs of the premixer, such as the duct length, contraction/expansion ratio, and different spray control parameters, such as spray velocity and spray cone angle. Both single droplet [1-6] and turbulent spray [7-8] vaporization process have been studied extensively in the literature. Abramzon and Sirignano [5] developed a two-dimensional transient droplet vaporization model based on the assumption of Hill’s vortex in the liquid phase. Their model included the effects of variable thermophysical properties, non-unitary Lewis number, effects of Stefan flow, effects of droplet internal circulation and transient liquid heating with vaporization. The details of the mathematical model are given by Sirignano [9]. This vaporization model has been shown to be very accurate for predicting single droplet vaporization [5, 10]. Torres et al. [11] developed an efficient one-dimensional multi-component fuel vaporization model and implemented it into a multi-dimensional CFD code: KIVA-3V. Their efficient computational algorithm showed very promising computational speed for three-dimensional spray simulations while capturing the droplet vaporization rate which compared quite well to the experiment.

To satisfy the compact design requirement for LPP premixer, a common technique is to inject the pre-atomized liquid fuel perpendicularly into the high temperature crossflow air. Gu et al. [12] systematically studied the pre-atomized liquid fuel dispersion and vaporization process in a crossflow premixer for both cold injections and pre-heated injections and showed the importance of transient droplet heating on the droplet vaporization rate. Liquid jet injected into a crossflow of air has been studied extensively in the literature and most of the researchers [13-15] have proposed correlations to predict the liquid jet penetrations based on liquid-to-gas momentum flux ratio. Stenzler et al. [16] extended the liquid jet penetration correlations by including the effects of the aerodynamic Weber number and liquid viscosity based on their experimental studies on different liquids under different crossflow temperatures. However, for a fixed liquid to air momentum flux ratio, compared to continuous liquid jet injection, liquid ejected from the nozzle in the form of pre-atomized droplets will encounter higher total drag forces due to larger total surface areas. Thus, for crossflow injections with pre-atomized sprays, smaller SMD would require higher liquid to air momentum flux ratio in order to attain the same penetrations. Thus, the correlation of liquid jet penetrations summarized from those experiments [13-16] would not apply for pre-atomized liquid injections. In addition, for sprays injected into high temperature crossflow of air, considerable portions of liquids would be vaporized as it penetrate through the air and the loss of liquid momentum will result in further reduction in spray penetrations. The current study proposes a vaporization performance correlation for pre-atomized fuel injections as a function of inlet air temperature, fuel to air momentum flux ratio and spray travel distance from injection point.

2. Computational Model

KIVA-4 code was utilized as the numerical tool for the current study. KIVA is a computer program developed by Amsden et al. [17] from Los Alamos National Laboratory (LANL), and it can be used to solve transient, three dimensional, chemically reacting fluid flows with sprays, where the liquid phase is treated as discrete particles with two-way coupling between two phases. Unlike direct numerical simulations (DNS), the discrete liquid phase is solved with several physical sub-models in order to track its change of location, radius, deformation and temperature without tracking its interface. Most of the physics based sub-models are developed based on the correlations from experiments. The main assumptions for those models are summarized as following: 1-D model is assumed for each droplet by considering it to be spherically symmetric with only variations in radial direction; Fickian diffusion is assumed when the droplet consists of multi-species where each of species have the same diffusion rate; Phase equilibrium is assumed such that Raoult’s law is used to calculate the vapor mass fraction for each vapor species at the gas-drop interface; The important physics sub-models are briefly discussed in this section and more details about KIVA’s mathematical model and numerical algorithms can be found in KIVA-II’s manual [17].

2.1 Physical sub-models

The equation of motion for a single spherical droplet is given by:

$$ \frac{d\mathbf{u}_d}{dt} = \frac{\mathbf{u} + \mathbf{u}_s - \mathbf{u}_d}{\tau} + \mathbf{g} $$

(1)
where $\tau$ is the dynamic relaxation time of the droplet, which is defined as:

$$
\tau^{-1} = \frac{3}{8} \frac{\rho \varepsilon}{\rho' r_d} C_d \left| \mathbf{u} + \mathbf{u}^- - \mathbf{u}_s \right|
$$

where $C_d$ is the viscous drag coefficient, which is defined as:

$$
C_d = \frac{24}{\text{Re}_d (1 + B_d)}
$$

with droplet Reynolds number defined as:

$$
\text{Re}_d = \frac{2 \rho \left| \mathbf{u} + \mathbf{u}^- - \mathbf{u}_s \right| r_d}{\mu_g(\hat{T})}
$$

where $\mu_g$ is the dynamic viscosity of air, which is calculated at the average film temperature defined by $\hat{T} = \left( T_g + 2T_s \right)/3$.

Comparing with the original drag model implemented in KIVA, this drag model incorporated the Stefan flow correction for regimes where strong evaporation will reduce the drag coefficient for the vaporizing droplet as proposed by Renksizbulut and Yuen [18]. This drag model is valid for low droplet Reynolds number in the range of $\text{Re}_d < 30$ [9]. For current co-axial flow applications, the droplet Reynolds number is very small [O(10) initially], and hence this modified drag model is applicable.

For a spherically symmetric droplet with only variations in radial direction, the interface mass conservation condition for each vaporizing fuel species $i$ can be written as:

$$
\rho_u (v_u - \dot{r}_d)(Y_{gs,i} - Y_{ls,i}) + \rho_u D_i \frac{\partial Y}{\partial r} \bigg|_{r_u} + \rho_{gs} D_{gs,i} Sh_{gs,i} \left( Y_{gs,i} - Y_{gs,i} \right) = 0
$$

Summing Eq.(5) over all the fuel species, one can obtain the rate of change of droplet radius:

$$
\dot{r}_d = v_u - \frac{\rho_u}{2 \rho_u r_d} \sum_{\text{fuel}} D_{gs,i} Sh_{gs,i} (Y_{gs,i} - Y_{gs,i})
$$

where $Y_{gs,i}$ is the average vapor mass fraction of fuel species $i$ within the computational cell traversed by the droplet. $Sh_{gs,i}$ is the Sherwood number for fuel species $i$ and is given by:

$$
Sh_{gs,i} = \left( 2.0 + 0.6 \text{Re}_d^{1/3} \text{Pr}_{gs,i}^{1/3} \right) \ln \left( 1 + B_d \right)
$$

where $\text{Pr}_{gs,i} = \frac{\mu_g(\hat{T})c_p(g)}{K_g(\hat{T})}$ is the gas Prandtl number.

### 2.2 One-dimensional equations for discrete droplet phase

Continuity, species transport and energy equations are solved within each droplet with the assumption that those properties only change in the radial direction:

$$
\frac{\partial \rho_i}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho_i v_r \right) = 0
$$

$$
\frac{\partial \left( \rho_i Y_{i,i} \right)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho_i v_r Y_{i,i} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho_i D_i \frac{\partial Y_{i,i}}{\partial r} \right)
$$

The interface condition on droplet surface temperature is determined by the energy balance equation:

$$
\sum_{\text{fuel}} L \rho c_p(\hat{T}) \left( \dot{r}_d - v_r \right) Y_{gs,i} + D_i \frac{\partial Y}{\partial r} \bigg|_{r_u} = k_g \frac{T_g - T_i}{2 r_d} N_u - k_i \frac{\partial T}{\partial r}
$$

where the first term on the right hand side is the heat flux to the droplet interface from the gas side and the second term is the heat flux to the droplet interface from the liquid side, and the difference between the two terms yields the net heat flux at the interface, which should be equal to the heat flux due to vaporization, which is represented by the term on the left hand side of Eq. (8). The Nusselt number is calculated by the Ranz-Marshall correlation [9]:

$$
N_u = \left( 2.0 + 0.6 \text{Re}_d^{1/3} \text{Pr}_{gs,i}^{1/3} \right) \ln \left( 1 + B_d \right)
$$
\[
\frac{\partial(\rho T)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho \nu T\right) = \frac{1}{c_p r^2} \frac{\partial}{\partial r} \left(r^2 k \frac{\partial T}{\partial r}\right)
\]

\[
+ \frac{\rho D}{c_p r^2} \sum_i \left[ \frac{\partial}{\partial r} \left(r^2 h_{i,j} \frac{\partial Y_{i,j}}{\partial r}\right) - h_{i,j} \frac{\partial}{\partial r} \left(r^2 \frac{\partial Y_{i,j}}{\partial r}\right) \right]
\]

To solve for \( \rho_l, \nu, Y_{ls,i}, T \), an additional equation for average liquid density can be written in terms of mass fraction of each species and their density:

\[
\rho_l = \left( \sum_i Y_{ls,i}/\rho_{ls,i} \right)^{-1}
\]

More details on the numerical algorithms to solve the above 1-D liquid phase equations can be found in [12,17].

Once the 1-D liquid phase equations are solved, the mass fraction of each vaporizing species can be determined using Raoult’s law for relatively low ambient pressures. Raoult’s law states that:

\[
p_{gs,i} = X_{b,i} p_{sat,i}(T_s)
\]

where \( p_{gs,i} \) is the partial pressure for fuel species \( i \) at the droplet surface in the gas phase, \( p_{sat}(T_s) \) is the saturation pressure for fuel species \( i \) at droplet surface temperature, \( T_s \), \( X_{b,i} \) is the mole fraction of fuel species \( i \) at the droplet surface in the liquid phase, which can be calculated by:

\[
X_{b,i} = \frac{Y_{b,i}/MW_i}{\sum_{fuel} Y_{b,i}/MW_i}
\]

\[
Y_{gs,i} = \frac{X_{gs,i} MW_i}{\sum_i X_{gs,i} MW_i} = \frac{p_{gs,i} MW_i}{\sum_i p_{gs,i} MW_i}
\]

3. Validation

In this section, comparisons between simulations and experimental data from Dâïff et al. [1] were presented to validate the vaporization model. In our simulation, all the cases are setup with the exact same initial conditions as reported by Dâïff et al. [1]. Unlike in a spray environment, the far field fuel vapor mass fraction was considered to be zero since there were no other droplets vaporizing in the neighborhood, and velocity and temperature of the external air were held constant during the simulations. Moreover, in order to maintain the same physical conditions as in experiments, the droplet velocity was maintained to be zero.

Figure 1 shows comparisons between the simulations and the experiments for single droplets of pure heptane and decane. The computational parameters for both cases are listed in Table 1. The transient change in diameter of both blended and pure decane droplets shows very good agreement with experiments. The validation of the vaporization model as described in this section is extracted from one of our numerical experiments [12] and presented here for completeness.

4. Results and Discussions

The corrupting influence from the momentum and drag coupling on the discrete droplet phase is relatively small for larger droplets and this influence is also small even for small droplets when they are away from the nozzle tip [19]. Thus, for all the subsequent pre-mixer simulations, mono-dispersed spray was adopted with an initial droplet size of 80 micron diameter, which is relatively large but is still within the range of practical sprays. The spray cone angle is fixed at 100°, which is optimum for good spray dispersions.

Two types of liquid fuels are investigated here: Jet-A and RME. Jet-A is the primary conventional fuel used in the aviation industry. RME is a biodiesel which can be blended in jet-A. RME has already been tested in blends with Jet-A fuel as a potential surrogate fuel in the aviation industry [20]. Thus, it is important to study both fuels and compare their vaporization characteristics. Both jet-A and RME are comprised of more than one species with different transport properties. In order to avoid numerical complexity, averaged properties of all the species are used and tabulated in Table 2 such that both fuels can be considered to be single-component fuels. Since the fuel vapor pressure is an important parameter for the liquid fuel vaporization process, it is plotted versus temperature for both fuels and is shown in Figure 2. The properties of Jet-A fuel are taken from the tabulated data of KIVA-4 fuel library while RME’s properties are used from reference [10]. It can be seen that vapor pressure is a monotonically increasing function of temperature for both fuels. Vapor pressures for both Jet-A and RME are very low at room temperature, indicating that both of them are non-volatile in nature.

4.1 Computational Setup for Crossflow Premixer

The computational domain in Figure 3 represents a typical simplified version of rectangular pre-mixer with a length of 300 mm and 60mm x 60mm cross-section. The pre-mixer has six bounding surfaces with the following set of boundary conditions: the left side is assigned as velocity inlet boundary condition with fixed velocity and temperature and the right side is pressure outlet boundary condition. All other surfaces are assigned law-of-wall boundary conditions. To resolve the boundary layer, the resolution of the computational grid is chosen such that \( y^+ \) is less than 300. Figure 3 also
shows the contour plot of the gas phase velocity in the streamwise direction at two cross-sectional planes of Z=70 mm and Z=230 mm respectively. The two-way coupling effects can be clearly observed from the velocity contour plot where the velocity near the center of slice decreased due to the inter-phase drag from the discrete droplet phase.

4.2 Spray Simulation Results and Analysis

The main purpose of this study is to quantify the vaporization performance for each fuel under different operation conditions. To achieve this, the fuel vapor mass flow rate at the outlet is calculated since it indicates how much percentage of the liquid fuel has been vaporized through the pre-mixer chamber. The fuel vapor mass flow rate at the outlet can be calculated as:

\[ \dot{m}_v = \sum \rho v z A \]  \hspace{1cm} (20)

where index c represents each computational cell at the outlet. Most of the variables, such as density, pressure and temperature are all cell-centered in KIVA-4. But velocities in KIVA-4 solver are all nodal values. Thus, the cell-centered value for \( V_z \) is calculated by averaging over all the neighboring nodes for each cell.

In order to have a comprehensive view of cross-flow vaporization performance dependencies on different parameters, such as inlet air temperature, fuel/air momentum flux ratio and spray travel distance from injection point, several different sets of simulations were conducted in this section.

Three important dimensionless parameters are defined here,

1. Fuel/air momentum flux ratio is defined as,
\[ qFa=\frac{(\rho_F \times u_F^2)}{(\rho_{air} \times u_{air}^2)} \]

2. Fuel air temperature difference in dimensionless form, \( T_{e}=\frac{(T_{air} - T_f)}{T_f} \)

3. Traverse distance in dimensionless form, \( z^*=(z-z_0)/L \)

Thus, the fuel vaporization performance could be a very complex function, \( vp(\%) = f(T_d, qFa, z^*) \), with three independent variables.

In order to study the separate effects, the fuel vaporization performance needed to be compared at a fixed fuel/air momentum flux ratio for different inlet air temperatures, and vice versa. To fix the fuel/air momentum flux ratio at different inlet air temperatures, the fuel injection velocity is varied at different inlet air temperatures to compensate the change of the air density. Meantime, since the inlet air mass flow rate will also change due to density change at different temperatures, the fuel injection mass flow rate is also varied in order to maintain a constant stoichiometric ratio between the air and the fuel. For this study, air/fuel stoichiometric ratio is fixed at 17.3, giving the equivalence ratio to be 14.7/17.3=0.85, which is a reasonable value for lean combustions. For jet-A, the fuel/air momentum flux ratio is 73.3 when inlet air temperature is 800k and fuel injection velocity is 2m/s, which corresponds to the baseline test parameters.

Table 3 and Table 4 summarized the values for all the important parameters used for both fuels during the subsequent simulations. The inlet air temperature is varied from 400k to 800k with 50k increment, and fuel/air momentum flux ratio is fixed at three different levels, 33.3, 73.3 and 113.3. Both parameters are varied in a relatively large range in order to clearly show their influence on the fuel vaporization performance. Figure 4 shows the fuel trajectories at three different levels of fuel/air momentum ratios to illustrate how the spray is dispersed throughout the premixer.

Figure 5 plots the jet-A fuel vapor mass fraction along the pre-mixer channel at different inlet air temperatures from 400k~700k. At each temperature, one can observe that the fuel vapor mass fraction increases with increase in the fuel/air momentum flux ratio. The fuel vapor mass fraction reached a maximum value of 0.016, 0.037, 0.048 and 0.053 at the premixer exit for inlet air temperatures varying from 400k to 700k. Since air-fuel stoichiometric ratio is fixed at 17.3, the maximum fuel vapor mass fraction would be \( 1/(1+17.3)=0.055 \), which is evident from Figure 5d where it shows that jet-A almost completely vaporizes at the pre-mixer exit.

First, the total vaporization performance for jet-A fuel was summarized at different simulation conditions, as shown in Figure 6a, where one can observe jet-A’s total vaporization performance versus the dimensionless temperature, \( T_d \) at three different fuel/air momentum flux ratios. By curve fitting the data at qF/air=73.3, the fuel vaporization performance can be expressed as a function of the dimensionless temperature, \( T_d \). We found that a third order polynomial function fits very well with the simulation data, expressed as:

\[ vp(\%) = a_0 T_d^3 + a_1 T_d^2 + a_2 T_d + a_3 \]  \hspace{1cm} (21)

where \( a_0=-12.252, a_1=91.790, a_2=28.850, a_3=-27.279 \).

As seen from both Figure 5d and Figure 6, the effect of fuel/air momentum flux ratio on the fuel vaporization performance is relatively weak since jet-A almost completely vaporized at air temperature of 700k. Thus, those data at such high air temperature were excluded for fitting the correlation function when considering the effects of fuel/air momentum flux ratio on the fuel vaporization performance. To compensate the effect of momentum flux ratio on fuel vaporization performance and fit the data onto the previous curve-fitted
function, a weighting coefficient is applied to all the scattered data, which is expressed as: \([q_{Fa}] / [q_{Fa}]_{ref}\)^n, where \([q_{Fa}]_{ref}\) is the reference fuel/air momentum flux ratio, chosen to be 73.3 in this case, and the power coefficient \(n\) is adjusted such that a best fit curve could be generated. By tuning \(n\) to be 0.21, all the scattered data fit quite well with the fitting function, which is plotted in Figure 6b. Thus, the jet-A’s total vaporization performance can be summarized as a function of dimensionless supplying air temperature, \(T_d\), and fuel/air momentum flux ratio, \(q_{Fa}\):

\[
vp(\%) = (a_1 T_d^3 + a_2 T_d^2 + a_3 T_d + a_0)^n \frac{(q_{Fa})}{73.3}^n
\]  
(22)

Furthermore, it is also important to predict jet-A’s vaporization performance at different travel distances, two cross-sectional data was monitored where \(z^*=0.6\) and \(z^*=0.8\). Smaller travel distance was not considered due to low vapor mass fractions. As before, a simple weighting function was applied to both cross-sections with the following functional form:

\[
vp(\%) = (a_1 T_d^3 + a_2 T_d^2 + a_3 T_d + a_0)^n \left(\frac{z^*}{73.3}\right)^n
\]  
(23)

We found that by tuning \(p=0.558\), the simulation data fit quite well with Eq. (23), which is shown in Figure 7. From the fitting function, one can approximate the Jet-A’s vaporization performance at specified inlet air temperatures, fuel/air momentum flux ratios and spray travel distances.

Since the vapor pressure of RME is much lower than jet-A, it was expected that higher inlet air temperature is needed for RME. It was found that the total vaporization performance for RME is only 5% when the inlet air temperature is 500K. Thus, to summarize a correlation function for RME, the inlet air temperature was chosen to be in the range of 550K to 800K, with 50K increment for each simulation. Figure 8 shows the RME vapor mass fractions along pre-mixer at different inlet air temperatures and fuel/air momentum flux ratios. Using a similar curve-fitting procedure for jet-A, a third order polynomial function fits the simulation data very well at \(q_{Fa}=73.3\) for RME’s total vaporization performance, which is shown in Figure 9a. However, to include the effects of fuel/air momentum flux ratio, we found that a simple weighting function couldn’t fit well with the simulation data. In this case, two constraining power functions were assumed with respect to \(q_{Fa}\):

\[
vp(\%) = a_1 T_d^3 + a_2 T_d^2 + a_3 T_d + a_0
\]

\[
\left(\frac{q_{Fa}}{33.3}\right)^{b_1} + \left(\frac{q_{Fa}}{33.3}\right)^{b_2}
\]

where \(a_1=34.027, a_2=-216.888, a_3=-81.046, b_1=-5.541, b_2=0.314\). Figure 9b shows that the proposed function fits very well with all the simulation data for RME’s total vaporization performance at different inlet air temperatures and fuel/air momentum flux ratios. Furthermore, to predict RME’s vaporization performance at different cross-sections, the following functions was proposed based on two cross-sectional data where \(z^*=0.6\) and \(z^*=0.8\).

\[
vp(\%) = \{a_1 T_d^3 + a_2 T_d^2 + a_3 T_d + a_0\}
\]

\[
\left(\frac{q_{Fa}}{33.3}\right)^{b_1} + \left(\frac{q_{Fa}}{33.3}\right)^{b_2}\}

\]

\[
(z^*)^c_1 (T_d)^{1-c_1/c_2}
\]

Where \(c_1=1.15, c_2=0.78\). Thus, this function is equivalent to Eq. (24) when \(z^*=1\). As shown in Figure 10, Eq. (25) fits the simulation data quite well at those two cross-sections.

5. Conclusion

Jet-A and RME was studied on their vaporization performance characteristics under different parameters, among which the inlet air temperature, fuel/air momentum flux ratio and spray travel distance are most important. At each inlet air temperature, three different fuel/air mass flux ratios are simulated, where \(q_{Fa}=73.3\) corresponds to the fuel/air momentum flux ratio at 2m/s of fuel injection velocity and 800K of inlet air temperature. It was found that at high inlet air temperatures, the effect of fuel/air momentum flux ratio on the fuel total vaporization performance is relatively weak while the effect is strong at low inlet air temperatures. Next, the scattered data of fuel vaporization performance at different levels of inlet air temperatures, fuel/air momentum flux ratios and cross-sections are curve-fitted step-by-step to form a correlation function, which can be used to approximate the fuel vaporization performance at specified inlet air temperature, fuel/air momentum flux ratio and spray travel distance.

**Nomenclature**

- \(a_d\): Droplet acceleration
- \(B_d\): Global Spalding mass transfer number
- \(C_D\): Droplet drag coefficient
- \(c_{pg}\): Specific heat of gas phase
- \(c_{pl}\): Specific heat of liquid phase
- \(D_{gi}\): Vapor mass diffusivity of ‘i’th species into gas phase
Dl Liquid mass diffusivity within the droplet

$g$ gravitational acceleration

$h_{i,i}$ Specific enthalpy of species $i$ in the liquid phase

$k_g$ thermal conductivity of gas phase

$k_{gs}$ thermal conductivity of gas phase at the droplet surface

$k_l$ thermal conductivity of liquid phase

$L$ Length from fuel injection point to the exit

$L_i$ Latent heat of vaporization of species $i$

$m_d$ Droplet mass

$m_{d}$ Droplet vaporization rate

$\dot{m}_d$ Droplet vaporization rate

$MW_v$ Molecular weight of fuel vapor

$Nu_g$ Nusselt number for gas phase

$Pr_g$ Prandtl Number for gas phase

$P_{atm}$ Atmosphere pressure on which the fuel boiling temperature is based

$P_g$ Pressure of surrounding gas phase

$P_{gs,i}$ Partial pressure of fuel species $i$ at droplet surface

$P_{sat,i}$ Saturation pressure of fuel species $i$

$q_{Fa}$ Fuel/air momentum flux ratio

$\mathcal{T}_d$ Instantaneous droplet radius

$Re_d$ Reynolds number of the droplet exposed to external gas flow

$Sh_{g,i}$ Sherwood number for species $i$

$Sc_{g,i}$ Schmidt number for species $i$

$t$ Time

$\mathcal{T}$ Film temperature

$T_d$ Dimensionless inlet air temperature

$T_s$ Droplet surface temperature

$T_g$ Gas phase temperature

$u$ Mean gas phase velocity

$u'$ Turbulent gas phase velocity

$u_d$ Droplet velocity

$v_{ls}$ Liquid velocity at the droplet surface

$V_{pj}$ Volume of droplet ‘$j$’

$A_{pj}$ Surface area of droplet ‘$j$’

$X_{gs,i}$ Vapor mole fraction of species $i$ at droplet surface

$X_{hs,i}$ Liquid mole fraction of species $i$ at droplet surface

$Y_{gs,i}$ Vapor mass fraction of species $i$ at droplet surface

$Y_{hs,i}$ Liquid mass fraction of species $i$ at droplet surface

$Y_{li}$ Liquid mass fraction of species $i$ within the droplet

$z_0$ z coordinate of fuel injection point

$z^*$ Dimensionless spray travel distance in z direction

$\mu_g$ Dynamic viscosity of gas phase

$\rho_g$ Density of the gas phase

$\rho_{gs}$ Density of the gas phase at the droplet surface

$\rho_l$ Density of the liquid phase

References


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<tr>
<th>Fuel Name</th>
<th>Jet-A</th>
<th>RME</th>
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<td>653</td>
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**Table 1**: Summary of experiment conditions of evaporating droplet from Dāif et al. [1]

<table>
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<tr>
<th>Inlet air temperature (K)</th>
<th>Inlet air velocity (m/s)</th>
<th>Inlet air mass flow rate (g/s)</th>
<th>Fuel injection mass flow rate (g/s)</th>
<th>Fuel injection velocity (m/s)</th>
<th>Fuel injection velocity (m/s)</th>
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<td>10</td>
<td>19.5</td>
<td>1.13</td>
<td>1.5</td>
<td>2.22</td>
<td>2.76</td>
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<tr>
<td>700</td>
<td>10</td>
<td>18.1</td>
<td>1.05</td>
<td>1.44</td>
<td>2.14</td>
<td>2.66</td>
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</table>

**Table 2**: Properties of Jet-A and RME

<table>
<thead>
<tr>
<th>Inlet air temperature (K)</th>
<th>Inlet air velocity (m/s)</th>
<th>Inlet air mass flow rate (g/s)</th>
<th>Fuel injection mass flow rate (g/s)</th>
<th>Fuel injection velocity (m/s)</th>
<th>Fuel injection velocity (m/s)</th>
<th>Fuel injection velocity (m/s)</th>
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<tbody>
<tr>
<td>550</td>
<td>10</td>
<td>23.1</td>
<td>1.34</td>
<td>1.56</td>
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<td>2.86</td>
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<tr>
<td>600</td>
<td>10</td>
<td>21.1</td>
<td>1.22</td>
<td>1.49</td>
<td>2.21</td>
<td>2.75</td>
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<tr>
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<td>1.43</td>
<td>2.13</td>
<td>2.64</td>
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<tr>
<td>700</td>
<td>10</td>
<td>18.1</td>
<td>1.05</td>
<td>1.38</td>
<td>2.05</td>
<td>2.55</td>
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<tr>
<td>750</td>
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<td>16.94</td>
<td>0.98</td>
<td>1.33</td>
<td>1.98</td>
<td>2.46</td>
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<tr>
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<td>15.88</td>
<td>0.92</td>
<td>1.29</td>
<td>1.92</td>
<td>2.38</td>
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**Table 3**: Summary of Jet-A parametric studies

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>a₀</th>
<th>a₁</th>
<th>a₂</th>
<th>a₃</th>
<th>n</th>
<th>p</th>
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<tbody>
<tr>
<td>Jet-A</td>
<td>-12.2515</td>
<td>91.7896</td>
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<td>-216.888</td>
<td>281.6537</td>
<td>-81.0458</td>
<td>-5.54149</td>
<td>0.31412</td>
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</table>

**Table 4**: Summary of RME parametric studies

**Table 5**: Summary of coefficients of curve-fitting function for both fuels
Figure 1: Comparisons between the model and the experiment data for single droplet vaporization
Figure 2: Vapor pressure versus temperature for Jet-A and RME

Figure 3: 3-D view of Computational domain with converged velocity field
Figure 4: RME fuel trajectories projected onto X-Z plane for qFa=33.3,73.3,113.3
Jet-A vapor mass fraction along the channel (T_{air}=400K)

Jet-A vapor mass fraction along the channel (T_{air}=500K)
**Figure 5:** Jet-A vapor mass fraction along the pre-mixer at $q_F = 33.3, 73.3, 113.3$, a) $T_{air} = 400K$, b) $T_{air} = 500K$, c) $T_{air} = 600K$. d) $T_{air} = 700K$
Figure 6: Jet-A total vaporization performance vs dimensionless inlet air temperature at \(qFa=33.3, 73.3, 113.3\)

a) original simulation data  
b) weighted simulation data for \(qFa=33.3, 113.3\)
Figure 7: Jet-A vaporization performance vs dimensionless inlet air temperature at $q_{Fa}=33.3, 73.3, 113.3$ a) weighed simulation data at $z^*=0.6$ b) weighed simulation data at $z^*=0.8$
Figure 8: RME vapor mass fraction along the pre-mixer at $q_{Fa}=33.3, 73.3, 113.3$, a) $T_{air}=600\text{K}$, b) $T_{air}=700\text{K}$, c) $T_{air}=800\text{K}$
Figure 9: RME total vaporization performance vs dimensionless inlet air temperature at qFa=33.3, 73.3, 113.3 a) simulation data with curve fit at qFa=33.3 b) simulation data with curve fit for qFa=33.3, 113.3
Figure 10: RME vaporization performance vs dimensionless inlet air temperature at $q_{Fa}=33.3, 73.3, 113.3$ a) simulation data with curve fit at $z^*=0.6$ b) simulation data with curve fit at $z^*=0.8$