Multicomponent Fuel Vaporization at High Pressures

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Abstract
We extend our multicomponent fuel model to high pressures using a Peng-Robinson equation of state, and implement the model into KIVA-3V. Phase equilibrium is achieved by equating liquid and vapor fugacities. The latent heat of vaporization and fuel enthalpies are also corrected for at high pressures. Numerical simulations of multicomponent evaporation are performed for single droplets for a diesel fuel surrogate at different pressures.

1 Introduction

Predicting combustion performance in engines depends on predicting spatial and temporal variations in liquid fuel vaporization. Predicting droplet vaporization at high pressures is important in diesel engines where pressures can exceed critical pressures of hydrocarbons. While single component droplet vaporization at elevated pressures has been studied extensively (e.g. [1]-[4]) less is known about multicomponent droplet vaporization at elevated pressures. Raoult’s law, which applies at standard pressures, is no longer valid at high pressures. Jin and Borman [5] use a Redlich-Kwong equation of state to study a high pressure vaporization of a binary pentane and octane droplet. Stengele, et. al. [6] compare experimental and theoretical results of two component droplet vaporization under high pressure.

Our model shares many of the same features as [5] and [6]. The inert gas species is assumed soluble in the liquid fuel, liquid side interior diffusion is tracked, and the gas side gradients are modeled with Nusselt and Sherwood numbers. We use a Peng-Robinson [7] equation of state to compute the phase equilibrium at the droplet interface and correct the latent heat of vaporization and enthalpy for high pressure. The model is an extension of the multicomponent model developed in [8] and [9] for standard pressures. Unlike [5] and [6] however, we embed our algorithm in KIVA-3V, with the hope of performing
full spray simulations in engines once the gas dynamics in KIVA-3V have been generalized to high pressures.

The rest of the paper is divided into the following sections. Section 2 gives some of the equations solved to model evaporation in spray droplets. Section 3 discusses phase equilibrium, latent heat and enthalpy corrections at high pressure. Section 4 compares single droplet evaporation using Raoult’s law and a Peng-Robinson equation of state at different pressures. Section 5 concludes, and section 6 gives the nomenclature.

2 Interfacial constraints

For a spherically symmetric droplet, we have an interface condition for fuel species $i$,

$$
\rho_s (v_s - r_s')(Y_{g,i} - Y_{l,i}) + \rho_s D_l \frac{\partial Y_i}{\partial r} |_{r_s} - \rho_g D_{gi} S h_{gi} \left( \frac{Y_{g,i} - Y_{g,i}}{2r_s} \right) = 0,
$$

(1)

an equation for the surface regression rate,

$$
r'_s - v_s = \frac{\rho_g \sum_{i,j=1} D_{gi} S h_{gi} (Y_{g,i} - Y_{g,i})}{2\rho_s r_s (1 - Y_{g,i})},
$$

(2)

and an interface condition on temperature

$$
\sum_{j_{gas}} L_{j_{gas}} \rho_{j_{gas}} \left[ (r'_s - v_s) Y_{j_{gas},i} + D_l \frac{\partial Y_{j_{gas},i}}{\partial r} |_{r_s} - \lambda_{j_{gas}} \frac{\partial T}{\partial r} |_{r_s} + \lambda_{j_{gas}} N u_y \frac{T_{\text{gas}} - T_s}{2r_s} \right] = 0,
$$

(3)

where $r'_s = v_s = \frac{d r_s}{d t}$ is the time rate of change of the droplet radius. These equations are coupled to a conservation of mass equation for each species and an energy equation within the interior of the droplet using an interior discretization [9].

3 Phase Equilibrium

At atmospheric pressures, one can express $Y_{g,i}$ in terms of $Y_{l,i}$ using Raoult’s law. Raoult’s law states,

$$
p_{g,i} = X_{l,i} \rho_{vap,i},
$$

(4)

where $p_{g,i}$ is the partial pressure of species $i$ in the gas phase at the droplet surface, $X_{l,i}$ is the mole fraction of species $i$ in the liquid phase at the droplet surface, and $\rho_{vap,i}$ is the equilibrium vapor pressure for a pure species $i$ at
surface temperature, $T_s$. The quantities $X_{i,t}$ and $Y_{g,s,i}$ are determined from the relationship between mole and mass fractions

$$X_{i,t} = \frac{Y_{i,t}}{\sum_j Y_{j,t}} \quad Y_{g,s,i} = \frac{X_{g,s,i} W_i}{\sum_j X_{g,j} W_j}$$

(5)

where $W_i$ is the molecular weight of species $i$.

At higher pressures, one must use an equation of state to determine phase equilibrium. We employ the Peng-Robinson equation of state,

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b) + b(V-b)}$$

(6)

where

$$a = \sum_{i=1}^{N} \sum_{j=1}^{N} X_i X_j a_{ij}, \quad b = \sum_{i=1}^{N} X_i b_i, \quad a_{ij} = (1 - k_{ij})(a_i a_j)^{\frac{1}{2}},$$

$$a_i(T) = 0.45724 \frac{R^2 \rho c^2}{P_{tc}} \alpha_i(T_i, \omega_i), \quad b_i = 0.07780 \frac{RT_i c}{P_{tc}},$$

$$\alpha_i = 1 + m_i(1 - T_i^{\frac{1}{2}}), \quad m_i = 0.37464 + 1.54226 \omega_i - 2.6992 \omega_i^2.$$ (9)

Here $T_{ic}$ is the critical temperature for species $i$, $P_{tc}$ is the critical pressure for species $i$, $T_i = \frac{T}{T_{ic}}$ is the reduced temperature, $\omega_i$ is the acentric factor, and $k_{ij}$ is the interaction parameter for species $i$ and $j$.

Mole fractions on the gas side are calculated from mole fractions on the liquid side by equating liquid and vapor fugacities,

$$f_i^v = f_i^l.$$ (10)

4 Results

Figure 1 shows calculations comparing droplet lifetimes of a diesel surrogate (62.5% n-decane, 37.5% α-methyl naphthalene) [12] using Raoult’s law and Peng-Robinson at different pressures. A 1 mm droplet initially at 363K evaporates in a fixed 400K ambient temperature. We see that while the droplet lifetimes are similar for 1 bar, the difference in droplet lifetime grows as the pressure increases. Raoult’s law overestimates the droplet lifetime at high pressures.

We also show a full 3D engine calculation for a gasoline direct injection engine experimentally studied at Sandia National Laboratory by Dick Steeper. The spray is injected at -90 CAD before top dead center at a 74° cone angle into a cylinder pressure of approximately 2 bars. The injection velocity is 10,900 $\frac{m}{s}$ and the fuel temperature is 90°C. The spray is represented by 2000 spray
droplets each with a droplet radius of 38 μm. A total of 14.4 milligrams of fuel is injected for an injection duration of 1.47 milliseconds. Since the pressures are relatively low, we do not employ the high pressure corrections for this calculation. We compare a multicomponent seven species fuel blend (synfuel - a gasoline surrogate [13]) to the single component “KIVA gasoline”, previously used by KIVA-3V to model gasoline. The seven species fuel is composed of by mass 24.23% cyclohexane, 19.11% iso-octane, 17.35% toluene, 17.03% isopentane, 12.71% ethylbenzene, 8.49% n-decane, and 1.08% naphthalene. Figure 2 plots two perpendicular cross sections which show the total vapor fuel mass fraction contours at −80° CAD and −70° CAD before top dead center. The left hand plots show the synfuel contours and the right hand plots show the KIVA gasoline contours. We note the higher concentration of the KIVA fuel vapor cloud, which shows that KIVA gasoline evaporates more quickly than synfuel.

5 Conclusion

We have implemented a high pressure multicomponent fuel evaporation algorithm into KIVA-3V. The high pressure algorithm currently uses the Peng-Robinson equation of state to calculate the phase equilibrium by equating liquid and vapor fugacities and corrects for latent heats and enthalpies at high pressures.

Preliminary results show that Raoult’s law overestimates droplet lifetimes at
Figure 2: Top left: Total fuel vapor mass fraction contours for synfuel in a 3D GDI engine at $-80^\circ$ CAD before top dead center. Top right: Fuel vapor contours for KIVA gasoline at $-80^\circ$ CAD. Bottom left: Contours for synfuel at $-70^\circ$ CAD. Bottom right: Contours for KIVA gasoline at $-70^\circ$ CAD. KIVA gasoline fuel vapor is more concentrated near the spray axis than synfuel.
high pressures when compared to Peng-Robinson. We hope to soon implement a general equation of state into the gas dynamics and perform full 2D and 3D spray calculations.

6 Nomenclature

Symbols

\begin{align*}
D & \quad \text{Mass diffusion coefficient} \\
f & \quad \text{fugacity} \\
k_{ij} & \quad \text{Peng-Robinson interaction parameter} \\
L & \quad \text{Latent heat of vaporization} \\
Nt_{bg} & \quad \text{Gas Nusselt number} \\
p & \quad \text{Pressure} \\
p_{\text{vap}} & \quad \text{Pure species vapor pressure} \\
r_s & \quad \text{Droplet radius} \\
r_s' & \quad \text{Time rate of change of droplet radius} \\
R & \quad \text{Universal Gas constant} \\
Sh_{bg} & \quad \text{Gas Sherwood number}
\end{align*}

Subscripts

- $i$ \quad \text{Species } i \\
- $g_s$ \quad \text{Gas phase at droplet surface} \\
- $i_C$ \quad \text{Critical} \\
- $g_\infty$ \quad \text{Gas phase in droplet cell} \\
- $i_R$ \quad \text{Reduced} \\
- $l$ \quad \text{Liquid phase} \\
- $g$ \quad \text{Gas phase} \\
- $l_s$ \quad \text{Liquid phase at droplet surface}

References


