Numerical Simulation for Evaporating Fuel Spray of Ethanol-Fuel Blends with taking into account the Vapor-Liquid Equilibrium

Background and Objective

- Alcohols are promising alternative to fossil fuels because it can be produced from biomass resources
- Alcohol-fuel blends are azeotrope and have unique vapor-liquid equilibrium characteristic different from blends composed of aliphatic hydrocarbons
- Incorporate a vapor-liquid equilibrium (VLE) calculation available for alcohols-fuel blend into 3D-CFD code
- Develop an understanding of effects of VLE characteristic on evaporation process in a fuel spray as well as the effect of the latent heat of vaporization, (LHV) especially for ethanol-fuel blends

Vapor-Liquid Equilibrium

- The VLE calculation code is developed principally based on predictive Soave-Redlich-Kwong method [1]
- The VLE satisfies the following relation:

$$y_i\phi_i^V = x_i\phi_i^L \qquad (i=1,2,\ldots,n)$$

where the fugacity coefficients for liquid and vapor phases are calculated as follows:

$$\ln\phi_i = \frac{b_i}{b}\left(\frac{pv}{RT}-1\right) - \ln\frac{p(v-b)}{RT} - \ln\left(\frac{v+b}{v}\right)\left[\frac{1}{A_1}\left(\ln\gamma_i + \ln\frac{b}{b_i} + \frac{b_i}{b} - 1\right) + \frac{a_i}{b_i RT}\right]$$

where the volume v is determined by the cubic Soave-Redlich-Kwong equation of state:

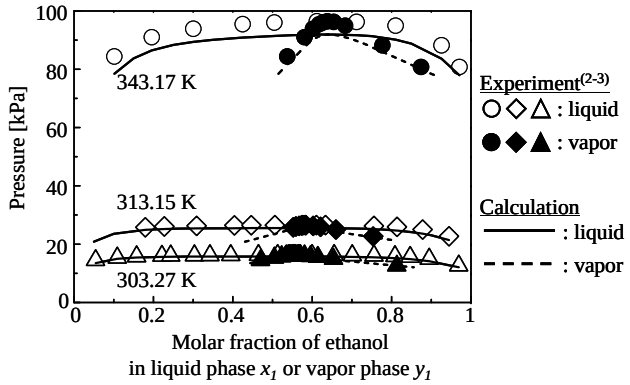
$$p = \frac{RT}{v-b} - \frac{a}{v(v+b)}$$

the parameters a and b in the mixture are determined by the modified Huron-Vidal 1st order model and the linear mixing rule as follows:

$$a = b\left\{\sum_{i=1}^{n} x_i \frac{a_i}{b_i} + \frac{RT}{A_1}\left(\sum_{i=1}^{n} x_i \ln\gamma_i + \sum_{i=1}^{n}\ln\frac{b}{b_i}\right)\right\} \qquad b = \sum_{i=1}^{n} x_i b_i$$

The activity coefficients γ_i are calculated by the UNIFAC method with the group interaction parameter replaced by a cubic function of temperature [1].

- The calculated results for n-heptane-ethanol system capture the azeotropic behavior are in good agreement with experiments [2,3] as shown below.



Calculation Condition

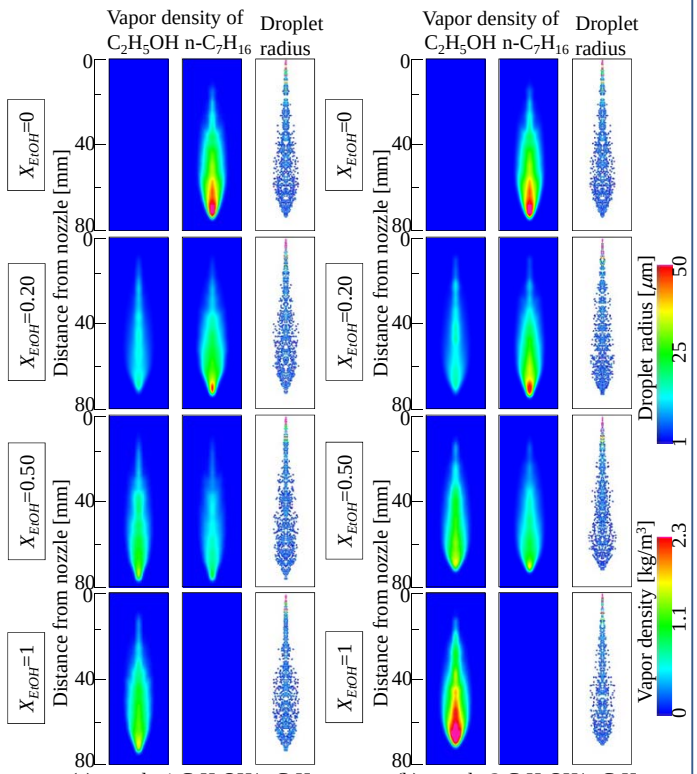
- The above calculation code was incorporated into "multi-component model"[4] developed basd on KIVA3V, and was used for calculating the VLE of fuel components and nitrogen as an ambient gas
- The ambient pressure of 1.51 MPa, temperature of 600 K and the injection pressure of 15 MPa were set
- To isolate the effect of the VLE characteristic and the LHV, the two blends are calculated:

"Pseudo-1 C_2H_5OH-n-C_7H_{16} blends" which take into account the VLE and the LHV of C_2H_5OH but pseudo-1 C_2H_5OH is assumed to have transport properties (density, viscosity, surface tension, etc) identical with n-C_7H_{16}

"Pseudo-2 C_2H_5OH-n-C_7H_{16} blends" which take into account the VLE of C_2H_5OH but pseudo-2 C_2H_5OH is assumed to have transport properties and the LHV identical with n-C_7H_{16}

Results

- Ethanol evaporates faster than n-heptane when the mixing fraction is not significant, e.g., less than 0.50.
- The high LHV of C_2H_5OH significantly suppresses the evaporation.
- The evaporation quantity reaches a maximum at the mixing fraction of ethanol around 0.10 or 0.20.



(a) pseudo-1 C_2H_5OH/n-C_7H_{16} (w/ LHV of C_2H_5OH)

(b) pseudo-2 C_2H_5OH/n-C_7H_{16} (w/o LHV of C_2H_5OH)

<References>

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2. Barro, C., Rogalski, M. and Péneloux, A., *Fluid Phase Equilibria*, Vol.8, Issue 1, pp.55-73, 1982.
3. Janaszewski, B., Oracz, P., Goral, M. and Warycha, S., *Fluid Phase Equilibria*, Vol.9, Issue 3, pp.295-310, 1982.
4. Kobashi, Y., Fujimori, K., Maekawa, H., Kato, S., Kawano, D. and Senda, J., "Modeling of Auto-Ignition and Combustion Processes for Dual-Component Fuel Spray," *SAE Int. J. Engines* 4(2):2193-2206, 2011.

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