The influence of non-ideal vapor-liquid-equilibrium on vaporization of multicomponent hydrocarbon fuels

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Abstract

In this work, the differences between non-ideal vapor-liquid-equilibria (VLE) and the effect on vaporization for multicomponent hydrocarbon fuels, which are representative for engines or gasifiers, are investigated. The VLE for a general multicomponent system is given by

$$\widetilde{y}_i \phi_i^v p = \gamma_i \widetilde{x}_i f_i^+$$

where $\widetilde{x}_i$ is the molar fraction of the liquid, $\widetilde{y}_i$ the molar fraction of the vapor, p the pressure of the system, ϕ_i^v the fugacity coefficients of the vapor, γ_i the activation coefficients of the liquid, and f_i^+ the fugacity of a selected reference state. For an ideal VLE the fugacity and the activation coefficients are equal to unity one ($\phi_i^v = \gamma_i = 1$) and fugacity is equal to the saturation pressure of the pure component. The equation for the ideal VLE is also called Raoult's law and most standard models, e.g. in CFD codes, for droplet vaporization use this relation. Here, the fugacity coefficients are determined using the binary Non-Random-Two-Liquids (NRTL) approach.

The VLE differences at 1.0 atm between Raoult and non-ideal approaches are illustrated for the binary mixture iso-octane/ethanol in Fig. 1. The non-ideal VLEs show an azeotrope point at around 0.4 kg/kg ethanol and lower boiling and condensation temperatures compared to Raoult's law. The software Aspen Plus is used to determined the non-ideal approaches. Figure 1 shows furthermore the in this work used NRTL-model and experimental data from Wen [1]. Iso-octane/ethanol mixtures are suitable to descripe engine fuels like E10. Significant differences between the Raoult and all the non-ideal approaches can be seen both for the condensation and the boiling curve. The VLE results are then applied for single droplet vaporization using the formulation of Law [2] modified for convective environments, which can be considered as base model for most CFD applications. The binary droplet mixture of iso-octane/ethanol results in a ternary VLE within e.g. the surrounding nitrogen gas atmosphere. The droplet life time and the vaporization rates of the single components and their mixtures, which corresponds among other to E10 and E90, are compared between ideal and non-ideal behavior. Based on the deviations in the VLE approach, a parametric study of non-ideal VLE-behavior for a pressure range between 0.5-20.0 bar, a gas temperature range of 0-$600\,^{\circ}$C and particle Reynolds number below break-up and atomization, which are typical vaporization conditions in IC engines and gasifiers, is performed. The observed differences suggest that non-ideal VLE have a significant influence on droplet vaporization of complex hydrocarbon mixtures under realistic conditions for technical systems.

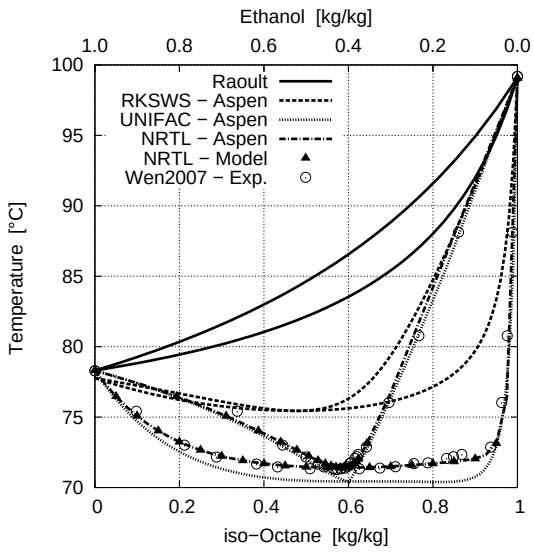

Figure 1. Ideal and non-ideal (real) VLE of iso-octane and ethanol at 1.0 atm

[1] Wen, C.C. and Tu. C. H., *Fluid Phase Equilibrium* Vol. 258, p. 131-139 (2007).
[2] Law, C.K., *Combustion and Flame* Vol. 26, p. 219-233 (1976).

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