



Modeling of vapor-liquid equilibrium of gasoline-ethanol blended fuels for flash boiling simulations

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ABSTRACT

Flash boiling is a physical phenomenon which governs the non-equilibrium phase change of a high temperature fluid as it is depressurized below its vapor pressure. The modeling of this process is of importance to a number of industrial applications and requires the vapor-liquid equilibrium properties of the fluid under consideration. The highly non-ideal nature of gasoline-ethanol fuel blends makes vapor-liquid equilibrium calculations extremely difficult for such fluids. A simple model known as GEFflash (Gasoline-Ethanol Flash), based on existing literature and fundamental chemical engineering thermodynamics is proposed to calculate the properties of gasoline-ethanol fuel blends that are required to perform flash boiling simulations. In addition, a second model based on the chemical engineering software Aspen Plus is also proposed and the predictions of the two models are validated against experimental data available in open literature. The results indicate that both models reproduce the trend in experimental data for vapor pressures and saturated liquid density for blends with different ethanol contents. The GEFflash model does not match the vapor mole fraction predictions of the Aspen Plus model for fuels with low ethanol content (E20 and E40). However, the vapor mole fractions for high ethanol content fuels (greater than E60) are accurate over the majority of the temperature range tested.

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1. Introduction

The phenomenon of flash boiling can be explained by considering the flow of a hot fluid through a nozzle, as shown in Fig. 1. The elevated vapor pressure of this high temperature fluid makes it susceptible to vaporization since any depressurization can cause the pressure to drop below the vapor pressure. Once the local pressure decreases below the vapor pressure, the fluid attains a metastable state and any disturbance in the fluid can spawn tiny vapor bubbles known as nuclei. This process is known as nucleation and can occur in two ways: heterogeneous and homogeneous. Heterogeneous nucleation takes place due to disturbances created by imperfections on nozzle walls, or dissolved impurities in the fluid, whereas homogeneous nucleation occurs due to microscopic fluctuations in the fluid density occurring at high degrees of superheat [1]. Once these nuclei are formed, they grow into larger bubbles due to continued vapor formation at their walls. In case the pressure downstream of the nozzle is significantly below the vapor pressure of the fluid, these bubbles continue to grow and eventually burst to form a spray of liquid droplets distributed in vapor. This process of formation of liquid droplets is known as atomization and the entire process starting from nucleation is known as

flash boiling. The amount of vapor formed inside the nozzle greatly affects the characteristics of the ensuing spray and hence flash boiling simulations of the flow inside the nozzle are extremely important.

The most direct application of the nozzle flow case explained above is the flow through a fuel injector nozzle in an internal combustion engine. Kim et al. [2] showed that flash boiling can improve engine performance. Kawano et al. [3] studied the effect of flash boiling on the spray, combustion, and the exhaust emissions and concluded that flashing reduced smoke emission due to better atomization. In addition, flash boiling also has applications in other industries. For example, flashing is used in a certain type of desalination method known as Multi-Stage Flash Distillation (MSF) [4]. An efficient method employed in paper drying is known as impulse drying and uses flash vaporization of the water in the paper [5]. Flash evaporation may be applied in wine making to improve the wine quality [6]. In geothermal power plants based on water-based geothermal fields, flashing is used to convert the geofluid into vapor which is then passed through a turbine to generate power [7]. The study of flash vaporization is also important in order to address safety concerns occurring from loss of cooling accidents (LOCA) in light water nuclear reactors [8].

Flash boiling is similar to cavitation in that it is a phase change process in which the energy required for phase change is provided by interphase heat transfer. However, one major difference

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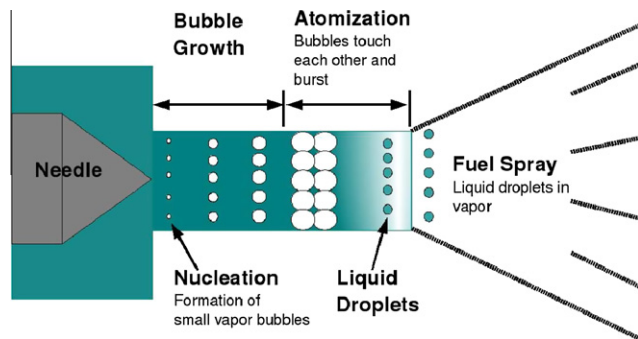


Fig. 1. Process of flash boiling in nozzle, adapted from [9].

between these two phenomena is that flash boiling takes place under the condition of thermal non-equilibrium [10]. Therefore any effective modeling of the flash boiling process requires a method that can account for the non-equilibrium phase change process. The Homogeneous Relaxation Model (HRM) has been used for simulating flash boiling flows by a number of authors (see [11–13]). This model is based on the simple concept that the local, instantaneous mass fraction of vapor will relax to its equilibrium value over an empirically correlated relaxation time. Gopalakrishnan and Schmidt [10] implemented this model into the open source computational fluid dynamics library OpenFOAM [14]. The fluid's vapor-liquid equilibrium (VLE) properties are required to provide closure to the model. Gopalakrishnan and Schmidt [10] simulated flash boiling in water and used curve fits to obtain the required properties. However, such curve fits are not available for most fluids of interest in industrial applications and hence programs capable of performing VLE calculations are required. Lee et al. [15] simulated the flash boiling of a multi-component surrogate for the aviation fuel JP8. The properties for the JP8 surrogate were obtained through a look-up table generated by the SUPERTRAPP program [16]. Similarly, Neroorkar et al. [17] used the REFPROP database and code library [18] which employs the equation of Span and Wagner [19] to obtain the properties of hexane.

In recent times, research has pursued the development of alternative energy resources to replace fossil fuels. A possible alternate fuel is ethanol since it can be made from biomass and therefore may be considered as a renewable fuel [20,21]. In the past few decades, 10% ethanol by volume has been added to automotive gasoline due to its ability to boost the fuel's octane rating. However, with the increased focus on reducing dependence on fossil fuels, auto manufacturers have been manufacturing cars that are capable of running on gasoline containing 85% ethanol. This fuel known as E85 has a lower vapor pressure than pure gasoline and hence the application of flash boiling to improve its atomization becomes critical in order to reduce unburnt hydrocarbon emissions and improve fuel efficiency. Ethanol, however, has a highly polar nature and when around 20% ethanol is mixed with gasoline, it forms a positive azeotrope having a higher vapor pressure than either pure gasoline or ethanol [22]. As a result, the above mentioned methods are not sufficient to model the VLE of gasoline-ethanol (G-E) fuel blends. Bennett et al. [23] tried to model the VLE of ethanol-hydrocarbon mixtures using a modified Peng-Robinson equation of state and van der Waals mixing rules and found that this method was not applicable to such non-ideal mixtures. Pumphrey et al. [24] proposed an approach for calculating the vapor pressure of G-E blends by treating them as pseudo binary systems of ethanol and gasoline. Balabin et al. [25] and Kar et al. [22] used the Clausius-Clapeyron equation, assuming the vapor to be an ideal gas, to find the enthalpy of vaporization of G-E mixtures from their vapor pressure measurements. Additionally, VLE of complex mixtures of hydrocarbons with alcohols have been modeled through the use

of the cubic plus association equation of state (CPA EOS) ([26]) and by combining the Peng-Robinson equation of state with a group contribution method to calculate the binary interaction parameters ([27]). In this case, the CPA EOS is an attractive option since all parameters required by the EOS can be obtained by regressing vapor pressure and liquid density data and no experimental critical properties or accentric factors are required. However this method has yet to be applied to GE blends.

It can be observed that there is a need to develop and test a model which can provide the VLE properties and volatility information required for accurate flash boiling simulations of G-E fuel blends. In the current work, a computationally inexpensive modeling procedure is proposed that couples some of the existing models developed for G-E blends with fundamental chemical engineering thermodynamics to provide the required closure for flash boiling models. A model based on the process engineering software Aspen Plus is also proposed and is used for validation in cases where experimental data are unavailable.

2. Modeling procedure

This section describes the steps followed in building a model for properties of G-E blends using a binary mixture approximation based on the idea of Pumphrey et al. [24]. The model developed is known as the Gasoline-Ethanol Flash model (GEFlash) and the following sub-sections present the formulations used to calculate the different properties: vapor pressure, enthalpy of vaporization, mass fraction of vapor, and, saturated liquid and vapor densities. Finally, the last sub-section describes the methodology followed to combine these models into one framework.

2.1. Vapor pressure

The model of Pumphrey et al. [24] was used to calculate the vapor pressure of the G-E blends. According to this method, the vapor pressure of a G-E blended fuel can be obtained by Eq. (1)

$$P_{sat} = x_e \gamma_e P_{e,sat} + x_g \gamma_g P_{g,sat} \quad (1)$$

where the subscripts *e* and *g* stand for ethanol and gasoline respectively. x , γ , P_{sat} represent the molar fractions, the activity coefficients, and vapor pressure of the component. The activity coefficients are calculated using the Wilson equation formulation [28] given as follows

$$\ln(\gamma_e) = -\ln(x_e + \Lambda_{eg}x_g) + x_g \left(\frac{\Lambda_{eg}}{x_e + \Lambda_{eg}x_g} - \frac{\Lambda_{ge}}{x_g + \Lambda_{ge}x_e} \right) \quad (2)$$

$$\ln(\gamma_g) = -\ln(x_g + \Lambda_{ge}x_e) - x_e \left(\frac{\Lambda_{eg}}{x_e + \Lambda_{eg}x_g} - \frac{\Lambda_{ge}}{x_g + \Lambda_{ge}x_e} \right) \quad (3)$$

The parameters Λ_{eg} and Λ_{ge} were obtained by Pumphrey et al from their experimental data as equal to 0.1665 and 0.3527 respectively. This method was implemented in this work, and Fig. 2 is a verification that the implementation is accurate.

2.2. Enthalpy of vaporization

The Clausius-Clapeyron equation was used by Kar et al. [22] and Balabin et al. [25] to calculate the enthalpy of vaporization of the G-E blends. This method can be explained as follows. The Clausius-Clapeyron equation for pure substances is given as

$$\frac{dP_{sat}}{dT_{sat}} = \frac{H_{fg}}{T_{sat}v_{fg}} \quad (4)$$

where P_{sat} and T_{sat} are the saturation pressure and temperature of the liquid, H_{fg} is the enthalpy of vaporization, and v_{fg} is the difference in the specific volumes of saturated liquid and vapor.

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