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A proposed combination model for predicting surface tension and surface properties of binary refrigerant mixtures

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ABSTRACT

A combination model is proposed to describe the surface tension and surface properties of binary refrigerant mixtures combining the Laaksonen and Kulmala equation with the phase equilibrium between the bulk liquid and surface phases to predict the surface tension, surface composition and surface mole density of the binary refrigerant mixtures. Also, the present model is combined with the volume-translated Peng–Robinson (VTPR) equation of state to describe the fugacity coefficients of the components and molar volumes of the bulk and surface phases. This proposed combination model is subsequently applied for 13 binary refrigerant mixtures and compared with the gradient theory. The results of this model show that the surface tensions predicted by this model agree well with experimental data for these mixtures (overall AAD ~4.35). Compared with the gradient theory (overall AAD ~5.67 and 3.94 for density and temperature dependant influence parameter), the proposed combination model performs well.

Un modèle combiné proposé pour la prévision de la tension superficielle et des propriétés de surface de mélanges binaires de frigorigènes

Mots clés : Tension superficielle ; Composition superficielle ; Équation d'état de PR en termes de volume ; Mélanges de frigorigènes

1. Introduction

Surface tension is one of the basic and useful thermophysical properties with respect to the vapor–liquid interface that plays a fundamental role in many aspects of chemical processes; for example, surface tension is an important parameter for the calculations of heat exchanger and the heat transfer assessment. The liquid–vapor surface tension influences and controls many processes in chemical or reservoir engineering

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Nomenclature

A	fitting coefficient of the influence parameter
a	attractive parameter in Heyen EOS
AAD	average absolute deviation (%)
b	covolume in the Heyen EOS
B	fitting coefficient of the influence parameter
C	fitting coefficient of the influence parameter
c	temperature-dependent volume translation coefficient
calc	calculated result
exp	experimental
f_0	Helmholtz free energy density
i, j	components i and j
k_{ij}	binary interaction parameter for the attractive parameter in the VTPR EOS
L	liquid
l_{ij}	binary interaction coefficient for the influence parameter of gradient theory
N	the number of experimental points
P	pressure
R	ideal gas constant
ref	reference variable
S	surface phase
T	temperature
T_r	reduced temperature
V	vapor
VTPR	volume translated Peng–Robinson
x_i, y_i	mole fraction of each component i in liquid and vapor phases
z	position in the interface
Z_c	critical compressibility factor

Greek letters

κ	influence parameter
μ	chemical potential
ρ	mole density
σ	surface tension
ν	molar volume of phases
ω	acentric factor
Ω	grand thermodynamic potential
δ_a	average absolute deviation of surface tension

applications, especially for analyzing the heat transfer through heat-exchanging surfaces with bubbles or fluid drops. Additionally, surface tension depends on composition, molecular forces, and molecular size and describes the nature of molecular forces at the interface. Therefore, the knowledge of surface properties is important to broaden the understanding of interface heat and mass transfer (Zhao et al., 2010; Lin and Duan, 2003; Tjahjono and Garland, 2010).

It is generally quite difficult to measure the surface tension and properties with direct experimental methods, so one needs reliable theoretical predictions of surface tension and properties. The properties of bulk phases are usually known, but the properties of vapor–liquid interface are unknown. Therefore, the surface tension of mixtures should be related to bulk-phase compositions and properties. Several approaches have been applied to correlate and predict surface tension of mixtures, including the parachor method and its derivatives (Tjahjono and Garland, 2010; Sugden, 1924; Weinaug and Katz, 1943), the corresponding states principle (Guggenheim, 1945; Zuo and Stenby, 1997; Queimada et al., 2006; Kim et al., 2009), Monte Carlo simulation (Attard and Moule, 1993), the perturbation theory (Toxvaerd, 1972; Haile et al., 1976), the density functional theory (Teixeira and Telo da Gama, 1991; Winkelmann et al., 1994; Fu et al., 2001), the gradient theory (Khosharay and Varaminian, 2013; Miqueu et al., 2011) and activity coefficient models like Wilson, NRTL, and UNIFAC (Rafati and Ghasemian, 2008; Rafati et al., 2011; Nath, 1999). On the other hand, the models which apply density (or volume) in combination with surface tension (such as the parachor method, the gradient theory and etc) are generally better than the models which utilize only surface tension information because the size and interactions of the molecules affected the preferential adsorption in the surface layer and these factors are related to volumetric properties (Tjahjono and Garland, 2010).

In recent years, some researchers have worked on the prediction and correlation of surface tension and properties of pure refrigerants and their mixtures. Zhelezny and Bysko (1999) applied scaling principles to predict the surface tension of R116/R23, R22/R14, R134a/R152a and R22/R142b binary mixtures and presented the results of this investigation. Lin et al. (2008) applied the linear gradient theory in combination with VTPR and VTSRK EOSs and the temperature dependant influence parameter correlation to determine the surface tension of binary refrigerant systems. Vilaseca et al. (2010) combined the density gradient theory of van der Waals in with the soft-SAFT EOS to determine the surface tension of the CFCs and HCFCs and concluded that this model accurately predicts the surface tension and properties. Di Nicola and Moglie (2011) used semi-empirical correlating methods on the basis of corresponding state theory for surface tension of pure refrigerants. Khajeh and Modarress (2012) used quantitative structure–property relationship (QSPR) models to calculate surface tension of 224 refrigerant compounds. Based on the corresponding states principle theory, Di Nicola and Pierantozzi (2012) proposed two new equations to predict the surface tension of binary refrigerant mixtures.

In the present work, the Laaksonen and Kulmala (1991) equation is used in combination with the phase equilibrium between the bulk liquid and surface phases to predict the surface tension, composition and density of binary refrigerant mixtures. In this work, the fugacity is applied to perform phase equilibrium calculations. The volume-translated Peng–Robinson (VTPR) equation of state (Lin et al., 2007) is used to calculate the fugacity coefficients of the components and molar volumes of the bulk and surface phases. Molar volumes of pure refrigerants can be calculated with the help of VTPR EOS. To identify the advantages of the proposed combination model, the well recognized gradient theory in combination with the VTPR EOS is also used to predict the surface tensions refrigerant mixtures. Subsequently, the results of the proposed combination model are compared with the results of the gradient theory. The density based and temperature dependant correlations (Oliveira et al., 2008) are applied for the influence parameters of