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Thermodynamic properties of lubricant/refrigerant mixtures using statistical mechanics and artificial intelligence

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ABSTRACT

In this research, the volumetric properties of sixteen lubricant/refrigerant mixtures are predicted using the developed statistical mechanical equation of state at a broad range of temperatures, pressures and mole fractions. The equation of state have been examined using corresponding states correlation based on just one input parameter (density at room temperature) as scaling constants. Besides, the artificial neural network (ANN) based on back propagation training with 19 neurons in hidden layer was tested to predict the behavior of binary mixtures of lubricant/refrigerant. The AADs% of a collection of 3961 data points for all binary mixtures using the EOS and the ANN at various temperatures and mole fractions are 0.92% and 0.34%, respectively. Furthermore, the excess molar volume of all binary mixtures calculated from obtained densities of ANN, and the results shown these properties have good harmony with literature.

Propriétés thermodynamiques des mélanges de lubrifiant et de frigorigène à l'aide de la mécanique statistique et de l'intelligence artificielle

Mots clés : Frigorigène ; Lubrifiant ; Volume molaire en excès ; Mécanique statistique ; Réseau neuronal artificiel

1. Introduction

There is a major demand for an appropriate molecular thermodynamic model to represent both volumetric and equilibrium properties of newly processed fluids especially in engineering application. IUPAC and the Thermophysical Properties Division of NIST have identified the information of the properties of mixtures of lubricants with substitute HFC refrigerants as a high priority research area, and there is a need to develop methods to predict compatibility regimes and properties (Marsh and Kandil, 2002). The polyol esters (POEs) and the polyalkylene glycols (PAGs) have been proposed as refrigerant oils. The most favorable applications of POE and PAG lubricant/refrigerant mixtures need the study of their physical properties such as density. In the last years new oils based on carbonate molecules

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Nomenclature

K	Boltzmann factor [J K^{-1}]
ω	Pitzer acentric factor [–]
λ	adjustable parameter [–]
ρ	number density [mol m^{-3}]
T_C,	critical temperature [K]
P_c	critical pressure [Pas]
R	universal gas constant [J mol^{-1} K^{-1}]
B_2	second virial coefficient [M^3 mol^{-1}]
T_r	reduced temperature [–]
α	the scaling parameter [M^3 mol^{-1}]
b	van der Waals co-volume [M^3 mol^{-1}]
T_B	Boyle temperature [K]
V_B	Boyle volume [M^3 mol^{-1}]
ρ_r	density at room temperature [Mol m^{-3}]
G_{ij}	pair distribution function [–]
η	packing fraction of the mixture [–]
T_{cmix}	traditional pseudocritical temperature [K]
x	mole fraction [–]
ANN	artificial neural network [–]
w_i	represents the weights [–]
BP	back propagation [–]
MLP	multilayer percepetron [–]
RBF,	radial basis function networks [–]
GR	ghost recon networks [–]
CFB	cascade forward back propagation [–]
SSE	square error [–]
AAD	absolute average deviation [–]
MSE	mean square error [–]
R^2	coefficient of determination [–]
MARE	mean absolute relative error [–]

have been proposed (Hayashi et al., 1996; Takahata et al., 1994; Takeno et al., 1992) as candidates for stationary air conditioners due to their thermal stability, lubricity, and miscibility with refrigerants. Dialkyl carbonates have been proposed as alternative lubricants in low environmental impact air conditioners due to their miscibility with hydrofluorocarbon (HFC), good viscosity, and thermal stability (Hayashi et al., 1996; Takahata et al., 1994; Takeno et al., 1992). Besides their inherent interest, thermodynamic properties of the dialkyl carbonate/n-alkane mixtures permit us to find parameters for molecular models that are useful to predict thermophysical properties for HFCs/carbonate systems (Garcia et al., 1996, 1998).

In the past years, refrigerants have been found as hydrate formers. Generally the most refrigerants used in the industry belong to three groups: chlorofluorocarbon (CFC), hydrochlorofluorocarbon (HCFC) and hydrofluorocarbon (HFC). The class of HFCs is known as good candidates to protect the world's environment (Eslamimanesh et al., 2011; Miguel et al., 2000). The ozone depletion potential (ODP) and global warming potential (GWP) of HFCs are lower than other groups'. For example, the ozone depletion potential is zero for HFC134a, HFC152a, and HFC32 because of the absence of chlorine atoms. Also the global warming potential of above HFCb refrigerants is less than those of CFC12 and HCFC22, because they have more hydrogen atoms and so have a shorter atmospheric life-time (Lisal and Vacek, 1996).

The study of the thermophysical properties of lubricant/refrigerant mixtures is necessary for the successful transition to new environmentally alternative refrigerants (Geller and Davis, 1995; Mang, 1982; Mastrangelo, 1959; Spauschus, 1988, 1997). It is very important to obtain accurate and reliable measurements of the solubilities, densities, and viscosities of these mixtures because they are extremely important for the design of refrigeration compressors. Moreover, information of these thermophysical properties for lubricant/refrigerant systems is very rare.

Because direct measurement of the applicable thermophysical properties over a wide range of temperatures and pressures is difficult, attempts to expand procedures for estimating thermophysical properties have been offered in the past (Goharshadi et al., 2007; Yousefi and Karimi, 2012, 2013). Equations of state (EOS) play a central role to model the thermophysical properties of fluids. The EOS attempts to express the relationship between temperature, pressure, and volume for fluids or mixtures of substances. If the EOS of a system is established, all thermodynamic behavior of the system can be calculated using statistical mechanical tools. Concerning the vast applicability of different refrigerants, accurate information of the pressure–density relation of these systems over an extended range of temperature and pressure is extremely useful in predicting thermophysical properties. The theories of liquids have been expanded over the past years based on perturbation theories (Yousefi and Karimi, 2012, 2013). Therefore, an analytical equation having a statistical–mechanical basis in molecular theory is very desirable.

However, these models have some limitations because of the use of many adjustable parameters or mixing rules. Therefore, they need a sufficient amount of data for calibration and justification purposes that makes them computationally inefficient. In such cases, an artificial neural network (ANN) can be a proper option to model the different thermodynamic properties. In other words, the relationship between the physical and thermodynamic properties is extremely nonlinear. Therefore, the ANN technique is a particularly capable algorithm to approximate a certain property such as density using learned the relations between the input and output data (Yousefi and Karimi, 2013). As a result, thermodynamic properties can be modeled by the ANN technique as an alternative tool (Karimi and Yousefi, 2012; Lazzus, 2009). Recently, The ANNs have been severely applied to different fields (Esen et al., 2008a, 2008b, 2008c, 2009, 2017). The main reason for this fast progress and different applications of the ANN is their capability to virtually approximate any function in a stable and efficient way.

Tao–Mason (TM) equation of state (Tao and Mason, 1994) has been successfully developed for fluids and their mixtures (Karimi et al., 2011a, 2011b; Yousefi et al., 2009). Moreover, the applications of equation of state and artificial neural networks approaches (Yousefi and Karimi, 2012, 2013) were studied to predict the properties of pure polymers.

This study focused on the potential of the new versions of both the TM EOS and ANN to estimate thermodynamic properties of lubricant/refrigerant mixtures (such as: Decane/DMC, DMC/Octane, HFC/TEGDME, HFC/TriEGDME, TEGDME/Heptane, CO2/PEC9, CO2/PEC7, CO2/PEC5, Diethyl carbonate/n-dodecane, DMC/n-dodecane, TEGDME /n-dodecane, TEGDME