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Ph.D. Dissertation
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Study of Thermophysical properties of Natural gases, CO_2-Nobel gases, Refrigerants and Carbon Nanotubes- based fluid

By:

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In The Name of God

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THESIS

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Declaration

I, Fakhri Yousefi, declare that this thesis represents my own work effort. Where other sources of information have been used, they have been acknowledged.

I also declare that my research and the subject of my thesis is not repetitive and I guarantee that I am not willing to publish these results without the permission of Shiraz University. According to the intellectual and moral ownership regulation, all right reserved by Shiraz University.

Fakhri Yousefi

5 November 2009

Dedicated to:

My Parents,

My Husband,

, My Dear Daughter and Son (Medisa & Eliya)

For Their Love, Endless Support and Encouragement

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ABSTRACT

Study of Thermophysical properties of Natural gases, CO2-Nobel gases, Refrigerants and Carbon Nanotubes- based fluid

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Part I. It is the purpose of this work to extract unlike intermolecular potential energies of five carbon dioxide-based binary gas mixtures including CO_2-He, CO_2-Ne, CO_2-Ar, CO_2-Kr, and CO_2-Xe from viscosity data and compare the calculated potentials with other models potential energy reported in literature. Then, dilute transport properties consisting of viscosity, diffusion coefficient, thermal diffusion factor, and thermal conductivity of aforementioned mixtures are calculated from the calculated potential energies and compared with literature data. Rather accurate correlations for the viscosity coefficient of afore-cited mixtures embracing the temperature range 200K<T<3273.15K is reproduced from the present unlike intermolecular potentials energy. Our estimated accuracies for the viscosity are to within $\pm 2\%$. In addition, the calculated potential energies are used to present smooth correlations for other transport properties. The accuracies of the binary diffusion coefficients are of the order of $\pm 3\%$. Finally, the unlike interaction energy and the calculated low density viscosity have been employed to calculate high density viscosities using Vesovic-Wakeham method.

Also Viscosities, diffusion coefficients, thermal conductivities and thermal diffusion factors for seven binary gaseous mixtures H_2–CO_2, H_2–N_2, H_2–CH_4, H_2–C_2H_6, N_2–CH_4, N_2–C_2H_6, CH_4–C_2H_6, one ternary gaseous mixture N_2–CH_4–C_2H_6 and one quaternary gaseous mixture H_2–N_2–CH_4–C_2H_6 were determined based on the principle of the corresponding states of viscosity together with the inversion technique. The calculated transport properties have been compared with those obtained from other methods and also from experimental data. Our estimated accuracies are to within 3% for the viscosity, 5% for the binary diffusion coefficient and 14% for the thermal conductivity.

Part II. Tao and Mason (J. Chem. Phys. 1994, 100, 9075-9084) developed a statistical-mechanical-based equation of state (EOS) for pure substances. In the

present study, we have successfully extended this EOS to fluid mixtures, selecting refrigerant fluid mixtures as the test systems. The considered refrigerant mixtures are R32 + R125, R32 + R134a, R134a + R152a, R125 + R143a, R125 + R134a, R32 + R227ea, R134a + R290, and R22 + R152a. The second virial coefficient, B(T), necessary for the mixture version of the Tao-Mason (TM) EOS, was determined using a two-parameter corresponding-states correlation obtained from the analysis of the speed of sound data and two constants: the enthalpy of vaporization ΔH_{vap} and the molar density ρ_{nb}, both at the normal boiling point. Other temperature-dependent quantities, including the correction factor $\alpha(T)$ and van der Waals covolume b(T), were obtained from the Lennard-Jones (12-6) model potential. The cross parameters $B_{12}(T)$, $\alpha_{12}(T)$ and $b_{12}(T)$, required by the EOS for mixtures, were determined with the help of simple combining rules. The constructed mixture version of the TM EOS was extensively tested by comparison with experimental data. The results show that the molar gas and liquid densities of the refrigerant mixtures 1.3% and 2.69%, respectively, over the temperature range of 253-440 K and the pressure range of 0.33-158 bar. The present EOS was further assessed through comparisons with the Ihm-Song-Mason (ISM) and Peng-Robinson (PR) equations of state. In the gas phase, the TM EOS outperforms the two other equations of state. In the liquid phase, there is no noticeable difference between the TM EOS and the PR EOS, but both work better than the ISM EOS.

Part III. We used some extended models for calculation of thermal conductivities of suspension of multi-walled CNTs in (α-olfin) oil, decene (DE), distilled water (DW), ethylene glycol (EG) and single-walled CNTs in epoxy and poly methylmethacrylate (PMMA). Also we utilized a hybrid model based upon mega-trend-diffusion technique and neural network to estimate the expected domain range of real data and generate a number of virtual data points to reduce the error of estimated function with respect to a small actual dataset and build the robust prediction model. Then we compared the obtained results with actual data. The results show good harmony with the literature values. DNN-MLP model possesses a high ability to predict thermal conductivity ratio with an absolute average error of 3.26%. The results demonstrated good agreement between the predicted and the experimental values of thermal conductivity ratio (r=0.991). The standard deviation in relative errors was 2.3%. This value showed the dispersion around the average value was small.

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