Thermodynamic Modeling of Alkanolamine and Ethylene Glycol Systems Using SAFT Equation of State

Arash Pakravesh

Department of Physical Chemistry, Faculty of Chemistry and Petroleum Science, Bu-Ali Sina University, Hamedan, Iran

1. Background

Accurate thermodynamic modeling of pure alkanolamines and ethylene glycols and their mixtures plays a key role in the design and development of various industrial processes such as chemical, petroleum, natural gas, paper, tobacco, cork, and ink industries. Thermodynamic modeling is even more important in separation processes, such as acid gas removal, because more than 40% of the total cost of such processes is related to the separation unit. From a theoretical perspective, alkanolamines and glycols offer a unique study opportunity due to their hydroxyl groups, which lead to strong self-association. Analyzing their thermodynamic behavior is useful for understanding these interactions. Thermodynamic models, such as equations of state (EoSs) can be used to model alkanolamine and ethylene glycol systems [1,2]. The associating nature of alkanolamines and ethylene glycols has led to the increased use of advanced EoSs like SAFT (Statistical Associating Fluid Theory) for modeling their pure and mixture properties. In this study, the PρT-SAFT EoS [3] was employed to model the thermodynamic behavior of monoethanolamine (MEA), diethanolamine (DEA), methyldiethanolamine (MDEA), 2-amino-2-methyl-1-propanol (AMP), monoethylene glycol (MEG), diethylene glycol (DEG), and triethylene glycol (TEG) and their mixtures, including vapor-liquid equilibrium, volumetric properties, and second-order derivative thermodynamic properties.

2. Method

The PρT-SAFT EoS [3] is a $P\rho T$ reparameterization of the SAFT EoS, achieved by utilizing a more advanced computational method and fitting experimental $P\rho T$ data instead of VLE data for parametrization. The PρT-SAFT EoS has five adjustable parameters to represent the thermodynamic behavior of pure associating fluids, which are estimated from $P\rho T$ data over a wide range of T and P. The PρT-SAFT EoS is formulated as follows:

$$a^{res} = a - a^{ideal} = a^{seg} + a^{chain} + a^{assoc}$$

3. Results

Based on the availability of experimental data, calculations were performed in this section for the following thermodynamic properties: density, isobaric heat capacity, sound velocity, isobaric thermal expansivity, isothermal compressibility, saturated vapor pressure, and saturated liquid density. The average absolute deviation percentage (%AAD) is used to compare the PρT-SAFT EoS results and experimental data:

$$\%\text{AAD} = \frac{100}{N_P} \sum_{i=1}^{N_P} \left| \frac{Y_i^{\text{cal}} - Y_i^{\text{exp}}}{Y_i^{\text{exp}}} \right|$$

4. Conclusions

In this work, the thermodynamic behavior of three pure ethylene glycols (MEG, DEG, and TEG), four pure alkanolamines (MEA, DEA, MDEA, and AMP), eleven binary mixtures, and five ternary mixtures composed of them were calculated and compared with available experimental data using the PρT-SAFT EoS.
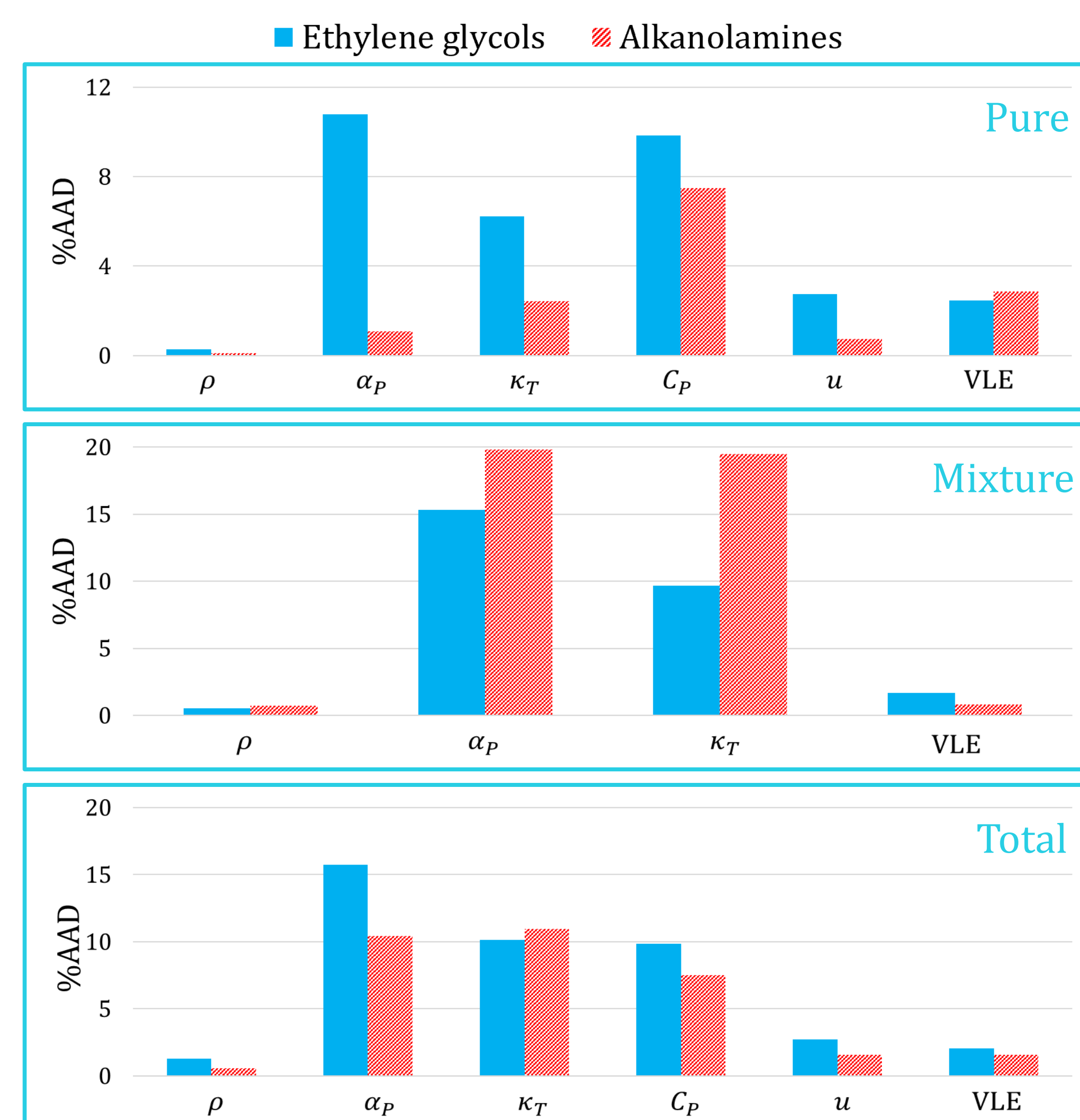
Overall, the PρT-SAFT EoS demonstrates promising potential for the thermodynamic modeling of pure alkanolamines, ethylene glycols, and their binary and ternary mixtures.

5. References

[1] Arash Pakravesh and Hosseinali Zarei. Journal of Chemical and Engineering Data, Article ASAP, DOI: 10.1021/acs.jced.4c00390.

[2] Arash Pakravesh, Amir H. Mohammadi, and Dominique Richon. International Journal of Thermophysics 46.2 (2025): 30.

[3] Arash Pakravesh, Fatemeh Zarei, and Hosseinali Zarei. Fluid Phase Equilibria 538 (2021): 113024.