Extension of Structural (s)-SAFT-γ Mie equation of state for branched alcohols + *n*-alkanes mixtures

R.M. Slabbert, A.J. Burger*, A. Schulze-Hulbe
Department of Chemical Engineering, Stellenbosch University, Banghoek Str, Stellenbosch, South Africa
Telephone: +27 21 808 4494 *Email: ajburger@sun.ac.za

Introduction

- The group contribution (GC) approach: powerful method for predicting phase equilibria and derivative properties
- GC has been successfully implemented in the frameworks of SAFT EoS's
- SAFT-γ Mie's accuracy approaches that of SAFT-VR Mie, despite its inherently predictive nature [4]
- However: SAFT-γ Mie is unable to differentiate between isomers → structural (s)-SAFT-γ Mie addresses this shortcoming by accounting for the relative position of functional groups in molecules

Objectives

1. Generation of VLE data for 12 binary systems consisting of *n*-alkanes and methyl-branched alcohols at 101.32 kPa
2. Determine the phase behaviour SAFT-γ Mie and (s)-SAFT-γ Mie with existing parameters and refining them as required

Methodology

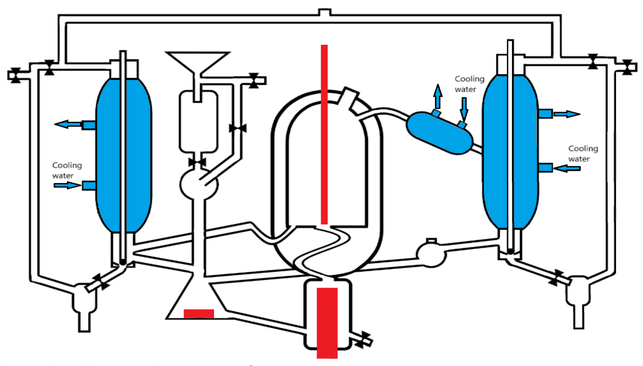
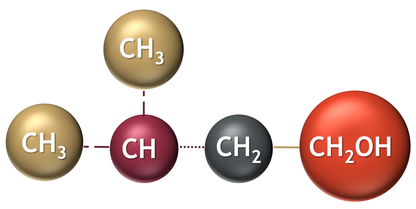


Fig 1: Experimental set-up

- Modified Gillespie still used to experimentally produce the data for binary VLE sets under isobaric conditions (1.0132 bar)

- 2-methyl-1-butanol



3-methyl-1-butanol

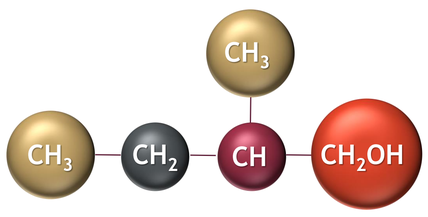


Fig 2: Illustration of how 2-methyl-1-butanol and 3-methyl-1-butanol are split into groups.

Experimental confirmation

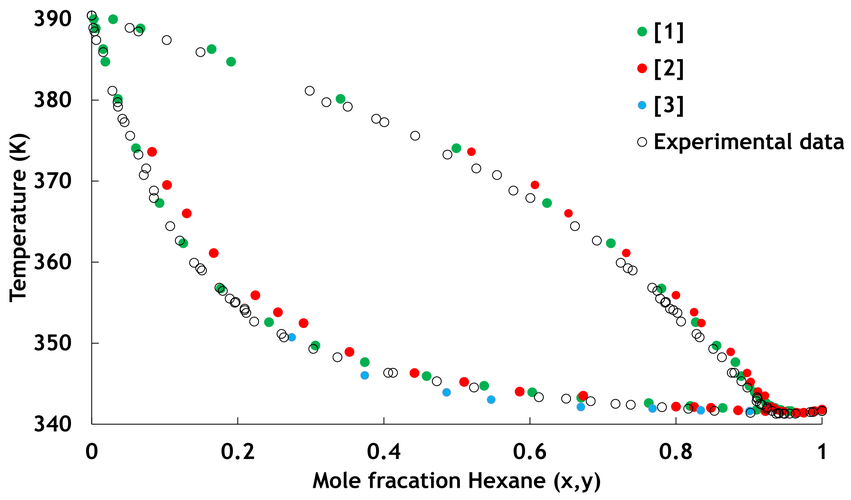


Fig 3: Experimental data of binary system n-hexane + 1-butanol compared to data generated by [1], [2] and [3]

Preliminary Results

- CR in the figure below indicates that combining rule has been used for dispersion energy of CH_2OH - CH
- The regression indicates that the dispersion energy for CH_2OH - CH was regressed using binary data 2-methyl-1-butanol + n-heptane
- (s)-SAFT-γ Mie used parameter from [6] as well as values regressed by research group

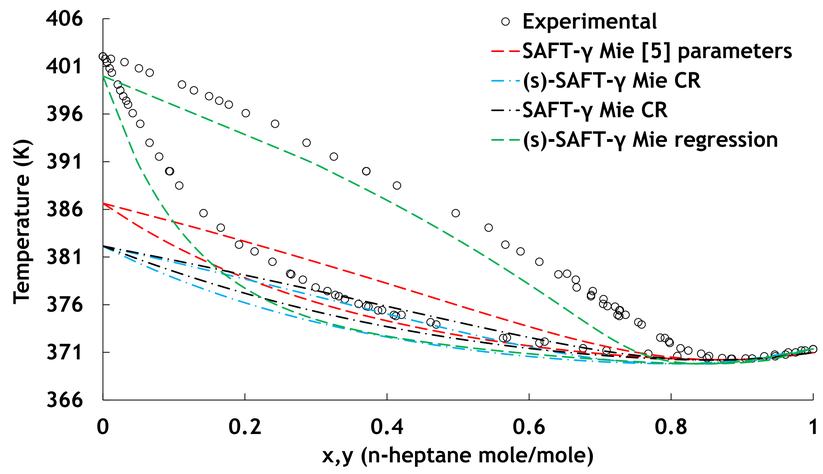


Fig 4: Experimental data of binary system n-heptane + 2-methyl-1-butanol with the predictions of SAFT-γ Mie and (s)-SAFT-γ Mie

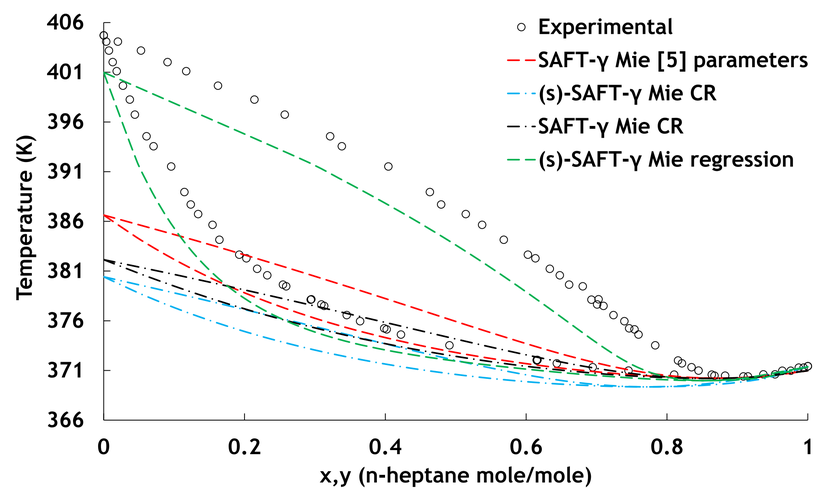


Fig 5: Experimental data of binary system n-heptane + 3-methyl-1-butanol with the predictions of SAFT-γ Mie and (s)-SAFT-γ Mie

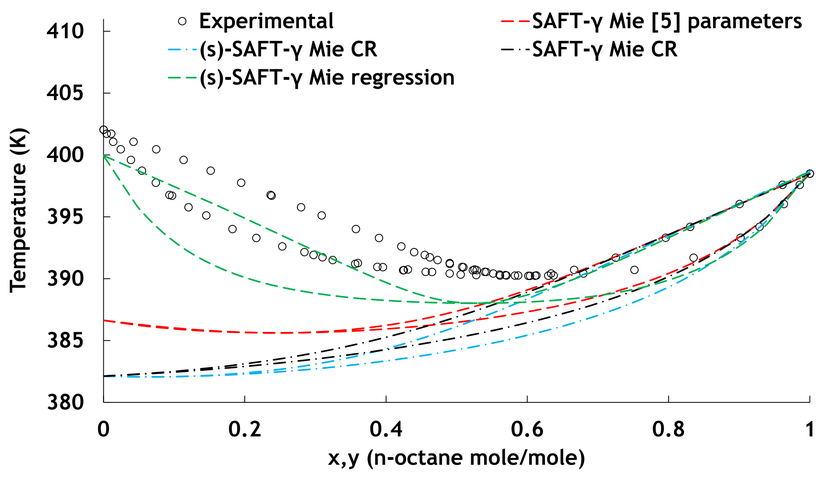


Fig 6: Experimental data of binary system n-octane + 2-methyl-1-butanol with the predictions of SAFT-γ Mie and (s)-SAFT-γ Mie

Preliminary Conclusion

- (s)-SAFT-γ Mie has shown robust predictive capabilities for binary mixtures of *n*-alkanes and methyl- branched alcohols
- Further work is in progress to determine relative capabilities of (s)-SAFT-γ Mie relative to SAFT-γ Mie

[1] Dominguez, M. et. al. (1997) J. Chem. Eng. Jpn., 1997, 30, p.484-490
[2] Govindaswamy, S. et. al. (1976). J. Chem. Eng. Data, 21, p.366-369
[3] Rhim, J. N. et. al. (1981), 19, p.199
[4] Dufal, S., Papaioannou, V. et. al. (2014). Journal of Chemical & Engineering Data, 59(10), pp.3272-3288.
[5] Haslam, A.J. et al. (2020), 65(12), pp. 5862-5890
[6] *Shaahmadi, F. et. al. (2021). The Journal of Chemical Physics, 154(24), p.244102.*
[7] Papaioannou, V. et. al. (2014). The Journal of Chemical Physics, 140(5), p.054107.

The financial assistance of Sasol South Africa (Pty) Ltd towards this research is hereby acknowledged. Opinions expressed and conclusions arrived at are those of the authors and are not necessarily to be attributed to Sasol South Africa (Pty) Ltd