

Supporting Information

Using the SAFT- γ -Mie to generate coarse-grained force fields usable in molecular dynamics simulations: Describing the micellar phases of polyalkylglycols in aqueous solutions

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S.1 – Atomistic MD simulation details

The Gromacs 2020.6 software was used to perform the atomistic molecular dynamics simulations, using the leap-frog algorithm to integrate the equations of motion. A timestep of 2 fs was used and the cut-off distance was set to 1.4 nm. Beyond the cut-off distance, dispersion interactions were corrected by adding the missing energy and pressure to the system and electrostatic interactions were approximated with the Particle-Mesh Ewald (PME) algorithm^{1,2}. All bonds containing hydrogen atoms had the bond distance constrained using the LINCS algorithm³. The OPLS-AA⁴ force field was chosen to model the ethylene oxide and propylene oxide oligomers where the degree of polymerization equals 8. Initial configurations of cubic boxes containing 300 molecules were randomly generated with packmol⁵. An initial energy minimization step was performed before an equilibration stage in the NpT ensemble for a total of 1 ns. Production runs in the NpT ensemble were conducted for a total of 10 ns. Temperature and pressure were kept constant using the Nosé-Hoover^{6,7} thermostat with a coupling constant of 0.5 ps and the Parrinello-Rahman⁸ barostat using a coupling constant of 10 ps.

S.2 – SAFT- γ -Mie derivative properties

S.2.1 – Isothermal compressibility coefficients

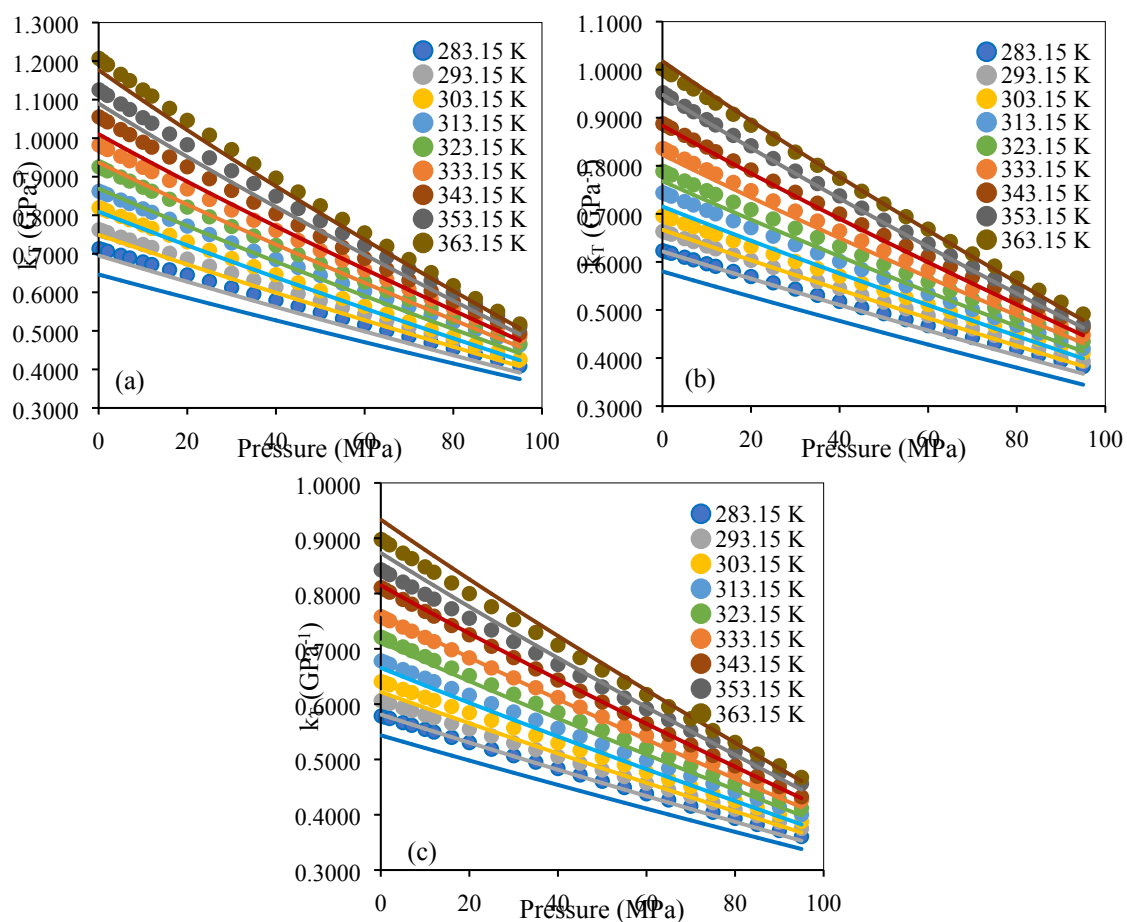


Figure S1 – Experimental (markers) and SAFT- γ -Mie (lines) isothermal compressibility coefficients for diglyme (a), triglyme (b) and tetraglyme (c) as a function of pressure and temperature.

S.2.2 – Isobaric expansion coefficients

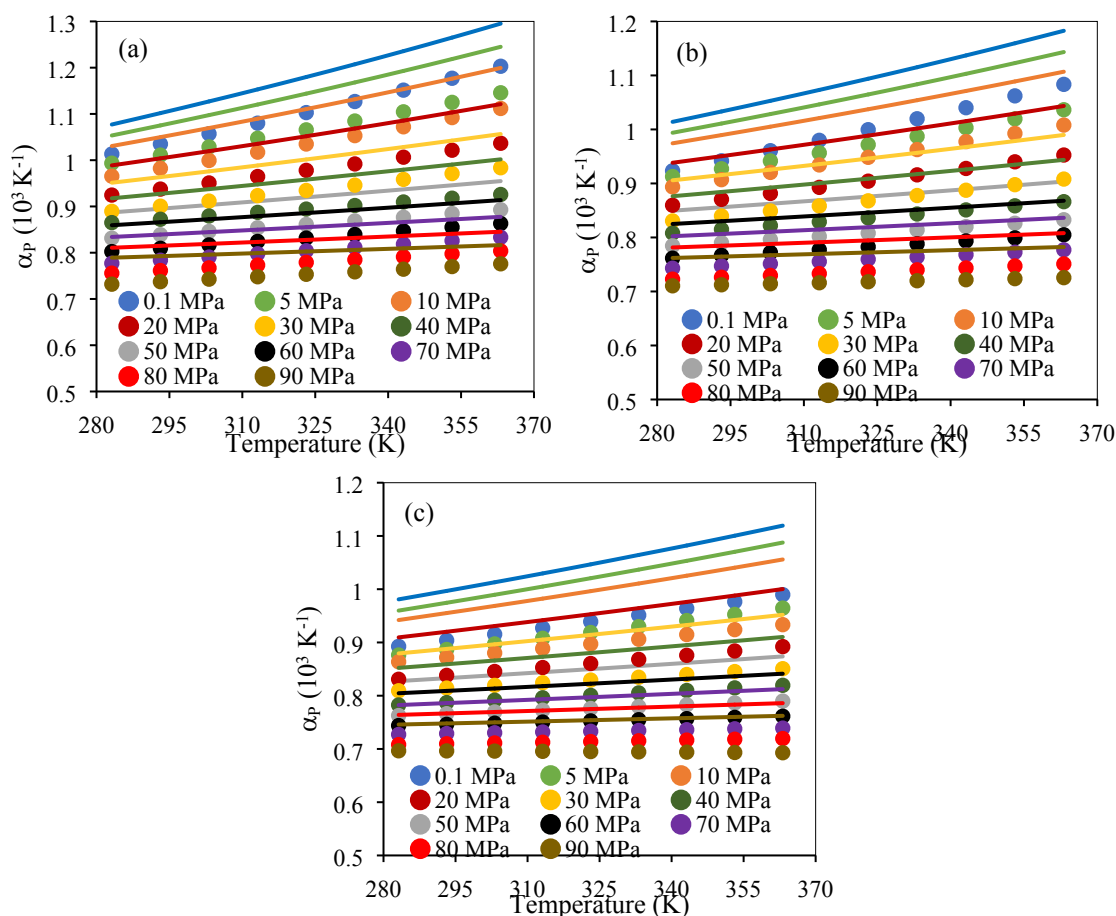


Figure S2 - Experimental (markers) and SAFT- γ -Mie (lines) isobaric expansion coefficients for diglyme (a), triglyme (b) and tetraglyme (c) as a function of temperature and pressure.

¹ Essmann, U.; Perera, L.; Berkowitz, M. L.; Darden, T.; Lee, H.; Pedersen, L. G. A Smooth Particle Mesh Ewald Method. *J. Phys. Chem.* **1995**, *103* (15), 31–34.

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³ Hess, B.; Bekker, H.; Berendsen, H. J. C.; Fraaije, J. G. E. M. LINCS: A Linear Constraint Solver for Molecular Simulations. *J. Comput. Chem.* **1997**, *18* (12), 1463–1472.

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⁵ Martínez, L.; Andrade, R.; Birgin, E. G.; Martínez, J. M. Packmol: A Package for Building Initial Configurations for Molecular Dynamics Simulations. *J. Comput. Chem.* **2009**, *30* (10), 2157–2164.

⁶ Nosé, S. A Molecular Dynamics Method for Simulations in the Canonical Ensemble. *Mol. Phys.* **1984**, *52* (2), 255–268.

⁷ Hoover, W. G. Canonical Dynamics: Equilibrium Phase-Space Distributions. *Phys. Rev. A* **1985**, *31* (3), 1695–1697.

⁸ Parrinello, M.; Rahman, A. Polymorphic Transitions in Single Crystals: A New Molecular Dynamics Method. *J. Appl. Phys.* **1981**, *52* (12), 7182–7190.