Free Energy Studies of Triethylene Glycol

Richard Olsen [C, S], Bjørn Kvamme and Tatiana Kuznetsova
Department of Physics and Technology, University of Bergen, Bergen, Hordaland, Norway
richard.olsen@ift.uib.no

Due to the hygroscopic nature of triethylene glycol (TEG) it is commonly used as a dehumidifier in ventilation systems, but is even more common in industry where it is used both to remove water from natural gas [1], as well as a thermodynamic hydrate inhibitor to prevent the formation of clathrate hydrates [2]. After TEG has been utilized, it is usually regenerated to prevent it from reaching other stages of processing. However, after regeneration, there will inevitably remain trace amounts of TEG. Thus, it is important to gain detailed knowledge on how leftover TEG may affect materials present in later stages of processing. This can be achieved by studying the interface between bulk mixtures (e.g. water and methane) and solid materials of interest, such as calcite (i.e. concrete in pipes), hematite (i.e. rust in pipes), and zeolites (i.e. molecular sieve). Free energy differences and chemical potentials are important tools for investigating the preferred trajectory a physical system will undertake during its lifetime. Therefore, it is of interest to estimate the difference in free energy between TEG on a surface of importance and of TEG in a bulk environment. It is difficult to measure free energies and chemical potentials at the interface between a bulk environment and a surface. Therefore, these properties often need to be estimated using theoretical tools. In our work, we used molecular dynamics (MD) simulations. There exists many methods to perform such estimates from MD data, such as temperature thermodynamic integration, thermodynamic integration and free energy perturbation. These have been considered and the most important have been used to study the free energy of TEG in bulk water and methane.

References

[1] Elsarrag, E., Magzoub, E. E. M., and Jain, S. Mass-transfer correlations for dehumidification of air by triethylene glycol in a structured packed column. Ind. Eng. Chem. Res. 43 (2004), 7676.
[2] Mohammadi, A. H., Eslamimanesh, A., Yazdizadeh, M., and Richon, D. Glycol loss in a gaseous system: Thermodynamic assessment test of experimental solubility data. J. Chem. Eng. Data 56 (2011), 4012.