Water solution of 1,4-dioxane: Molecular dynamics method

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We investigate physical properties of water solution of 1,4-dioxane using molecular dynamics and two force fields to describe dioxane molecules: Smith's model [1] and modified OPLS-AA [2]. The obtained results may be useful for simulations of polymer membranes in Red/Ox flow batteries. One of the features of the Smith's force field is an additional term in the formula of non-bonded interactions, which explicitly describes hydrogen bonds in solution. Water interactions are represented by three versions of TIP4P model developed in 1983, 2004 and 2005. The solution density, enthalpy of solvation and viscosity are calculated over the whole range of dioxane concentrations. A combination of Green–Kubo formula with double exponential method [3] is applied to calculate viscosities. Results of the calculations are compared to the experimental data [4, 5]. We discover that the Smith's force field is able to reproduce the experiment accurately whereas the OPLS-AA model demonstrates significant discrepancies with the experimental data. These discrepancies imply that the dioxane affinity to water is excessive in this model. The structural analysis of the solution confirms this implication.

[1] Smith G D, Borodin O and Bedrov D 2002 *J. Comput. Chem.* **23** 1480–1488
[2] Dodda L S, Cabeza de Vaca I, Tirado-Rives J and Jorgensen W L 2017 *Nucleic Acids Res. Spec. Publ.* **45** W331–W336
[3] Zhang Y, Otani A and Maginn E J 2015 *J. Chem. Theory Comput.* **11** 3537–3546
[4] Goates J R and Sullivan R J 1958 *J. Phys. Chem.* **62** 188–190
[5] Besbes R, Ouerfelli N and Latrous H 2009 *J. Mol. Liq.* **145** 1–4