Salting out and interfacial tension of methane with electrolyte solutions from computer simulations

Samuel Blazquez[1]
I. M. Zerón[1], M. M. Conde[2], J. L. F. Abascal[1] and C. Vega[1]
[1]*Departamento de Química Física, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain*
[2]*Departamento de Ingeniería Química Industrial y Medio Ambiente, Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid, 28006 Madrid, Spain*
samuelbl@ucm.es

The solubility of methane in water decreases when a small amount of salt is present. This is usually denoted as the salting out effect (i.e., the methane is expelled from the solution when it contains small amounts of salt). The effect is important, for instance the solubility is reduced by a factor of three in a 4 m (mol/kg) NaCl solution. Some years ago, we showed that the salting out effect of methane in water could be described qualitatively by molecular models using computer simulations [1]. However, the salting out effect was overestimated. In fact, it was found that the solubility of methane was reduced by a factor of eight. This points out to limitations of the force field used. In this work [2] we have carried out direct coexistence simulations to describe the salting out effect of methane in water using a recently proposed force field denoted as Madrid-2019 [3] based on the use of scaled charges for the ions and the TIP4P/2005 force field for water [4]. For NaCl the results of the Madrid-2019 force field significantly improve the description of the salting out of methane as can be seen in Fig. 1. For other salts the results are quite reasonable. Thus, the reduction of charge of the ions seems also to be able to improve the description of the salting out effect of methane in water.
Besides, we shall show that the brine-methane interface exhibits an increased interfacial tension as compared to that of the water-methane system. It is well known that electrolytes tend to increase the surface tension of liquid water, and this seems also to be the case for the interface between water and methane.

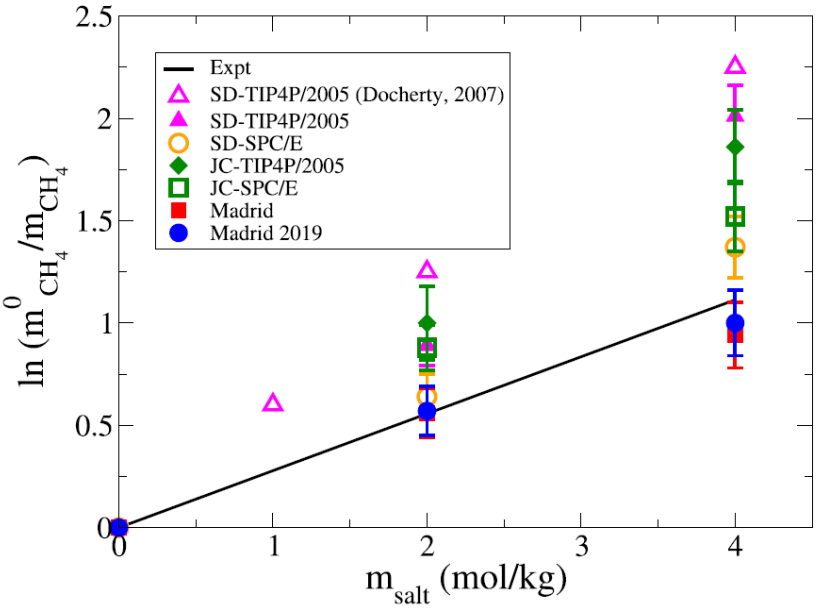

Figure 1: Salting out of methane calculated from computer simulations with different models

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