Assessing diffusivities of organic compounds in ionic liquids

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While equilibrium dissolution of volatile compounds in ionic liquids (ILs) has been studied for numerous systems, diffusivities of such compounds in the ILs have not commonly been assessed in most studies [1, 2]. We thus report on the diffusivity of methanol and ethanol in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [BMIM][NTf2].

Transient absorption of the single-component vapours in [BMIM][NTf2] was measured using sorption microgravimetry: IL was first degassed by exposing it to vacuum and then exposed to the vapours while mass of the solution was measured over time. Experimental data were evaluated by using Fick's second law.

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{1}$$

The model of the transient absorption into the one-dimensional liquid body upon its idealized instantaneous exposure was taken from the literature [3]. This model was then modified to reflect the realistic pressure dependences in the apparatus.

The knowledge of the diffusivities of volatile components in ILs enables to utilize extraction units outside equilibrium and, potentially, enhance their performance. Besides that, knowledge of diffusivities of volatile compound in ILs allows for the targeted preparation of IL-based separation membranes.

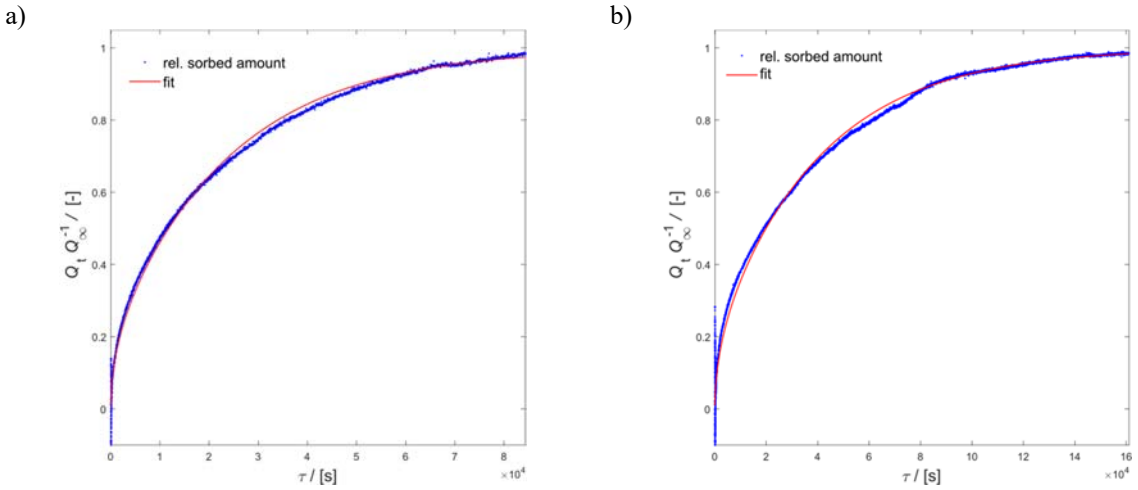

Figure 1: Transient absorption of methanol (a) and ethanol (b) vapour in [BMIM][NTf2].

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References

[1] A. Chapeaux, L. D. Simoni, T. S. Ronan, M. A. Stadtherr, J. F. Brennecke: *Extraction of alcohols from water with 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide*. Green Chemistry **10**, 1301–1306 (2008).

[2] A. Heintz, S. P. Verevkin, D. Ondo: *Thermodynamic properties of mixtures containing ionic liquids. 8. Activity coefficients at infinite dilution of hydrocarbons, alcohols, esters, and aldehydes in 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide using gas−liquid chromatography.* Journal of Chemical & Engineering Data **51**, 434–437 (2006).

[3] J. Crank: *The mathematics of diffusion*. Clarendon Press: Oxford, 1975.