Modelling facilitated transport in Polyvinyl amine membranes for CO2 capture: insights from Molecular Dynamics and PC-SAFT EoS.

Modelling facilitated transport in Polyvinyl amine membranes for CO_2 capture: insights from Molecular Dynamics and PC-SAFT EoS.

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Background

In the context of CO_2 removal from gas streams, the project NANOMEMC[2] (www.nanomemc2.eu) focuses on Facilitated Transport (FT) membranes based on Polyvinyl mine (PVAm). Such materials bear amine groups that, in presence of humidity, promote reactions that boost the transport of CO_2 while not affecting the other gases. A possible reaction route is shown in **Figure 1**.

Very few modelling studies are present in the literature concerning these fixed sites FT membranes despite their selectivity comparable to the most common absorption processes. Aim of the present work is to provide a detailad deep investigation on the transport properties of PVAm, to partially fill this lack, for the ternary system of CO_2/H_2O/PVAm. Molecular Dynamics (MD) and PC-SAFT[1] Equation of State (EoS) were used to achieve a reliable interpretation of the physical sorption process of CO_2 in such a complex, strongly polar environment.

Modelling and Simulating Strategies

PC-SAFT EoS: H_2O has been treated as 2B self-associating molecula (Huang and Radosz[2]); the induced (by H_2O) association has been considered for the PVAm with 2 and 3 sites (2B and 3B scheme) while the CO_2 studied as 0 or 2 (2B) association sites, not allowing for the self association even in the latter case.

MD simulations: molecular models of solvated PVAm membranes were constructed by explicitly considering a binary mixture of short chains (20 monomers) of PVAm and H_2O. Structural characteristics of these systems, such as pore size distribution and pore limiting diameter were obtained at different levels of hydration and correlated to self-diffusion of water in these structures. Chemical reaction(s) not explicitly included in the calculations.

Results

Figure 2 shows the main results achieved in terms of physical solubility of CO_2 in the swollen polymer while the self diffusion coefficient of H_2O in the polymer matrix, from MD simulations as well as from the scaling model of Phillies (1989) and experimental data, is depicted in **Figure 3.**

Conclusions

Physical sorption of CO_2 in swollen by water PVAm has been predicted by PC-SAFT EoS by two associating approach. The 2B scheme for CO_2 allows to elucidate the role of relative on the adsorption process. MD prediction on self diffusion of H_2O in PVAm agree with both experimental data and Phillies scaling model.

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Figure 1

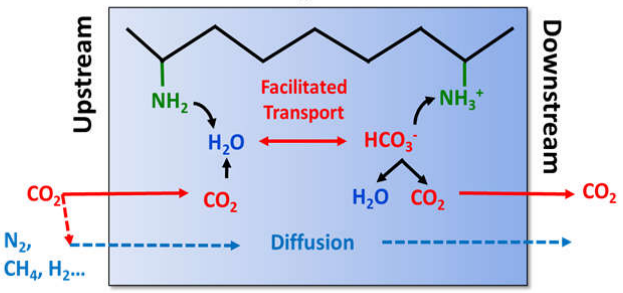

Figure 2

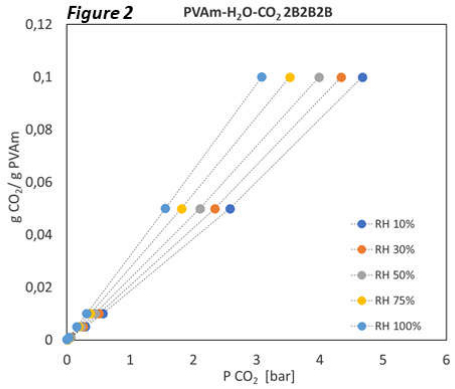

Figure 3