Modelling water sorption in Facilitated Transport Membranes with PC-SAFT Equation of State: the case of Polyvinyl amine

"This is a post-peer-review, pre-copyedit version of an abstract published in "EUROMEMBRANE 2018: Book of Abstract". The final authenticated version is available online at: http://euromembrane2018.org/programme/final-program/

ISBN: 9788409032471

Acknowledgements. *Performed in the framework of the European Project H2020 NANOMEMC2 "NanoMaterials Enhanced Membranes for Carbon Capture", GA No. 727734*

Modelling water sorption in Facilitated Transport Membranes with PC-SAFT Equation of State: the case of Polyvinyl amine

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Keywords: Facilitated Transport, gas separation, PC-SAFT, CO_2 capture, water sorption, Polyvinyl amine

Introduction

Facilitated transport membranes have great potential for carbon dioxide removal. By coupling the solution diffusion mechanism and the facilitation effect of the chemical reaction, CO_2 transport in such systems is substantially higher compared to other gases, like nitrogen and methane. The presence of water is needed in the membrane to activate the reaction mechanism, and affects the sorption and diffusion of all the gases in the membrane. The present work focuses on the modelling of water sorption in purified Lupamin® (polyvinylamine (PVAm)), with the PC-SAFT Equation of State (EoS) (Gross and Sadowski, 2001). The work is aimed at finding the best parameters and association schemes to model the water sorption in PVAm with the PC-SAFT model, in order to use it to model more complex situations such as the multicomponent sorption in the system.

Material and Methods

Within the SAFT theory, the PVAm-water mixture has been treated by using different approaches, in particular water has been considered as a self-associating species, while for PVAm we considered two schemes, one without association and one with water-induced association. Several association schemes, following the original notation given by Huang and Radosz (1991), were then tested to achieve the best agreement with experimental data. In particular, water association was modelled with the 2B and 4C association schemes, by using the pure component parameters from Diamantonis and Economou (2011), while PVAm was treated considering the 0, 2B and 3B association schemes. The PC-SAFT parameters for PVAm were retrieved by fitting the water sorption data.

Results and Discussion

When PVAm is considered as non-associating, no reasonable agreement is achieved between PC-SAFT model and the experimental data, for all the water association schemes used, as shown in Figure 1a, where, for the sake of brevity, only the results for water 2B association scheme are presented. When PVAm is considered as associative (induced) species, better results are achieved. Figure 1b shows the results obtained with the 2B association scheme for both PVAm and water. It can be seen that the PC-SAFT EoS is able to describe well the experimental data over the entire range investigated. Moreover, by increasing the number of PVAm association sites from 2 to 3, an improvement in the model description capability it is obtained, as figure 1c reports. The best fitting is achieved by considering 4 association sites for water and 3 for PVAm, as shown in figure 1d, even if the differences among the last two cases are quite small.

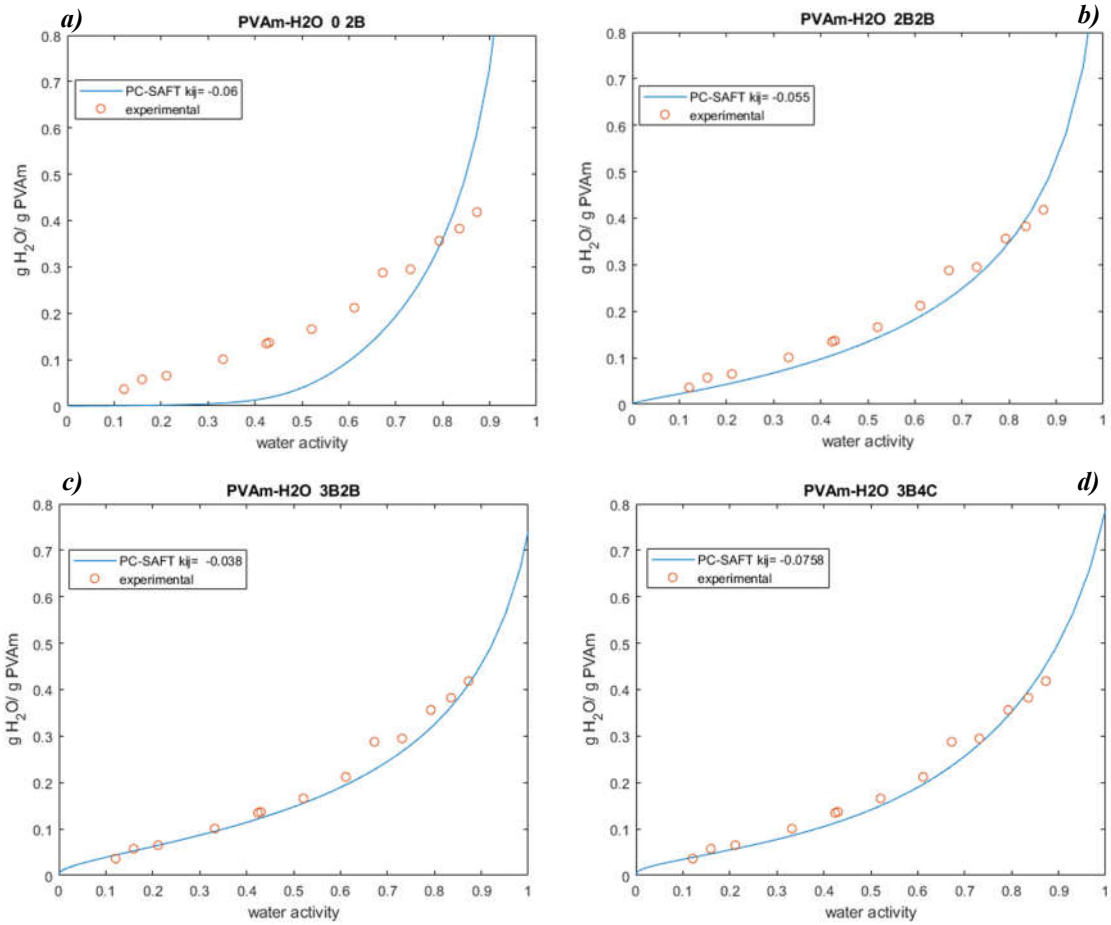

Figure 1. Water sorption on PVAm as function of water activity, red circles are experimental data, blue lines are PC-SAFT calculations for the association scheme considered: ***a)*** PVAm=0, H_2O=2B. ***b)*** PVAm=2B, H_2O=2B. ***c)*** PVAm=3B, H_2O=2B. ***d)*** PVAm=3B, H_2O=4C.

Conclusions

PC-SAFT EoS has been used to model the water sorption in purified PVAm (Lupamin®). The hydrogen bonding interactions between water and PVAm were modelled by using different association schemes. For each scheme, except the one that neglects the presence of association sites in PVAm, the equation of state proved capable to properly describe the experimental water sorption data. In particular, the best agreement was reached considering 3 association sites for PVAm and 4 association sites for water.

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