Membrane Modelling of Post-Combustion CO₂ Capture with Non-ideal Effects

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Our modern age is undeniably dependent on fossil fuels, although enormous amounts of efforts have been devoted to utilize sustainable energies. Due to its energy-efficient nature, membrane gas separation technology has gained industrial applications in controlling greenhouse gas emissions for a number of key industries. For example, hollow fiber and spiral wound membrane modules are commercially used for carbon capture in the natural gas industry. However, membrane technology faces some challenges that may restrict wider implementation. Part of this is the lack of detailed models to accurately simulate membrane gas separation processes, given the current state of the art is based on utilizing empirically based models utilizing reported gas permeances. However, non-ideal effects imposed by operating conditions as well as the nature of the feed gas may alter the structural properties of membranes, compared to the empirical findings, adversely affect the performance of a membrane module and subsequent carbon capture process. As such, there is need for detailed model development to address these challenges, as larger scale membrane processes will be commissioned once the performance of commercial membrane modules can be accurately simulated.

Mathematical models are required to evaluate the overall performance of gas separation membrane modules operating in the presence of non-ideal effects. These models can also predict the design parameters of membrane modules and facilitate process optimization. Many studies have been developed to model gas separation processes through membranes, but these neglect non-ideal effects by assuming ideal gas behaviour, negligible pressure loss at both retentate and permeate sides, assume isothermal process conditions, ignore concentration polarization effects and generally do not account for competitive sorption effects of mixed gas systems. Examples of where non-ideal behaviour is important is in pressure drop induce expansion resulting in gas cooling due to the Joule-Thomson effect; while is often ignored, since the process is assumed adiabatic.

This presentation will report on membrane model development that approaches permeability as a function of parameters, such as temperature and pressure, as well as the impact of concentration polarization in gas separation processes has on performance. In the present study, the developed model will be used to accurately describe the performance of a poly-dimethyl siloxane (PDMS) membrane for carbon dioxide separation. The model will represent the performance of the module for post-combustion carbon dioxide capture operating on an industrial process. In order to find a rigorous solution to the model, non-ideal effects will be added to the mass, momentum and energy equations and the results will be compared with the case of ideal treatment. The outcomes clearly demonstrate the importance of accounting for non-ideal behaviour in membrane modelling. The mathematical model is programmed in Aspen Custom Modeller (ACM) so it can be readily applied in process simulators such as Aspen Plus or Aspen Hysys. While previous models can rarely take multicomponent permeation into account, connecting to the large library of Aspen physical properties will further extend the applicability of the developed model and highlights its viability, given it can easily be incorporated into the larger suite of chemical engineering process units available through
Aspen Tech software. Ultimately, this simulation model will be used on large scale process designs to better review and predict the potential of membrane gas separation in other carbon capture applications.