

## Application of Maxwell Stefan equations to characterize silicalite membranes

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Inorganic membranes composed of zeolites such as silicalite are able to separate a wide variety of gas mixtures near atmospheric conditions and are therefore well suited to be used in tandem with, or to replace many gas separation processes such as absorption and cryogenic distillation. Due to the highly ordered and regular pore network inside zeolites, different gas molecules will interact with the zeolitic pores at different rates leading to the separation of gas mixtures by surface diffusion.

In order to characterize silicalite membranes to be used for the separation of multi-component gas mixtures, a rigorous model is required that accounts for both intermolecular and intramolecular interactions, as well as interactions between the gas molecules and the adsorbent. To this end, the Maxwell Stefan equations have been used to calculate the exchange diffusivities between gas molecules in the presence of similar, and different molecular species in silicalite membranes.

In this study, defect free membranes were fabricated by impregnating silicalite particles into ceramic supports composed of  $\text{TiO}_2$ . The membranes were then characterized by conducting binary gas permeation experiments at different feed pressures and compositions using synthetic post combustion flue gas mixtures composed of  $\text{CO}_2$  and  $\text{N}_2$ . For a membrane whose  $\text{CO}_2$  permeance was found to be a maximum of  $2.64 \times 10^{-6} [\text{mol} \cdot \text{m}^{-2} \cdot \text{Pa}^{-1} \cdot \text{s}^{-1}]$ , the exchange diffusivity of  $\text{CO}_2$  in the presence of  $\text{N}_2$  was found to decrease from  $2.32 \times 10^{-10}$  to  $2.5 \times 10^{-11} [\text{m}^2 \cdot \text{s}^{-1}]$  as a function of  $\text{CO}_2$  log mean partial pressure difference, and the exchange diffusivity of  $\text{N}_2$  in the presence of  $\text{CO}_2$  was found to increase as a function of  $\text{N}_2$  log mean partial pressure difference without bound beyond  $3.2 \times 10^{-11} [\text{m}^2 \cdot \text{s}^{-1}]$ . Although these diffusivities are not independent of operating conditions as desired, the observed trends better describe the transport of gas molecules as required for industrial separation process design.