

A Mechanism for Diffusion of CO₂ in Silica-Supported Amine Sorbents

Abstract

A two-dimensional reaction-diffusion model and associated sensitivity study has revealed that the stability of diffusive intermediates strongly influences the capacity for CO₂ uptake in highly loaded, silica supported PEI sorbents. Experiments show that humidity drastically increases the CO₂ capacity of these sorbents. Quantum chemistry shows, however, that zwitterions are unstable under polar conditions similar to those found in PEI. Physically-bonded moieties involving water, amines and CO₂ are proposed as better alternatives for diffusive intermediates. A continuum model was established based on these new intermediates. Qualitative and quantitative results – including the results of a sensitivity analysis – will be presented and compared with experimental data.