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Modeling the Transport Properties of CO_2/Polyamine Reactive Mixtures at Multiple Length-Scales SALOMON TURGMAN-COHEN, Kettering University, FERNANDO ESCOBEDO, Cornell University — Polyfunctional amine oligomers have been utilized as phase changing sorbents for carbon dioxide capture applications. Knowledge of the dynamic properties of these mixtures is essential to the design of efficient separation processes. The reactive character of polyamine/CO_2 blends and the severe variation in their transport properties as a function of CO_2 concentration renders these mixtures challenging to probe experimentally. We implement a multiscale modeling strategy in which polyamine/CO_2 mixtures are approximated by an ionic speciation model. Molecular dynamics (MD) simulations of such models are used to probe the diffusion coefficient and viscosities at various concentrations of ionic species and absorbed CO_2. The results of MD simulations are applied to a simple mass transfer model to predict optimal thicknesses of amine films and the kinetics of the absorption process. The latter is compared to experimental thermogravimetric results.

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