Molecular Dynamics Simulations of Viscosity Evolution of Aqueous Amine CO_2 Capture Solutions: Monoethanolamine versus Piperazine

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Chemical absorption of CO_2 by aqueous amine solutions is currently the most mature technology to capture CO_2 from post-combustion flue gases. A density-functional-theory-based fast virtual screening of the CO_2-capture performance has been developed for various aqueous amine solutions such as monoethanolamine (MEA) and piperazine (PZ). An important issue in developing high-performance amine solutions for CO_2 capture is that the viscosity of amine solutions containing PZ increases rapidly with the CO_2 loading. A new design of a fast-CO_2-absorbing component as fast as PZ but not as viscous as PZ is therefore desirable. For this purpose, using molecular dynamics simulations combined with Green-Kudo (GK) and Stokes-Einstein (SE) equations, we compute the transport behavior (viscosity and diffusivity) of aqueous PZ solution as a function of CO_2 loading at different conditions and compare our findings to the experimental data. The calculation indicates that the SE method predicts lower viscosities than the GK method. The CO_2-loading-dependent viscosities calculated with the GK method reproduce the experiments.