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Transport properties of carbon dioxide and ammonia in water - ethylene glycol mixtures from molecular dynamics simulations¹

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The endothermic decomposition of ammonium carbamate has been proposed as a novel heat sink mechanism for aircraft thermal management (Johnson *et al.* SAE Technical Paper 2012-01-2190, 2012, doi:10.4271/2012-01-2190]. The products of this decomposition are carbon dioxide and ammonia which need to be efficiently removed in order to better control the decomposition reaction. Molecular dynamics simulations can provide insight into the transport properties of carbon dioxide and ammonia in the carrier fluid. In this work, an extensive set of molecular dynamics simulations was performed to better quantify the concentration dependence of solubility and diffusivity of carbon dioxide and ammonia in water, ethylene glycol, and their mixtures at standard temperature and pressure and at elevated temperature. The simulation results confirm the experimental observations that ammonia is more soluble than carbon dioxide in either water or ethylene glycol and that both carbon dioxide and ammonia are more soluble in ethylene glycol than in water. The simulations of water - ethylene glycol mixtures show that increasing the molar fraction of ethylene glycol leads to increased solubility of carbon dioxide and ammonia in the mixture.

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