Prediction Model for Fick Diffusion Coefficients in Liquids with Dissolved Gases Close to Infinite Dilution

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Systems based on liquids containing dissolved gases are relevant in many areas of chemical and energy engineering. Well-known examples include liquid organic hydrogen carriers for the storage of hydrogen or ionic liquids for carbon dioxide sequestration from flue gas. One key property required for optimizing process design is the Fick diffusivity (D_{11}). However, determining D_{11} for all mixtures is unrealistic. Therefore, predictive engineering models are necessary.

This work presents a simple and transferable model for calculating D_{11} in binary mixtures consisting of a liquid solvent with a dissolved gas close to infinite dilution of the gas. This model requires only pure-component properties of the solvent and solute and does not incorporate any mixture-specific interaction parameters. Properties required are solvent density and viscosity and the molar mass and molar core volume V_0 of both components. V_0 can be calculated for an arbitrary substance using a group contribution approach considering the volume of the constituent atoms. The model was developed and trained with the help of 451 experimental data points for binary mixtures of a liquid with a dissolved gas. The solvents include linear, branched, and cyclic hydrocarbons, alcohols, acids, ethers, and ionic liquids. The solutes include eleven gases with a wide range of molar mass, weight, and polarity. Overall, the model was trained to reproduce D_{11} values ranging over more than two orders of magnitude with an average absolute relative deviation (AARD) of 19%. With the help of a testing set, including 314 D_{11} values which were not included in the training set and span over seven orders of magnitude, the predictive capabilities of the model were tested and agreement with an AARD of 24% was found. The model is exceptionally easy to implement and its successful application, even for binary gas mixtures, suggests a realistic depiction of fluid behavior.