Solubility of gases and solvents in silicon polymers: molecular simulation and equation of state modeling - DTU Orbit (08/11/2019)

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The solubility of n-alkanes, perfluoroalkanes, noble gases and light gases in four elastomer polymers containing silicon is examined based on molecular simulation and macroscopic equation of state modelling. Polymer melt samples generated from molecular dynamics (MD) are used for the calculation of gas and solvent solubilities using the test particle insertion method of Widom. Polymer chains are modelled using recently developed realistic atomistic force fields. Calculations are performed at various temperatures and ambient pressure. A crossover in the temperature dependence of solubility as a function of the gas/solvent critical temperature is observed for all polymers. A macroscopic model based on the simplified perturbed chain-statistical associating fluid theory (sPC-SAFT) is used for the prediction and correlation of solubilities in poly(dimethylsilamethylene) and poly(dimethylsiloxane) and also the phase equilibria of these mixtures over a wide composition range. In all cases, the agreement between model predictions/correlations and literature experimental data, when available, is excellent.

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