Gas Mixture Solubilities in Polyethylene below Its Melting Temperature: Experimental and Molecular Simulation Studies

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The accurate knowledge of the transport properties of gases in polymeric materials is crucial for technological applications, since these properties govern the behavior of end products under specific use conditions. One example concerns offshore oil and gas production, where flexible pipes and risers might be in contact with water, hydrocarbons, gases and all carried fluids at high temperature and high pressure. Another interesting application is the case of plastic pipes used for gas distribution networks. In the context of new energies, hydrogen is taking a growing place and its introduction in existing distribution pipes as a mixture with natural gas can be an alternative to its transport. We present solubility values of gas mixtures (CH4 + CO2 and CH4 + H2) in polyethylene below its melting temperature. The objective of such studies is to assess the existence of specific interactions between the matrix and one type of penetrant molecule. Data were acquired using both experiments and molecular simulations. Experiments were performed on a medium density polyethylene with pure and mixed gases for temperatures in the range 308-313 K. Hence, the solubility coefficient of each component of a gas mixture was determined. Monte Carlo simulations in the osmotic ensemble were also used to predict gas concentrations in the polymer phase. A good agreement with experimental data is observed. This is a significant validation of the use of an *ad hoc* constraint in the osmotic ensemble simulations to mimic the overall effect of the crystalline regions and to predict quantitatively solubility data in this semicrystalline system.