Solubility of Gases in Conventional Solvents and Ionic Liquids at Pre-combustion and Natural Gas Sweetening conditions from Monte Carlo Simulations

Thijs Vlugt[C] and Mahinder Ramdin[S]
Delft University of Technology, Delft, Netherlands
t.j.h.vlugt@tudelft.nl

The aim of the present study is the removal of acid gases from the pre-combustion and natural gas sweetening process using physical solvents. In the pre-combustion process, a fuel is gasified to produce syngas, which is a mixture of carbon monoxide (CO) and hydrogen (H_2). However, the syngas also contains several impurities like carbon dioxide (CO_2), nitrogen (N_2) and sulfur compounds (e.g., hydrogen sulfide, H_2S). Similar impurities are also present in raw natural gas. These sour gases should be removed to meet customer and pipeline specifications. CO_2 should be removed to avoid dry ice formation during the liquefaction of the gas and due to the low caloric value of the gas, while H_2S is highly corrosive for the pipelines. The removal of the acid gases is typically performed in an absorber-stripper configuration using either a physical, a chemical solvent or a mixture of both (hybrid) solvents. The choice of the solvent is case specific and depends on many factors like the type and concentration of the impurities, the composition, the temperature, the pressure and ultimately the product specifications. However, chemical solvents (e.g., amines) are most widely used in the natural gas industry. Although amines are very effective in reducing the acid gas concentration, especially at low acid gas partial pressures, it have several serious drawbacks. These include their high energy requirement for solvent regeneration, volatility, corrosivity and the low CO_2/H_2S selectivity. Since the natural gas sweetening and the pre-combustion process operate at high pressures, physical solvents can be applied for acid gas removal and their use are in fact nowadays preferred over the traditional amine solvents. In the past decade, ionic liquids (ILs) have emerged as a promising physical solvent for acid gas removal. ILs are defined as salts with melting point lower than 100 ^{o}C and characterized by a very low vapour pressure, high thermal and chemical stability. The solubility data of acid gases are extremely important for the optimal design of absorption columns. However, experimental data of poorly soluble gases (e.g., CH_4, N_2 and H_2) and toxic gases (e.g., CO and H_2S) are scarcely reported in the literature. Moreover, experimental data for the solubility of gas mixtures in solvents, which requires an increased experimental effort, are even more scarce. Here we use Monte Carlo simulations to compute the solubility of the pure gases CO_2, CH_4, CO, N_2, H_2S, H_2, nitrous oxide (N_2O) in several conventional solvents (e.g., Selexol, Purisol, Rectisol and Fluor solvent) and ILs. In addition, solubility of some gas mixtures relevant for the natural gas sweetening and the pre-combustion process has been computed as well. The molecular simulation results are compared with available experimental data [1]. The results show that molecular simulation can be a powerful tool, in the absence of experimental data, to obtain gas solubilities in complex solvents.