Influence of Methanol Addition to the Speciation in the Water - CO_2 - Diethanolamine System

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The absorption of acid gases by aqueous amine solutions is an important industrial process. The solutions produced by the acid gas absorption contain various molecular and ionic species. Then the modeling of such system is made using electrolyte models that involve parameters which are determined by a data treatment of solubility data. Several problems are encountered applying this procedure. The first one comes from the lack of consistency between the published solubility data. The second one is linked to the presence, in the solution, of species involved in chemical equilibrium. In this case the use, during the parameter determination step, of a database restricted to phase equilibrium is generally not sufficient to ensure that the resulting model gives a precise representation of the liquid phase composition, a condition to get a model that may be extrapolated and included in a global model that includes kinetics. To get a realistic model, the best way is to include speciation values in the database used to determine the model parameters. This is the reason why we have constructed a new experimental device that allows getting not only solubility data but also speciation ones. The method, based on IR spectroscopy, has been applied successfully in our laboratory to the case of CO_2 absorption in aqueous methyldiethanolamine (MDEA) and diethanolamine DEA solutions. However, as, since several years, various new solvents systems have been developed that are mixtures of a chemical solvent such as alkanolamines and a physical one, we decided to extend our method to the determination of the speciation in such mixed solvent systems. In the present study we have considered the water - DEA - CO_2 - methanol system. Three solvent compositions have been considered, the measurement being made at 25C and at various CO_2 loadings. The values obtained allow determining the influence of methanol addition to the liquid phase composition. The results have been modeled using an electrolyte equation of state that could be applied to this mixed solvent system.