Modeling the Vapour Liquid Equilibrium of the Binary (Carbon Dioxide+Glycol) and Ternary (Carbon Dioxide+Glycol+Water) Systems

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The sequestration of carbon dioxide in depleted reservoirs and underground aquifers has become a promising technique to effectively reduce the carbon footprint of processing fossil fuels. Before the pipeline transmission and subsequent downhole injection of carbon dioxide into these reservoirs, the gas needs to be dehydrated to reduce the risk of hydrate formation, corrosion problems and the formation of liquid phases in the lines. In many cases, well designed acid gas compression and injection facilities can be utilized to avoid dehydration facilities. However, if dehydration of the acid gas stream is still necessary, glycol dehydration schemes are often used to reduce the water content of the acid gas to the appropriate level. Although effective in reducing the water content of acid gas mixtures, one concern with these facilities is the emission of glycols into the atmosphere during the solvent regeneration process. The design of these facilities requires accurate modeling techniques which can capture the vapour-liquid equilibrium (VLE) properties of these systems over the appropriate operating conditions. The cubic plus association (CPA) model has been very successful in modeling the VLE of binary mixtures containing associating and/or polar compounds (e.g. mixtures with water and glycols) and mixtures of these compounds with components which cannot self-associate (e.g. carbon dioxide). In this presentation, the ability of the model to predict the VLE of the CO2-glycol-water ternary system will be shown. The prediction of the ternary systems will be based on binary interaction parameters regressed from a databank which contains all of the known VLE data available in the open literature. In addition, the existing experimental binary and ternary VLE data will be reviewed based on the results obtained from the CPA and those from traditional cubic equations of state with local composition activity coefficient models.