

Vapour-liquid equilibrium for novel solvents for CO₂ post combustion capture

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Introduction

Vapour-liquid equilibria (VLE) of gas-solvent systems governs the distribution of molecular species between the vapour and liquid phases and is an important factor for the design of gas treating processes, including water-wash section and solvent losses due to volatility. For proper thermodynamic modelling accurate equilibrium data for the reactant-water systems for a wide range of temperatures, pressures and solvent concentrations are essential [1].

Presently, more research on aqueous solutions of novel promising solvents and solvent blends is in demand, including VLE data.

VLE data for promising novel solvent–water systems is rarely available in the literature. Almost all available references give total pressures as a function of temperature and liquid phase composition (P, T, x). The activity coefficients and vapour phase composition are then calculated from the total-pressure data based on the Gibbs-Duhem equation. Values of the limiting activity coefficients, γ_i^∞ , are important for the development of new thermodynamic models and for the adjustment of reliable model parameters or the choice of selective solvents for the absorption.

In this work VLE measurements provide experimental data on pressure, temperature and the composition of both phases (P, T, x, y) for novel binary and ternary CO₂ capture solvents. Assuming that the vapor phase is an ideal gas and that liquid properties are independent of pressure, activity coefficients, with pure solvent agent as reference state, can be calculated directly from the experimental data using the following correlation:

$$\gamma_i = \frac{y_i P}{x_i P_i^{sat}} \quad (1)$$

No VLE data were previously reported in the literature for the studied solvent systems.

Experimental set-up and results

Isothermal vapour-liquid equilibrium (VLE) measurements at 60, 80 and 100° C for different aqueous solutions of the solvent agents were performed using a modified Swietoslowski ebulliometer described in detail by Rogalski et al [3]. The equilibrium still, made of glass, has a volume of 200 mL. It is designed for operation at temperatures below 200°C and pressures of maximum 1 bar. The scheme of the experimental set-up is shown in the Figure 1[5].

The liquid in the ebulliometer is heated by an electric heater and partially evaporated. The stream of overhead liquid and vapour obtained is pumped by a Cottrell pump and passed to a thermometer placed inside the equilibrium chamber. The measured temperature corresponds to the equilibrium conditions established by the total pressure and the equilibrium composition of the liquid and vapour phases. The apparatus enables the withdrawal of samples of both vapour condensate and liquid phase. Gradual change of the composition of the solution in the apparatus can be made by introducing known quantities of one of the pure components[5].

Experimental activity coefficients were calculated using equation(1). Binary interaction parameters were determined by regression of the experimental data using Modfit, an in-house Matlab program for parameters estimation.

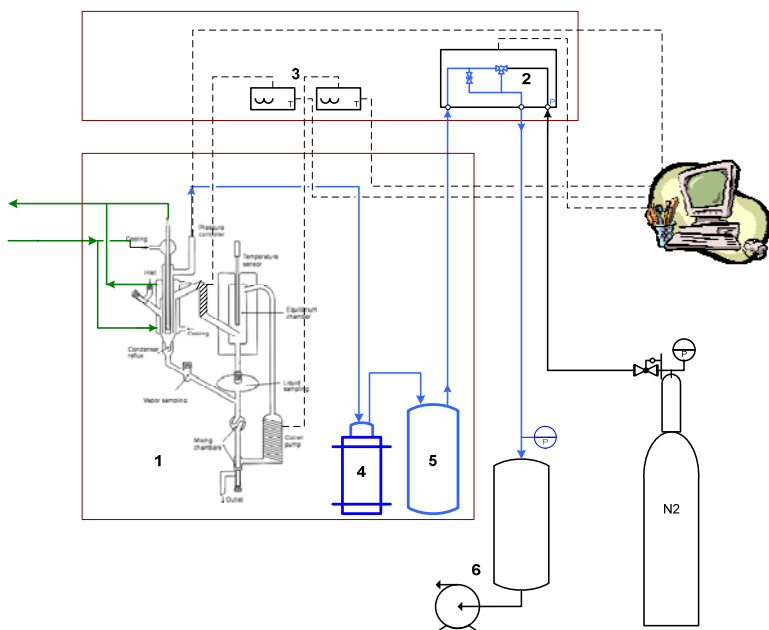


Figure 1. Experimental set-up. 1 – ebullimeter; 2 – pressure controller; 3 – temperature controllers; 4 – cold trap; 5 – buffer vessel; 6 – vacuum pump with buffer vessel[5].

The equilibrium Pressure as a function of Temperature diagram for one of the Solvents, measured with above mentioned Swietoslowski ebullimeter, is shown in Figure 2.

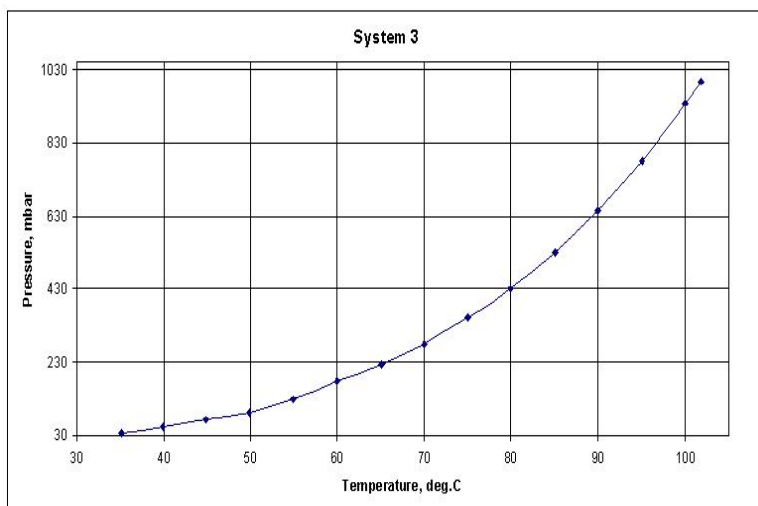


Figure 2. Equilibrium Pressure as a function of Temperature

Measured equilibrium data for different aqueous solutions of the solvent agents will be presented at the temperatures of 60, 80 and 100° C.

Conclusions

The ebullimeter enables an accurate determination of the vapour-liquid equilibrium of pure components and mixtures. The accuracy of the results obtained is limited only by the purity of the substances used and by the precision of the analytical methods used for the sample analyses.

There was obtained VLE data for novel solvent systems, which can be used for improvement of the thermodynamic models of the acid gas-solvent-water systems.

References

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