Phase Behaviour of Binary and Multicomponent Mixtures for CO_2-EOR: A Comparison Between Predictive Modelling and Experimental Data

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It is now clear that, to avoid dangerous climate change, a dramatic reduction in carbon dioxide emissions is required in the coming decades. Carbon capture and storage (CCS) is a promising large-scale clean-energy technology. Depleted oil and gas fields have been identified as promising sinks for CO_2. Furthermore, to partially offset CCS costs, the use of CO_2 in enhanced oil recovery (EOR) may be beneficial. For both CCS in depleted oilfields and CO_2-EOR, a full understanding of the phase behaviour of CO_2–hydrocarbon mixtures at reservoir conditions is required.

In order to simulate such processes, and to allow for the diverse chemical composition of the components present, several group-contribution-based thermodynamic models have been developed, notably SAFT-γ Mie. To date, the group parameter tables for SAFT-γ Mie are incomplete and/or lack validation in respect of some terms. To help address this, vapour-liquid equilibrium data (VLE) were measured for mixtures of (methylcyclohexane (MCH) + CO_2) and (MCH + N_2) at temperatures from (323 to 423) K and at pressures up to the critical. These data were used to optimise the interaction parameters involving MCH with N_2 or CO_2. Additionally, VLE data for (CO_2 + MCH + N_2) were measured at the same temperature and pressure conditions to validate the model. The measurements were carried out with a new analytical VLE apparatus equipped with on-line sampling and a gas chromatograph for compositional analysis. It was validated by means of saturated vapour pressure measurements on methanol and VLE measurements on (CO_2 + heptane). The results of these validation measurements were in good agreement with the literature. The experimental results for the (CO_2 + MCH + N_2) system have been compared with the predictions of both the SAFT-γ Mie approach and the Predictive-Peng-Robinson equation of state, with group contribution formulae for the binary interaction parameters.

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