Phase Behavior of CO_2 + Hydrocarbon Mixtures for CO_2 Sequestration through EOR. First step: Equation of state modeling of binary mixtures.

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Several scientific articles, as well as governmental reports and other sources around the world, have been recently proposing or concluding that CO_2 sequestration through EOR would be the most promising strategy, both technically and economically, for reducing CO_2 emissions globally.

Different decisions concerning for example whether a specific exploited reservoir is a good candidate for CO_2 -EOR or even the design of optimum long-term production strategies for new reservoirs can be based on specific phase equilibrium estimations, which depend essentially on the reservoir fluid composition and temperature. In particular, the minimum miscibility pressure (MMP) which indicates the minimum pressure necessary to get complete miscibility between CO_2 and the hydrocarbons mixture at a given temperature, is of special interest.

The best suited models for this type of calculations are equations of state, and modeling capabilities depend strongly on the type of mixing rules implemented and procedures for the estimation of interactions parameter values.

Binary mixtures of CO_2 with n-alkanes, from the lighter to the heavier ones, have been studied by an important number of authors, both experimentally and using different types of models. An important degree of inaccuracy or scatter can be realized when comparing data from different sources, specially for the more asymmetric systems (long chain alkanes). At the same time, modeling studies have generally achieved only partially accurate results in the correlation of phase equilibrium data in wide ranges of temperature and pressure.

During the last years we have dedicated some effort and a few publications to explore the possibilities that the flexible Cubic Mixing Rules (CMRs) offer for the modeling of asymmetric systems −where quadratic mixing rules fail- and to develop parameterization procedures. In this contribution, we present accurate results of predictive correlations for individual systems in wide ranges of temperature and pressure, based on a three-parameter cubic equation of state (the RK-PR EOS) coupled to CMRs. The objective functions in our optimization procedures present a balance between different type of experimental information, which made possible the achievement of a simultaneous proper description of both the critical and classical regions, which had not been possible before through different approaches. It is important to remark that, thanks to the third parameter in the RK-PR EOS and an adequate pure-compound parameterization procedure, good results are also obtained in the prediction of densities for the same mixtures.

The results achieved so far for the correlation of the complete series of CO_2 + n-alkane binary systems as a whole, with carbon number-dependent parameters, are also presented, discussing strengths and limitations.

Future work includes the study of prediction and correlation of ternary mixtures phase equilibria, as well as multi-component and in particular MMP calculations.