A New Approach to the Calculation of the Interfacial Tension for the (Carbon Dioxide + Water) System

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Accurate knowledge of the physical properties of the carbon dioxide + water system is becoming increasingly important in the optimization of carbon dioxide capture, utilization and sequestration (CCUS) processes. The interfacial tension between carbon dioxide and water is one important, but often overlooked, physical property. A robust, accurate and computationally efficient determination of the interfacial tension is very important for simulations required in CCUS.

There are a number of techniques to model the interfacial tension, which range from simple empirical correlations to those based on statistical thermodynamics. Unfortunately, the quicker, simpler methods suffer in their accuracy when modeling the carbon dioxide + water system over the full *T-P-x* range required in CCUS processes. Techniques derived from statistical thermodynamics and the theory of inhomogeneous fluids have been shown to be more accurate, however, due to their complexity, a number of the methods used to predict interfacial tensions are unsuitable for engineering applications.

Recently an alternative theory for the calculation of multicomponent interfacial profiles has been proposed. In this approach, the interfacial integration follows a minimum-effort path that is well-defined by any rational EoS. This has resulted in a procedure that independently solves the interfacial density profiles of the species in a robust and efficient way.

In this work, the new approach will be used to model the carbon dioxide-water interfacial tension data available in the open literature. In addition, we will show how different types of phase behaviour, as described by the EoS, affect the interfacial tension and the corresponding density profiles.