A New Fundamental Equation of State for the Binary Mixture of Carbon Dioxide and Argon

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Many studies and projects are addressing the problem of climate change caused by increasing atmospheric concentrations of greenhouse gases. One of the discussed mitigation approaches is carbon capture and storage (CCS). Its focus lies on the main greenhouse gas carbon dioxide. This technique involves separation and transportation of carbon dioxide and poses the challenge of safe storage. A knowledge of thermodynamic properties, like homogeneous densities or vapor-liquid-equilibrium properties, is mandatory to establish efficient and safe techniques. An accurate and realistic process design requires equations of state for such complex gas mixtures. The empirical and highly accurate model presented was developed in the form of the Helmholtz energy. As applied in the GERG-2008[1]for natural gases, the mixture model is based on EOS for the pure fluids, a corresponding states approach with up to four adjustable parameters per binary subsystem, and optionally a departure function, which contains multiple adjustable parameters. For the mixture carbon dioxide and argon, new highly accurate experimental data were obtained at Ruhr-Universität Bochum and SINTEF Energy Research. The data included density, speed of sound, and phase boundary measurements. Although the system was already described by a binary-specific function developed by Gernert and Span (2016)[2] as part of the “equation of state for combustion gases and combustion gas like mixtures” (EOS-CG), further improvement of the model became possible based on the new data sets. The new model is valid over the complete fluid state region and exhibits a reasonable extrapolation behavior. These results were achieved with the help of a new tool to enhance the adjustment procedure and to gain more knowledge about EOS, especially for mixtures. This tool is able to visualize the Helmholtz energy, the contribution of various terms, and their derivatives in three-dimensional diagrams. These functions lead to a better understanding of the influence of specific parameters or terms on the mathematical structure of the Helmholtz energy mixture model.

References:

[1]. Kunz, O., Wagner, W., *Journal of Chemical Engineering Data 11*, 2012, 3032-3091
[2]. Gernert, J., Span, R., *The Journal of Chemical Thermodynamics*, 2016, 274-293