## An Extended Fundamental Equation of State for Thermodynamic Properties of Mixtures Relevant for CCS-Applications

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Carbon capture and storage (CCS) is considered to be a key technology for a low-emission society. The safe and efficient design of CCS processes requires high-quality thermodynamic property data. In early studies, such properties were calculated for pure carbon dioxide. In reality, the captured, transported, and stored fluids are carbon-dioxide-rich mixtures with some components on a percent level and a variety of possible components contained on an impurity level. Some of these components have a significant impact on the thermodynamic behavior and especially on phase-equilibrium properties. The most accurate way to determine state properties of such highly non-ideal mixtures is by means of empirical multiparameter equations of state explicit in the reduced Helmholtz energy. In 2013, the development of a first reference model for CCS-relevant mixtures was completed and the model was later on presented by Gernert and Span [1] as the "equation of state for combustion gases and combustion gas like mixtures" (EOS-CG). It already allows for an accurate description of mixtures containing carbon dioxide, water, nitrogen, oxygen, argon, and carbon monoxide. Its mathematical structure enables the calculation of multicomponent-mixture properties by modelling each binary combination of the components. Over the last years, the model has been continuously updated and extended to additional components. For some binary systems with methane, hydrogen, and hydrogen sulfide, existing functions from the GERG-2008 model for natural gases of Kunz and Wagner [2] were adapted. Furthermore, new formulations were developed for binary mixtures with sulfur dioxide, hydrogen chloride, chlorine, monoethanolamine, and diethanolamine. Since some components were not described by accurate pure-fluid equations of state, new Helmholtz explicit formulations were developed.

References:

[1] Gernert and Span (2016), "EOS-CG: A Helmholtz Energy Mixture Model for Humid Gases and CCS mixtures", J. Chem. Thermodynamics 93, 274-293

[2] Kunz and Wagner (2012), "The GERG-2008 Wide-Range Equation of State for Natural Gases and Other Mixtures", J. Chem. Eng. Data 57, 3032