

Equation of State for Combustion Gases and Combustion Gas Like Mixtures

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The reduction of greenhouse gas emissions is the most prominent goal in energy technologies. Fossil power-generation with capture and storage of CO₂ (CCS) is considered a key technology in this context. Most CCS technologies result in high demands on thermodynamic-property models. Properties at high pressures need to be calculated accurately for mixtures of highly non-ideal gases like carbon dioxide and water (vapor) and for complex phase-equilibria. Corresponding demands were formulated, e.g., by the International Association for the Properties of Water and Steam (IAPWS) as IAPWS Certified Research Need (ICRN) *Thermophysical Properties of Humid Air and Combustion-Gas Mixtures*. As one of the projects funded by the E.ON research initiative, the project *Equation of State for Combustion Gases and Combustion Gas Like Mixtures* (EOS-CG) focuses on a thermodynamic-property model, which is sufficiently accurate for the relevant range of mixtures, temperatures and pressures (from humid air to compressed liquefied carbon dioxide). The recently internationally accepted standard for properties of natural gases, the GERG 2004 equation of state, is used as a starting point. Its performance for mixtures and states relevant to energy storage and CCS is analyzed in detail. For this purpose a comprehensive database has been built, comprising experimental p - ρ - T , vapor-liquid equilibrium, heat capacity and excess enthalpy data of the main combustion gas components nitrogen, oxygen, argon, carbon dioxide, water and their mixtures. Where available, the GERG 2004 is compared to data for the relevant binary and ternary mixtures. Deviations between experimental and calculated data are determined for liquid phase, phase equilibrium and vapor phase conditions. The quality of the experimental data is assessed depending on the denoted uncertainties, the age of the publication and the measurement method. This leaves very few data points of high quality but limited temperature and pressure range to compare the GERG 2004 with. For high temperatures and low pressures the comparison to an ideal mixture of real gases is performed to study its extrapolation behavior. For other p - T -regions not covered by experimental data the performance of the GERG model can only be investigated qualitatively. The contribution presented at the 17th *Symposium on Thermophysical Properties* will discuss the results of this comparative study. The accuracy of the formulation for all important mixtures in CCS processes will be presented with regard to process simulation application. It will be shown that the GERG 2004 performs well for dry air and regular combustion gas mixtures even far beyond its defined range of validity.