A New Model Combining Helmholtz Energy Equations of State with Gibbs Excess Models to Describe Reactive Mixtures

Tobias Neumann [C, S]
Thermodynamics, Ruhr-University Bochum, Bochum, North Rhine-Westphalia, Germany
and Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway
t.neumann@thermo.rub.de

Jana Poplsteinova Jakobsen
Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway

Monika Thol and Roland Span
Thermodynamics, Ruhr-University Bochum, Bochum, North Rhine-Westphalia, Germany

Carbon dioxide emissions have to be decreased to decelerate global warming. To stay below a 1.5 °C temperature increase the latest IPCC report [1] suggests four pathways of actions. Three contain the large-scale deployment of "carbon capture and storage" (CCS) technologies. On an industrial level, chemisorption is a feasible solution due to its relatively high efficiency and relatively low costs to capture CO2 produced, e.g., by burning fossil fuels. The most promising and already used sorbents are amine-based. In a chemical reaction between the CO2-rich gas stream and the liquid sorbent, CO2 is bound to the amine. To establish safe and efficient processes, knowledge of thermodynamic properties, e.g., of vapor-liquid and chemical equilibrium, as well as density data is of great importance. These properties are typically calculated from various different models. In particular, different approaches are used to simulate capture, transport, and storage processes. This leads to inconsistencies at the interfaces of the different process steps. Therefore, a new model was developed which reduces the inconsistencies by describing the required properties with a single equation of state that is applicable to capture and transport processes.

The new model is based on the well-established fundamental equations of state (EOS) in form of the Helmholtz energy, for example the EOS-CG 2019 [2]. This mixture model is the most accurate EOS for the calculation of thermodynamic properties of CO2-rich mixtures in the fluid state region. However, it cannot describe chemical reactions forming new components. Thus, the Helmholtz mixture model is combined with a Gibbs excess energy model in a consistent way. Due to the nature of the reactive mixtures, an e-NRTL model as proposed by Putta et al. [3] was chosen.

The structure of the new model as well as first results, which are validated with experimental data, will be presented.

References

[1] IPCC. Global warming of 1.5 °C. 2019. https://www.ipcc.ch/sr15/.

[2] S. Herrig, New Helmholtz-Energy Equations of State for Pure Fluids and CCS Relevant Mixtures, Ph.D. Thesis, Ruhr-Universität Bochum, 2018.

[3] Putta KR, Pinto DDD, Svendsen HF, Knuutila HK. CO2 absorption into loaded aqueous MEA solutions: Kinetics assessment using penetration theory. Int J Greenh Gas Control. 2016;53:338-353. doi:10.1016/j.ijggc.2016.08.009