

## New Fundamental Equations of State for Hydrogen-Rich Binary Mixtures

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Hydrogen is one of the most promising energy carriers of the future. However, the change to hydrogen and hydrogen mixtures as a sustainable and CO<sub>2</sub>-neutral energy supply is a step-by-step process towards decarbonization of primary energy sources. For example, new technology to inject synthetically produced hydrogen obtained from renewable excess energy sources (“power-to-gas”) into the natural gas grid offers the ability to offset products of carbonaceous energy sources. In this context, very high hydrogen concentrations can occur locally or temporarily in the natural gas grid. These have to be considered in the simulation of gas storage and grids, as well as transformation to the new technology. The thermodynamic property model GERG-2008 of Kunz and Wagner<sup>1</sup> is the current ISO standard for the calculation of natural gas properties and was developed particularly for conventional natural gas mixtures with high methane concentrations at typical pipeline conditions. Hydrogen was only considered as a trace element. To additionally obtain safety and accounting-relevant properties for synthetic hydrogen-rich mixtures with the same quality as for conventional natural gases, new binary mixture models in terms of the reduced Helmholtz energy are addressed in this work. Based on the reference equation for pure hydrogen by Leachman et al.,<sup>2</sup> a non-linear fitting algorithm developed by Lemmon and Jacobsen,<sup>3</sup> and the results of a comprehensive literature search, new multiparameter equations of state were developed for binary hydrogen mixtures. These can then be combined for multicomponent systems to obtain similar uncertainties in calculated properties. The pure-fluid equations required in the mixture model for the other components in each binary system either correspond to the equations used in the GERG-2008,<sup>1</sup> or to newer more accurate equations. Thus, the new mixture equations can be integrated into the GERG-2008<sup>1</sup> and the broad field of application of the model is maintained.

### References

<sup>1</sup> Kunz, O. and Wagner, W., *The GERG-2008 wide-range equation of state for natural gases and other mixtures: An expansion of GERG-2004*. *J. Chem. Eng. Data*, 2012, 57: 3032.

<sup>2</sup> Leachman, J.W., Jacobsen, R.T, Penoncello, S.G., and Lemmon, E.W., *Fundamental Equations of State for Parahydrogen, Normal Hydrogen, and Orthohydrogen*. *J. Phys. Chem. Ref. Data*, 2019, 38: 721.

<sup>3</sup> Lemmon, E. W. and Jacobsen, R. T., *A New Functional Form and New Fitting Techniques for Equations of State with Application to Pentafluoroethane (HFC-125)*. *J. Phys. Chem. Ref. Data*, 2005, 34: 69.