

Current Status of Thermodynamic Properties of Ortho-, Para- and Normal Hydrogen

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The usage of hydrogen has been hailed as a potentially game-changing countermeasure to current climate trends. For a safe and efficient application of large-scale hydrogen technology, accurate knowledge of the thermodynamic properties of hydrogen is important. Corresponding data are either obtained from laboratory experiments or derived from fundamental theories, also called ab initio approaches. To calculate thermodynamic properties in the entire fluid region in practice, equations of state are developed based on these data and on knowledge of the physical behavior of various thermodynamic properties.

Although hydrogen is often considered a very well-known pure substance, it poses particular challenges for the development of equations of state. As a matter of fact, “pure” hydrogen is a mixture of the spin isomers orthohydrogen and parahydrogen. The two spin isomers exhibit different thermodynamic properties, and their equilibrium composition changes with temperature. Hydrogen consists of more than 99 % parahydrogen at temperatures below 20 K. At standard conditions, hydrogen has a composition of about 75 % ortho- and 25 % parahydrogen and is called normal hydrogen. The change of the para-/orthohydrogen composition makes laboratory experiments considerably more difficult, especially at cryogenic temperatures, and also poses challenges for modeling.

The current reference equations of *Leachman et al. (2009)* largely depend on experimental data that were measured for rocket developments in the 1950s to 1970s; until recently, this data situation had not changed. However, in different research groups the newly awakened interest in thermodynamic properties of hydrogen resulted in activities that aim at a substantial improvement of the available database. The corresponding projects rely both on state-of-the-art experimental equipment and on ab initio approaches. First results show the expected limitations of the current reference equations of state. This work will present these findings and first steps towards new reference equations of state for hydrogen.