

## IAPWS Certified Research Need – ICRN

# Thermophysical Properties of Humid Air and Combustion-Gas Mixtures

### Closing Statement

In 2001/2002, the IAPWS Working Groups "Thermophysical Properties of Water and Steam" and "Industrial Requirements and Solutions" examined the published work and common industrial practice in the area of the thermodynamic and transport properties of humid air, combustion gases, and combustion gas related mixtures, which are required for accurate system design of power plants. They found that both the available information and the common technical practice were deficient in a number of respects. This resulted in the formulation of ICRN-14, Thermophysical Properties of Humid Air and Combustion-Gas Mixtures. ICRN-14 was approved in July 2002 at the IAPWS annual meeting in Buenos Aires, Argentina, with an expiration date of September 2005. At the 2005 annual meeting in Santorini, Greece, its validity was extended to September 2008. At the 2008 annual meeting in Berlin, Germany, it was discussed that ICRN-14 has supported relevant work in different places in the world. Some of the problems addressed in ICRN-14 have been solved by this work. Other problems, particularly phase equilibria in humid air and combustion gases at high pressure and temperature, are still not satisfactorily solved. Further experimental and theoretical work is required in these fields. However, ICRN-14 did not cover extended requirements that result mainly from carbon capture and storage (CCS) applications. It was decided to formulate an ICRN adapted to these new requirements and to allow ICRN-14 to expire. The expiration date of ICRN-14 was set to September 2011.

Over the last decade, thermophysical properties of humid air and combustion-gas mixtures have been addressed in research projects in many places in the world. This closing statement cannot yield a complete review of the scientific work done. Instead, three projects that are closely related to ICRN-14 will be discussed briefly as examples.

As part of the *Advanced Adiabatic Compressed Air Energy Storage (AA-CAES)* project funded by the European Commission, a working group was established that addressed both thermodynamic and transport properties of humid air. The work on thermodynamic properties was coordinated by Prof. Kretzschmar, University of Applied Science Zittau/Görlitz, the work on transport properties by Prof. Vogel, University of Rostock. Experimental work was carried out at PTB (Braunschweig), Imperial College, London, Ruhr-University Bochum, University of Natural Resources and Life Sciences, Vienna, and at the University of Rostock. The project substantially increased the amount of experimental data available for humid air and resulted in new, refitted formulations and in recommendations for the calculation of thermophysical properties of humid air. The results of the project are summarized in a PTB report [1] and in less detail in [2]. Publications on individual results are also available.

At the National Institute of Standards and Technology (NIST) in the USA and the University of Nottingham in the UK, Drs. Harvey and Wheatley and coworkers calculated second virial coefficients relevant for humid air and humid combustion gases from first principles, see e.g. [3,4]. This work has improved the understanding of the systems addressed by ICRN-14, particularly at low densities and high temperatures, where most experimental approaches become increasingly uncertain.

At Ruhr-University Bochum, Prof. Wagner, Prof. Span and coworkers attempt to improve the current standard for thermodynamic properties of natural gases and related mixtures, the GERG-2008 model [5], regarding the description of humid air and CO<sub>2</sub>-rich mixtures [6]. Like the work by Wheatley and Harvey [4], this work points to the fact that today the most challenging humid-gas problems are related to CO<sub>2</sub>-rich mixtures typical for power processes with CCS. A good example of the complexity of the resulting problems is given in the current, IAPWS-funded cooperation between Ruhr-University Bochum and the Czech Academy of Sciences, which addresses the consistent description of fluid and hydrate properties in the CO<sub>2</sub>/water system [7].

ICRN-14 has helped to initiate work on humid air and on humid gases in general at many institutes in the world. However, it does not adequately cover the problems considered most challenging today. Therefore, IAPWS allows ICRN-14 to expire as of September 2011. An ICRN adapted to the new demands will be formulated.

Plzeň, September 2011

## References

- [1] *S. Herrmann, H.-J. Kretzschmar, V. Teske, E. Vogel, P. Ulbig, R. Span and D. P. Gatley: Determination of Thermodynamic and Transport Properties of Humid Air for Power-Cycle Calculations. PTB-Bericht, Braunschweig (2009).*
- [2] *S. Herrmann, H.-J. Kretzschmar, V. Teske, E. Vogel, P. Ulbig, R. Span, and D. P. Gatley: Properties of Humid Air for Calculating Power Cycles. J. Eng. Gas Turbines and Power 132, 093001 (2010).*
- [3] *A. H. Harvey and P. H. Huang: First-Principles Calculation of the Air-Water Second Virial Coefficient. Int. J. Thermophys. 28, 556-565 (2007).*
- [4] *R. J. Wheatley and A. H. Harvey, Intermolecular potential energy surface and second virial coefficients for the water-CO<sub>2</sub> dimer. J. Chem. Phys. 134, 134309 (2011).*
- [5] *O. Kunz and W. Wagner: The GERG-2008 Wide-Range Equation of State for Natural Gases and other Mixtures: An Expansion of GERG-2004. To be submitted to J. Chem. Eng. Data (2011).*
- [6] *J. Gernert and R. Span: EOS-CG: An Accurate Property Model for Application in CCS Processes. Proc. Asian Thermophys. Prop. Conf., Beijing (2010).*
- [7] *V. Vins: Development of Thermodynamic Models for Hydrates in Water-Carbon Dioxide Mixtures. Report on the IAPWS Project, Annual IAPWS Meeting, Plzeň (2011).*