# U.S. National Committee to IAPWS
# 2013 Report on Activities of Potential Interest to IAPWS

**Communicated from the Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO:**

In a collaboration with the Ruhr University of Bochum, we have made substantial progress on an IAPWS project for development of an equation of state for the thermodynamic properties of heavy water. A young researcher from Bochum spent several months in Boulder in early 2013, collecting and evaluating the experimental database and developing preliminary fits for the EOS. There is modest improvement in the representation of the experimental data in comparison to the existing IAPWS formulation, but the new EOS should be significantly better in its extrapolation capabilities and also near the critical point.

In collaboration with the Dagestan Scientific Center of the Russian Academy of Sciences and the Kazan National Research Technological University, with support by IAPWS, measurements were performed of the thermal conductivity of ammonia-water mixtures in the temperature range from 278 K to 356 K at pressures to 20 MPa.
Reference: F.N. Shamsetdinov *et al.*, *Int. J. Refrigeration* **36**, 1347 (2013).

In NIST's Sensor Science Division (Gaithersburg, MD), a gravimetric apparatus has been constructed for measuring the saturation concentration of water as a function of temperature and pressure in compressed gaseous carbon dioxide (equivalent to a dew-point measurement) at pressures up to 5 MPa and temperatures up to 85 °C. These data are important for the design of systems for compression and transportation of $CO_2$ for carbon capture and sequestration. So far, data have been obtained on four isotherms at approximately 10 °C, 21.7 °C, 30 °C, and 40 °C. Preliminary data analysis indicates that the cross second virial coefficients between $H_2O$ and $CO_2$ obtained from these measurements are consistent with previous theoretical estimates [R.J. Wheatley and A.H. Harvey, *J. Chem. Phys.* **134**, 134309 (2011)], but have smaller uncertainty.

In July 2013, a new version (Version 3.0) was released of NIST Standard Reference Database 10 (NIST/ASME Steam Properties). This product implements IAPWS formulations "for general and scientific use" for thermodynamic, transport, and other properties of fluid water. The new version implements the new IAPWS thermal conductivity formulation, and has added a few additional properties, including the Prandtl number and the ionization constant. Unlike previous versions, Version 3.0 is compatible with personal computers using 64-bit operating systems. Further information may be found at http://www.nist.gov/srd/nist10.cfm.

**Communicated from the University of Maryland**

Research on supercooled water was continued:

- M.A. Anisimov, "Cold and supercooled water: a novel supercritical-fluid solvent", *Russ. J. Phys. Chem. B* **6**, 1-7 (2012).
- V. Holten and M.A. Anisimov, "Entropy-driven liquid-liquid separation in supercooled water", *Sci. Rep.* **2**, 713 (2012); Supplement www.nature.com/scientificreports.

- V. Holten, D.T. Limmer, V. Molinero, and M.A. Anisimov, "Nature of the anomalies in the supercooled liquid state of the mW model of water'. *J. Chem. Phys.* **138**, 174501, 1-10 (2013).
- J.W. Biddle, V. Holten, J.V. Sengers, and M.A. Anisimov, "Thermal conductivity of supercooled water", Phys. Rev. E **87**, 042302, 1-7 (2013).

Aqueous solutions:

- The Revised Guideline on the Critical Locus of Aqueous Solutions of Sodium Chloride was approved by IAPWS. It is based on D.A. Fuentevilla, J.V. Sengers, and M.A. Anisimov, "Critical locus of aqueous solutions of sodium chloride revisited", *Int. J. Thermophys.* **33**, 943-958 (2012); *ibid.* **34**, 384 (2013).
- D. Subramanian, J.B. Klaude, J. Leys, and M.A. Anisimov, "Thermodynamic anomalies and structural fluctuations in aqueous solutions of tertiary butyl alcohol", *Vestnik SPSU (Herald of St. Petersburg State University)* **4**, 140-153 (2012).
- D. Subramanian, "Self-assembly in aqueous solutions of a non-ionic hydrotrope", Ph.D. Thesis, (Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20742, 2012).

**Communicated from OLI Systems**

- Based on our previous work on the thermal conductivity of multicomponent electrolyte solutions (P. Wang and A. Anderko, Int. J. Thermophysics, 2012, 33, 235-258), a draft guideline for the computation of thermal conductivity of seawater has been prepared. This draft will be submitted for consideration by the IAPWS Subcommittee on Seawater at the London meeting in September 2013.

- A comprehensive model has been developed for the calculation of interfacial tension in liquid-liquid systems with or without electrolyte components. The model consists of an equation for computing the interfacial tension of two-liquid-phase nonelectrolyte systems and an expression for the effect of electrolyte concentration. The model has been shown to accurately predict the effect of salts on interfacial tension in a variety of water – salt – organic systems.

  Reference: P. Wang and A. Anderko, "Modeling interfacial tension in liquid-liquid systems containing electrolytes," Ind. Eng. Chem. Res., 52 (2013) 6822-6840