U.S. National Committee to IAPWS
2014 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 2013, collecting and evaluating the experimental database and developing preliminary fits for the EOS. A preliminary equation has been developed, and will be refined in the coming months, possibly augmented by some new data.

- In NIST's Sensor Science Division (Gaithersburg, MD), a gravimetric apparatus has been used to measure 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. These data are important for the design of systems for compression and transportation of CO_2 for carbon capture and sequestration. Data have been obtained on six isotherms at approximately 10 °C, 21.7 °C, 30 °C, 40 °C, 60 °C and 80 °C. The apparatus is currently being modified to take more data at conditions (in the same temperature range) with relatively high water vapor contents.

- The Properties Subcommittee of the ASME Research and Technology Committee on Water and Steam in Thermal Systems (which is the U.S. National Committee to IAPWS) completed the Third Edition of the book *ASME International Steam Tables for Industrial Use*, which was published in early 2014. This book documents and provides tables and charts (in both SI and U.S. customary units) based on IAPWS-IF97 and other IAPWS "industrial" recommendations. The main update for the Third Edition was the incorporation of the recently revised IAPWS thermal conductivity formulation.

Communicated from the University of Maryland

- Research on supercooled water:
  V. Holten, J.C. Palmer, P.H. Poole, P.G. Debenedetti, and M.A. Anisimov, "Two-state thermodynamics of the ST2 model for supercooled water", *J. Chem. Phys.* **140**, 104502 (2014).
  F.W. Bresme, J.W. Biddle, J.V. Sengers, and M.A. Anisimov, "Communication: Minimum in the thermal conductivity of supercooled water", *J. Chem. Phys.* **140**, 161104 (2014).
  V. Holten, J.V. Sengers, and M.A. Anisimov, "Equation of state for supercooled water at pressures up tp 400 MPa", submitted to *J. Phys. Chem. Ref. Data*.

- Research on aqueous solutions:
  D. Subramanian, C.T. Boughter, J.B. Klauda, B. Hammouda, and M.A. Anisimov, "Mesoscale inhomogeneities in aqueous solutions of small amphiphile molecues", *Faraday Discussions* **167**, 217-238 (2013).
  J. Leys, D. Subramanian, E. Rodenzo, B. Hammouda, and M.A. Anisimov, "Mesoscopic properties in solutions of 3-methylpyridine, heavy water, and an antagonistoic salt, *Soft Matter* **9**, 9326-9334 (2013).
  M.A. Anisimov, Mesostructures and dynamics in liquids and solutions", Sections D and E, *Faraday Discussions* **167**, 1-23 (2013).

D. Subramanian and M.A. Anisimov, "Mesoscale solubilization and phase behavior in aqueous solutions of hydrotopes", *Fluid Phase Equilibria* **362**, 170-176 (2014).
D. Subramanian, J.B. Klauda, P.J. Collings, and M.A. Anisimov, "Mesoscale phenomena in ternary solutions of tertiary butyl alcohol, water, and propylene oxide", *J. Phys. Chem. B* **118**, 5994-6006 (2014).

- Review on transport properties near the critical point including H_2O:
  J.V. Sengers and R.A. Perkins, "Fluids near critical points", in: *Transport Properties of Fluids: Advances in Transport Properties,* M.J. Assael, R.H. Goodwin, V. Vesovoc, and W.A. Wakeham, eds. (IUPAC, RSC Publishing, Cambridge, 2014), pp. 337-361.

Communicated from OLI Systems

- Within the framework of the Department of Energy's Critical Materials Institute, OLI Systems has initiated a project to develop a comprehensive thermodynamic model for rare earth metals in aqueous environments. This model is expected to provide a computational tool for designing and optimizing emerging processes related to recycling rare earth metal-containing products, broadening the supply of rare earth metals from unconventional sources and developing substitutes.

- A comprehensive model has been developed for systems containing water, carbon dioxide, hydrogen sulfide, and common chloride salts. The objective of this model is to predict both phase equilibria and speciation including pH.

- A previously developed model for the thermal conductivity of electrolyte systems including seawater (P. Wang and A. Anderko, Int. J. Themophysics, 2002, 33, 235-258) has been revised to incorporate new experimental data, optimize the concentration dependence of species-species interaction terms, and create a simple formulation for seawater in terms of salinity, temperature, and pressure.