# U.S. National Committee to IAPWS
# 2015 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 (Germany), we continue to work on an IAPWS project for an equation of state for the thermodynamic properties of heavy water. A preliminary equation has been developed, and is being refined and augmented by some new data.

  Work is beginning on a related IAPWS project to develop new transport property correlations for heavy water.

- In a collaboration with researchers at Fondazione Bruno Kessler (Italy), Nicolaus Copernicus University (Poland), and the University of Delaware (USA), a state-of-the-art flexible model for the water pair potential has been used to calculate second virial coefficients $B(T)$ for both $H_2O$ and $D_2O$. The calculations use the path-integral Monte Carlo method, which fully accounts for both intermolecular and intramolecular quantum effects. The results agree with experimental data, but cover a wider range of temperatures. The effect of molecular flexibility is found to be significant in comparison to the uncertainty of the calculations and of the experimental data. Some weaknesses in the current potential at larger distortions are being addressed, after which the calculations will be repeated and uncertainties will be estimated.

- 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 for six isotherms at approximately 10 °C, 21.7 °C, 30 °C, 40 °C, 60 °C and 80 °C. The data have been processed to yield cross second virial coefficients, which are found to agree with theoretical predictions. A paper on the work is in press: C.W. Meyer and A.H. Harvey, Dew-point measurements for water in compressed carbon dioxide, *AIChE Journal*, in press (2015) doi: 10.1002/aic.14818.

- NIST, in partnership with ASME, AIChE, and the University of Colorado-Boulder, recently hosted the 19$^{th}$ Symposium on Thermophysical Properties. The meeting included seven oral sessions plus a number of posters devoted to aqueous systems: see http://thermosymposium.nist.gov for information and abstracts of the presentations.

**Communicated from the University of Maryland, College Park**

- Research on supercooled water:

V. Holten, J. V. Sengers, and M. A. Anisimov, "Equation of state for supercooled water at pressures up to 400 MPa", J. Phys. Chem. Ref. Data **43** (4) 043101-0431024 (2014).

- Research on aqueous solutions:

M. B. Taraban, L. Yu, Y. Feng, E. V. Jouravleva, M. A. Anisimov, Z.-X. Jiang, and Y. B. Yu, "Conformational transition of a non-associative fluorinated amphiphile in aqueous solution" RSC Adv., **4**, 54565-54575 (2014).

A. E. Robertson (high-school senior), D. H. Phan (undergraduate student), J. E. Macaluso (undergraduate student), V. N. Kuryakov (graduate student), E. V. Jouravleva, C. E. Bertrand, I. K. Yudin, M. A. Anisimov, "Mesoscale solubilization and critical phenomena in binary and quasi-binary solutions of hydrotropes", Fluid Phase Equilibrium (special issue, to be published, 2015).

- Guideline on Thermodynamic Properties of Supercooled Water:

To be considered at the Annual Meeting of the International Association for the Properties of Water and Steam, Stockholm, Sweden, June 20-July 3, 2015

**Communicated from OLI Systems**

- Aqueous solution chemistry of rare-earth elements. OLI Systems is a member of the Department of Energy's Critical Materials Institute, which has been established to address the U.S. needs for critical materials, with particular emphasis on rare earth metals. OLI Systems provides simulation tools for rare earth metals in aqueous environments. In a recently completed project, we provided simulation tools for optimizing electrochemical recycling of rare earth elements. This work has been published in:

  T.E. Lister, P. Wang, and A. Anderko, "Recovery of critical and value metals from mobile electronics enabled by electrochemical processing", Hydrometallurgy, 149 (2014) 228-237

  Work is in progress on analyzing phosphogypsum-related systems as an alternative source of rare-earth elements.

- Aqueous CO2-H2S systems. The following paper has been published about a comprehensive model for systems containing water, carbon dioxide, hydrogen sulfide, and common salts:

  R.D. Springer, P. Wang, and A. Anderko, "Modeling the Properties of H2S – CO2 – Salt – Water Extreme Environments", SPE Journal, in press,
  DOI: http://dx.doi.org/10.2118/173902-PA.

- Thermal conductivity of seawater. A revised model for the thermal conductivity of seawater has been published:

P. Wang and A. Anderko, "Revised Model for the Thermal Conductivity of Multicomponent Electrolyte Solutions and Seawater", Int. J. Thermophysics, 36 (2015) 5-24

Based on this model, a simple formulation has been proposed as an IAPWS Guideline for seawater thermal conductivity.

- Aqueous solution chemistry of actinides. Work is in progress on developing a comprehensive model for the thermodynamic behavior of uranium, plutonium, neptunium, americium, and curium in multicomponent aqueous solutions.

**Communicated from Scripps Institution of Oceanography**

- Researchers from the U.S. contributed to two large review papers related to metrology for physical oceanography, with substantial Scripps involvement in Part 1 and Part 3,

  *Metrological challenges for measurements of key climatological observables: Oceanic salinity and pH, and atmospheric humidity. Part 1: Overview* by Feistel, Rainer; Wielgosz, Robert; Bell, Stephanie; Camoes, Maria; Cooper, Jeff; Dexter, Peter; Dickson, Andrew; Fisicaro, Paola; Harvey, Allan; Heinonen, Martti; Hellmuth, Olaf; Kretzschmar, Hans-Joachim; Lovell-Smith, J; McDougall, Trevor; Pawlowicz, Rich; Ridout, Paul; Seitz, Steffen; Spitzer, Petra; Stoica, Daniela; Wolf, Henning Article reference: MET-100397.R1

  *Metrological challenges for measurements of key climatological observables, Part 3: Seawater pH* by Dickson, Andrew; Camoes, Filomena; Spitzer, Petra; Stoica, Daniela; Fisicaro, Paola; Pawlowicz, Rich; Feistel, Rainer Article reference: MET-100472

- Scripps also continues involvement in SCOR Working Group (WG-145) that will — in part — address the need for a suitable activity coefficient model for seawater that can be used to further the goal of establishing a suitable seawater pH definition that is metrologically traceable. This group has met once, and is now planning its future work.