IAPWS Collaborative Grant Proposal, 2012

Development of a new Equation of State for Heavy Water

IAPWS Sponsors

Dr. Allan H. Harvey
Thermophysical Properties Division
Nat. Inst. of Standards & Technology
Boulder, CO 80305, USA
e-mail: aharvey@boulder.nist.gov

Prof. Dr.-Ing. Roland Span
Ruhr-Universität Bochum
Fakultät für Maschinenbau
Lehrstuhl für Thermodynamik
D-44780 Bochum, Germany
e-mail: roland.span@thermo.rub.de

Visiting Young Scientist
Mr. Stefan Herrig
Ruhr-Universität Bochum

The properties of heavy water (D_2O) are of significant scientific interest, and also of some industrial interest for certain nuclear power cycles. The current IAPWS formulation for the thermodynamic properties of D_2O was adopted in 1984 (with a minor adjustment for temperature scale in 2005 [1]), and is based on work performed in the group of Prof. Phil Hill over 30 years ago [2].

In the past 30 years, a modest amount of additional data has become available. We know of isochoric heat-capacity measurements [3,4], some new measurements of the density of the high-temperature liquid relative to that of ordinary water [5], some reanalyzed vapor density data [6], and some liquid heat-capacity data [7]. The preceding list is not necessarily complete; we have not yet performed a thorough literature search.

At least as important are the advances in the development of equation-of-state (EOS) technology over the past 30 years. Modern computer technology allows simultaneous optimization of EOS parameters to multiple data types, constraint of the EOS to proper extrapolation, smooth behavior of derivatives and better behavior in the critical region (the current IAPWS EOS for D_2O [2] is not recommended near the critical point), and a reduction in the number of adjustable parameters needed. This modern technology has been applied to numerous fluids (some of the advances were already applied to the IAPWS formulation for H_2O), and it should be possible to apply it to D_2O.

The proposed collaborative project combines the experience in EOS fitting of probably the two leading groups in that field; those at NIST and Bochum. Dr. Eric Lemmon of NIST would train the young researcher in advanced techniques for developing equations of state and guide him in applying the techniques to D_2O.

The production of a final EOS and accompanying paper could not be done in the timescale of an IAPWS collaborative project. Therefore, the goal of this project is to do the basic work necessary to get the project started and most of the way to completion. The student

would develop a complete database, be trained by Dr. Lemmon in the techniques of advanced fitting, and produce a preliminary EOS. This preliminary EOS would then be fine-tuned over the rest of 2013 in a collaboration involving the Boulder and Bochum groups, perhaps in conjunction with feedback and evaluation by the IAPWS TPWS Working Group. It is hoped that this would result in a new IAPWS Release that could be adopted in 2014 or 2015.

Budget

We propose a total budget of $7,500 for this project, which would last for 4 months beginning in early 2013. This would pay for the travel expenses of Mr. Herrig to Boulder (IAPWS would be invoiced for $1500 or the actual expense, whichever is smaller), and for 4 months of living expenses at $1500 per month.

References

[1] IAPWS, Revised Release on the IAPS Formulation 1984 for the Thermodynamic Properties of Heavy Water Substance (2005), available at www.iapws.org.

[2] Hill, P.G., MacMillan, R.D.C., and Lee, V., A Fundamental Equation of State for Heavy Water, *J. Phys. Chem. Ref. Data* **11**, 1 (1982).

[3] Mursalov, B. A.; Abdulagatov, I. M.; Dvoryanchikov, V. I.; Kamalov, A. N.; Kiselev, S. B., Isochoric Heat Capacity of Heavy Water at Subcritical and Supercritical Conditions, *Int. J. Thermophys.* **20**, 1497 (1999).

[4] Polikhronidi, N. G.; Abdulagatov, I. M.; Magee, J. W.; Stepanov, G. V., Isochoric Heat Capacity Measurements for Heavy Water Near the Critical Point, *Int. J. Thermophys.* **23**, 745 (2002).

[5] Tremaine, P., personal communication to A.H. Harvey (2011).

[6] Kell, G. S.; McLaurin, G. E.; Whalley, E., PVT properties of water. VII. Vapor densities of light and heavy water from 150 to 500 °C, *Proc. R. Soc. London, Ser. A* **425**, 49 (1989).

[7] Smirnova, N. N.; Bykova, T. A.; Durme, K. V.; Mele, B. V., Thermodynamic properties of deuterium oxide in the temperature range from 6 to 350 K, *J. Chem. Thermodyn.* **38**, 879 (2006).