IAPWS Certified Research Need – ICRN

Thermophysical Properties Associated with Ultra-supercritical Coal-fired Steam Generators

Closing Statement

In 2009, the IAPWS Working Groups "Physical Chemistry of Aqueous Systems" and “Power Cycle Chemistry” examined the published work in the area of thermophysical properties associated with ultra-supercritical coal-fired steam generators relevant to future electric power plants. This resulted in the formulation of ICRN-21, Thermophysical Properties Associated with Ultra-supercritical Coal-fired Steam Generators. ICRN-21 was approved in September 2009 at the IAPWS annual meeting in Doorwerth, The Netherlands, with an expiration date of September 2012. At the 2012 annual meeting in Boulder, Colorado, USA, it was decided to allow this ICRN to expire.

ICRN-21 described a need for thermophysical property data at temperatures up to 800 °C and pressures up to 50 MPa, to help in the design and operation of next-generation coal-fired plants being considered at the time. Of interest were thermophysical properties of supercritical steam, including the dielectric product and ion product, the diffusion characteristics of ions and neutral solutes under these conditions, and the degree of association of such ions and the solubility of salts formed. Both experimental work and computer simulations were envisioned as paths to improve understanding in these areas.

Subsequently, changes in market conditions have led to a situation where such ultrasupercritical coal-fired plants are no longer being considered, at least in the near or medium term. Therefore, this is no longer a major impetus for the research described in the ICRN.

For the most part, the needs mentioned in this ICRN have not been addressed, although we are aware of some efforts on molecular modeling of ion association [1,2] and diffusion [3] at relevant supercritical conditions.

Boulder, October 2012

References

[1] Chialvo, A.A., Gruszkiewicz, M.S., and Cole, D.R., Ion-Pair Association in Ultrasupercritical Aqueous Environments: Successful Interplay among Conductance Experiments, Theory, and Molecular Simulations, *J. Chem. Eng. Data* **55**, 1828 (2010).

[2] Plugatyr, A., Carvajal-Ortiz, R.A., and Svishchev, I.M., Ion-Pair Association Constant for LiOH in Supercritical Water, *J. Chem. Eng. Data* **56**, 3637 (2011).

[3] Ge, S., Zhang, X.-X., and Chen, M., A Molecular Dynamics Simulation of the Diffusivity of O_2 in Supercritical Water, *Int. J. Thermophys.* **31**, 2176 (2010).