PCAS WG Minutes

Dresden, Germany, 11-16 September, 2016

Present:
Andre Anderko (Chair) aanderko@olisystems.com
Masaru Nakahara nakahara@scl.kyoto-u.ac.jp
Vladimir Majer vladimir.majer@tul.cz

Andre Anderko opened the meeting. The agenda was approved without any additions. Masaru Nakahara was appointed clerk of minutes.

Minutes of the 2015 meeting were approved.

A round-table discussion of scientific work of the attendees was held. Andre Anderko described the work at OLI Systems on the aqueous solution chemistry of rare-earth elements, the properties of neutralizing amines and amine hydrochlorides, solution chemistry of actinides and thermodynamics of sodium phosphates, silicates and scale forming minerals. Vladimir Majer described his research on the solubility of gases in water and aqueous salt solutions. Masaru Nakahara reviewed his studies of self-diffusion coefficients of water using NMR over a wide range of thermodynamic conditions. Further, he described his work on the development of clean hydrogen fuel with formic acid used for chemical hydrogen storage.

The possibility of issuing ICRNs was discussed and no proposals were made.

PCAS Workshop (Monday)

The following presentation was made in the PCAS workshop:

Solubility of H_2S in NaCl(aq) over a wide range of temperatures and pressures: experimental data and correlation scheme (V. Majer)

In a discussion, it was indicated that this work could serve as a basis for a guideline.

PCC/PCAS Joint Workshop (Tuesday)

The following presentations were made:

Electrochemical corrosion potential monitoring in BWRs (Y. Wada)

Modeling actinide solution chemistry: Thermodynamic fundamentals for nuclear power industry (P. Wang and A. Anderko)

Update on geothermal chemistry (D. Addison)

TPWS/PCAS Joint Workshop (Thursday)

The following presentations were made:

Progress toward improved ideal-gas properties of ordinary and heavy water (J. Hrubý)

In discussion, it was indicated that the deviations from the previously accepted values (JANAF) are significant for heavy water.

Report of task group on isotopic fractionation (R. Feistel, A. Harvey, J. Hrubý, K. Maier)

Consensus has been reached that this task group should be kept inactive. Importance of fractionation anomalies in seawater has been indicated. J. Hruby raised the question of what to do with the report. Tentatively, it has been recommended to keep it internal to IAPWS.

Progress in modeling gas hydrates relevant for CCS using reference equations of state and extension of the model for mixed hydrates (S. Hielscher, A. Jäger, V. Vinš, R. Span, J. Hrubý, C. Breitkopf)

Carbon today and hydrogen in the future for chemical energy (M. Nakahara)

Rich Pawlowicz presented a request from ISO to IAPWS to assist in the development of a density model for produced water. A joint TPWS-PCAS task group has been formed to address this question, with R. Pawlowicz, A. Harvey, R. Feistel, and A. Anderko as members.

Guidelines

The following two guidelines have been discussed:

(1) Self-diffusion in high-temperature and supercritical water over wide density ranges by Masaru Nakahara and Ken Yoshida. The experimental work has been already published. It is planned to prepare a draft for the 2017 Meeting.
(2) Solubility of H_2S in water and aqueous solutions of NaCl and $CaCl_2$ by Vladimir Majer. Both the experimental work and the model have been published. Work on the guideline remains to be initiated.

Additionally, the following possible guidelines remain under consideration but no recent progress has been reported:

- Amine properties (James Bellows)
- Thermodynamics of hydration of gases and organic solutes (Josef Sedlbauer and Vladimir Majer)

Miscellaneous

Andre Anderko was nominated to be the PCAS representative for the Gibbs Award Committee.