16th ICPWS London, UK September 1-5, 2013

PCAS WG Minutes

Present: Masaru Nakahara (chair) Andre Anderko (vice chair, clerk of minutes) Masakatsu Ueno David Guzonas Liyan Qiu

nakahara@scl.kyoto-u.ac.jp aanderko@olisystems.com sk112652@mail.doshisha.ac.jp guzonasd@aecl.ca qiul@aecl.ca

- 1. **Opening remarks.** Masaru Nakahara opened the meeting and presented the agenda. Andre Anderko was appointed the clerk of minutes. Masaru Nakahara recognized the contributions of William Marshall, a former member of PCAS, who recently passed away.
- 2. Change of chair. Masaru Nakahara will step down as chair of the PCAS WG after the London meeting. As agreed at the Boulder meeting, Andre Anderko will take over as chair and Josef Sedlbauer will be appointed vice-chair.
- 3. **Progress report and future perspective.** Masaru Nakahara prepared a summary of the work of PCAS since the 2008 Berlin conference.

PCAS WG has discussed the fundamental thermodynamic and kinetic aspects of aqueous solutions and supercritical water to assist in the development of innovative approaches to a variety of problems encountered in power cycle engineering. In particular, the reactivity of such simple gases as hydrogen, carbon dioxide, and carbon monoxide, simple and complex organics like formic acid etc., and a variety of heavy metal oxides in supercritical water have been presented and discussed in relation to the power cycle chemistry. Attention has been paid to the free energy changes as a measure of the stability of the species involved. Information and opinions have also been exchanged on ionic conductivities and interfacial problems.

The group briefly discussed the future directions of PCAS activities. Andre Anderko proposed creating a list of research topics that would be of shared interest to PCAS members. Such topics should ultimately result in the creation of IAPWS releases or guidelines. As an example, Andre Anderko mentioned the properties of rare earth metals, which are attracting increasing attention. David Guzonas mentioned solubility and deposition of corrosion products. Masaru Nakahara mentioned solvation free energies of gases and organics.

- 4. **Possibility of an international collaboration project.** David Guzonas expressed interest in an international collaboration project, which would help him bring a foreign visitor for a short-term project at AECL. The group has agreed to support such a proposal at the next IAPWS meeting after the partner organization is established.
- 5. **Possible releases (guidelines).** Currently, PCAS is co-sponsoring a guideline for the thermal conductivity of seawater (based on the model developed previously by P. Wang and A. Anderko). This guideline is being prepared in collaboration with the Subcommittee on Seawater and is currently under review. Andre Anderko gave a brief talk at a joint TPWS-SCSW-ICRN-PCAS meeting about the progress towards the guideline.

Masaru Nakahara described a possible future release (or guideline) on self-diffusion in hightemperature and supercritical water, which would combine results of simulations and experimental data. Such release is currently contemplated but it has not been drafted yet.

- 6. **Possibility of an ICRN.** Currently, no ICRNs are being planned.
- 7. Membership. David Guzonas proposed his colleague Liyan Qiu as a new member of PCAS. Liyan Qiu is a research chemist at AECL, Canada. The group has endorsed Liyan Qiu's membership.

8. Contribution to press release:

- 1. PCAS continues to focus on the fundamental thermodynamic and kinetic aspects of aqueous solutions and supercritical water. Particular areas of focus are the reactivity of gases such as hydrogen, carbon dioxide, and carbon monoxide, simple and complex organics such as formic acid, and a variety of heavy metal oxides in aqueous solutions. An additional area of focus is the study of transport and interfacial properties.
- 2. A draft IAPWS guideline for the thermal conductivity of seawater has been prepared and is currently under review.