2010 IAPWS Annual Meeting
Niagara Falls, Canada

PCAS WG Minutes

Present: Masaru Nakahara (chair), Andre Anderko (vice chair, clerk of minutes), Mikhail Anisimov, Francis Brosseau, Jana Ehlerova, David Guzonas, Milan Sedlar, Peter Tremaine, Masakatsu Ueno

Monday, July 19, morning

1. **Opening remarks.** Masaru Nakahara made opening remarks. Andre Anderko was appointed clerk of minutes. Masaru Nakahara presented the meeting agenda, which was previously distributed by e-mail (PCAS Appendix A). The agenda has been adopted unchanged.

2. **Minutes of the 2009 Meeting** in Doorwerth were adopted as written.

3. **IAPWS Interntional Collaboration.** Mikhail Anisimov has indicated his intention to propose an international collaboration between his group at the University of Maryland (USA) and the group of Alexei Victorov at the St. Petersburg University (Russia) in the area of self-assembly of small molecules. A formal proposal is planned to be presented next year.

4. **Existing ICRNs.** The group discussed the ICRNs that were associated with previous activities.

   ICRN 17 (Research on Amines in the Power Industry)**.** Peter Tremaine suggested creating group contributions for high-temperature amines. Masaru Nakahara indicated that distributing partial molar properties for amines up to 300 °C would be useful.

   ICRN 21 (Thermophysical Properties Associated with Ultra Supercritical Coal-Fired Steam Generators).

   ICRN 22 (Steam Chemistry in the Turbine Phase Transition Zone). This ICRN is to be reviewed jointly with PCC

   ICRN 26 (Behavior of Aluminum in the Steam Water Cycle of Power Plants). This is a new proposal originating in PCC. The group discussed whether there was practical interest in aluminum in supercritical water. David Guzonas indicated that there was interest in accident containment scenarios. Al is used in pipe insulation and cladding.

ICRN 25 (Corrosion Mechanisms That Are Related to the Presence of Contaminants in Steam/Water Circuits, Particularly in Boiler Water). Peter Tremaine and Andre Anderko expressed support for this line of research.

ICRN 10 (pH Measurements and Potentiometric Studies of Supercritical Aqueous Solutions). This ICRN is up for renewal. Peter Tremaine expressed interest in moving the pH definition to molality to avoid single-ion activities. Peter Tremaine plans to look at this ICRN and rewrite it.

The group decided to analyze the ICRN documents and to conduct a further discussion related to ICRN's on Thursday.

5. **Releases.** No releases are currently worked.

6. **Membership.** David Guzonas became a member of PCAS. Masaru Nakahara raised the issue of membership of persons who have not participated in the activities of PCAS for a long time. Andre Anderko suggested sending out an e-mail with an inquiry whether they wish to participate. Masaru Nakahara expressed his plan to discuss this issue with other working group chairmen and finalize the policy by Thursday.

7. **Guidelines.** Masaru Nakahara opened discussion on creating a guideline on the basis of the IAPWS/IUPAC project "Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes and Gases" (Josef Sedlbauer, project coordinator). Originally, this project was supposed to result in the publication of a book. However, these plans have been changed and a new method of disseminating the results needs to be established. Jana Ehlerova presented some options regarding the publication of the results. They include an Excel format or a web-based application. Also, a report is scheduled for September. Jana Ehlerova distributed the current version of the report in an electronic form. Further discussion has been deferred until Thursday so that the members have time to familiarize themselves with the report.

Tuesday, July 20, morning

PCAS Workshop

The following presentations were given in the PCAS workshop:

1. Jana Ehlerova: Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes and Gases

Jana explained the project goals, timetable, rationale, and outlined the approach taken. She discussed the evaluation of the primary data. Over 5000 data points were retrieved from the literature. A database of recommended hydration properties for about 150 compounds was produced at 25 C, 0.1 MPa. The work is still unfinished, with about ½ of the compounds yet to be checked for consistency.

The question was raised as to what the output for IAPWS was to be, e.g., guidelines. A journal paper is almost completed. A brief update on the project budget was given – there have been no expenses claimed yet, and there is 8000 euro left. The expenses for the two young scientists will be claimed at the end of the project. There was a discussion on how the high temperature data will be reported. It was suggested that all the high temperature data be included, including the uncertainties. There was a question raised about the relationship between IAPWS and IUPAC on this work, and it was explained that a fraction of the budget was provided by each group.

2. Mikhail Anisimov: Can small molecules self-assemble in aqueous solutions

The types of molecules being considered were molecules like 3-methylpyridine and t-butanol. The results of dynamic light scattering showed unexpected behaviour, suggesting the formation of mesoscopic structures. It was noted that TBA is that last alcohol that is miscible with water. There have been anomalies reported for about 40 years – these have not yet been explained but there is evidence that impurities or gas bubbles may play a role. So the question arises as to whether the observed effects are real or artefacts, and are they genuine equilibrium structures or long-lived non-equilibrium structures? The question was raised as to whether this phenomenon can be used to create new materials.

3. Masakatsu Ueno: Electric Conductivities of 1:1 Electrolytes in High-Temperature Ethanol Along the Liquid-Vapor Coexistence Curve

There was a brief discussion of the density effect on transport properties; in low density solvents, transport is dominated by binary collisions whereas in high density solvents many-body effects dominate. Alcohols were chosen as the model solvent because water is complicated because of hydrogen. While alcohols are also hydrogen bonded, they are less so than water. The concept of dielectric friction was discussed and models were presented. It was found that non-hydrodynamic effects in EtOH and MeOH are well explained by HO theory at higher density, but at lower density limitations are observed. There was a discussion of other models for conductivity and there application to these data.

4. Milan Sedlar: Homogeneous Nucleation during Cavitation Processes

There was a brief introduction to sources of cavitation nuclei in water during cavitation. He pupose of the project was to create a model of the processes for incorporation into CFD codes. The concept of the critical nucleation work was explained, and the details of developing a model outlined. There was a discussion on the difficulties in incorporating such a model into CFD codes. There was some discussion on how easy it might be to extend the model to higher temperatures; the current focus was on low temperature applications. However, there was no obvious impediment to extending this to higher temperatures.

5. Francis Brosseau: Activity Transport Models for CANDU-6 Pressurized Heavy Water Reactors.

   The title study has been carried out to extend the previous work done by Peter Tremaine and co-workers. The reaction conditions examined are extened up to 550-600°C and 25-30 MPa.

6. Peter Tremaine: Deuterium Isotope Effects on Acid Ionization

   The solvent isotope (D_2O/H_2O) effect on the ionization constants has been discussed in relation to the substances used in the CANDU reactor. The importance of the zero-point energy difference has been pointed out.

Tuesday, July 20, afternoon

Joint PCC/PCAS Workshop

The first part of the workshop was devoted to the presentation of proposed ICRNs. The following two ICRNs were introduced at the workshop:

a. Jeff Bignold: **ICRN 25** (Corrosion Mechanisms That Are Related to the Presence of Contaminants in Steam/Water Circuits, Particularly inoiler Water)

b. Robert Svoboda: **ICRN 26** (Behavior of Aluminum in the Steam Water Cycle of Power Plants).

In the second part of the workshop, the following three presentations have been made:

1. Hiroshi Takaku: Combined Effect of Chloride and Sulfate Ions

2. Andre Anderko: Thermodynamic Modeling of High-Temperature Aqueous Chemistry in Power Plant Environments

3. Masaru Nakahara: Carbon Dioxide Fixation and Hydrogen Storage and Transportation in the Form of Formic Acid

PCAS Workshop - continued

One presentation was made after the end of the joint PCC/PCAS workshop:

1. David Guzonas: Corrosion in Supercritical Water-Cooled Reactor

Guidelines - continued

Discussion resumed on the guideline resulting from the project "Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes and Gases". Masaru Nakahara reported that he had discussed the format for the guideline with Allan Harvey, who will provide detailed feedback. Peter Tremaine indicated that it would desirable to publish high-temperature data in addition to the publication that is tentatively planned to be submitted to Chemosphere. The group concurred.

Thursday, July 22, morning and afternoon

Joint Workshop of TPWS, SCSW, and PCAS

The following presentations were given at workshop:

1. Soohaeng Yoo: The Phase Diagram of Water with Various Models

2. Kenji Yasuoka: Surface Tension of Water with Rigid Models

3. Masaru Nakahara: Scaled Formulation of self-Diffusion Coefficients for Water Over a Wide Range of Density and Temperature Including the Supercritical"

Following the joint workshop, discussions resumed within the PCAS group.

Press Release. Masaru Nakahara conveyed Jim Bellows' request to provide him with a contribution to the press release. The group decided that the press release should describe the project "Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes and Gases", which is nearing completion. Subsequently, Jana Ehlerova and Andre Anderko formulated the PCAS contribution to the press release.

ICRNs. Discussion of ICRNs was resumed.

ICRN 26. David Guzonas provided background information on the importance of aluminum chemistry. Accordingly, the results of ICRN would also be of value to the nuclear industry, in particular in clarifying the behavior of aluminum in post-LOCA (Loss of Coolant Accident) containment sump water interactions of aluminum hydroxide or oxyhydroxide on ion-exchange resins. Peter Tremaine moved to approve the ICRN and the rest of the group concurred. David Guzonas a Peter Tremaine proposed adding a friendly amendment to mention additional application areas as described here.

ICRN 20 on sensors. Masaru Nakahara stated that this ICRN expired but there was interest in PCC in renewing it. The group decided to agree with the changes proposed by PCC.

ICRN 10 on pH. David Guzonas raised a question whether this subject is of practical importance and indicated that the topic is too narrow. Peter Tremaine recommended sending it to PCC with a request to identify broader applications or, absent any changes, close it. The group concurred.

ICRN 25. Andre Anderko indicated that this topic is of great importance and is definitely worth investigating. However, Peter Tremaine and Andre Anderko stated that this ICRN does not have a sufficient focus and looks like a project vision for decades of research. The group recommends sending it back to PCC with a recommendation to put more focus so that it is not an open-ended project.

Mission Statement. Peter Tremaine drafted a mission statement in response to a general request that the working groups prepare/update their mission statements. The group introduced minor modifications and approved the draft. Masaru Nakahara will submit it to the Executive Committee.

PCAS Mission Statement 2010

1) To provide critically evaluated thermodynamic and transport property data for solutes and interfaces in high-temperature high-pressure aqueous solutions, of interest to the electric power industry and other industrial applications.
2) To develop new experimental techniques and modeling methods needed to obtain key thermodynamic transport property data for high temperature aqueous solutions and interfaces relevant to the IAPWS mission.

Finalizing the guideline. Masaru Nakahara reiterated the need to develop a schedule for finalizing the project on hydration. Jana Ehlerova indicated that the low-temperature part will be finished in September and the schedule for the high-temperature part has not been decided yet. Further inquiries will be forwarded to Josef Sedlbauer.

Future of PCAS. The future of PCAS was discussed. The low turnout at PCAS meetings remains a concern. Peter Tremaine proposed considering converting PCAS to a subcommittee and/or holding only joint workshops with other working groups. Andre Anderko indicated that the current model of presenting the majority of talks in joint workshops is a step in the right direction but more focus is needed. Masaru Nakahara indicated that it is desirable to preserve a separate PCAS workshop. This is partially due to the fact that PCAS's mission is to solve fundamental problems, which differentiates it from the other groups. For future ICRNs, Milan Sedlar indicated that he is going to prepare, jointly with Frantisek Marsik, an ICRN in the area of nucleation.

Adjournment. The meeting adjourned at 3:20pm.

The International Association for the Properties of Water and Steam
http://www.iapws.org

Physical Chemistry of Aqueous Systems Working Group (PCAS WG)

Schedule

Niagara Falls, Canada, 18 – 23 July, 2010

Sun 18	19:00	Informal Get-together, Cocktails and Registration
Mon 19	08:30	Opening Plenary Session - Executive Committee
	10:00	PCAS WG Meeting a) *Opening.* b)*Clerk.* c)*Approval of Previous Minutes*. d)*International Collaboration*
	13:30	PCAS WG Meeting e)*ICRN*. f)*Release*. g)*Membership*. h) *"Hydration Project" by Sedlbauer, Guideline*.
Tue 20	08:30	PCAS Workshop on "Basic Solution Chemistry and Physics Useful for Power Cycle Applications"
	1)	Jana Ehlerova instead of Josef Sedlbauer. The Joint IUPAC/IAPWS project. Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes and Gases.
	2)	Mikhail Anisimov. Self-Assemby of Small Molecules in Aqueous Solution.
	3)	Masakatsu Ueno. Electric Conductivities of 1:1 Electrolytes in High-Temperature Ethanol along the Liquid-Vapor Coexistence Curve. NaBr, KBr, and CsBr.
	4)	Milan Sedlar. Nucleation in Water during Cavitation Processes.
	5)	Dave Guzonas and Peter Tremaine. Activity Transport Models for CANDU-6 Pressurized Heavy Water Reactors.
	11:00	PCAS Task Group Meeting i)*Organics in Hot Water*. j)*Inorganics in Hot Water*
	1)	Peter Tremaine. Deuterium Isotope Effects on Acid Ionization Constants under Hydrothermal Conditions.
	2)	Francis Brosseau and Peter Tremaine. Critical Evaluation of Iron and Nickel Thermochemical Data under Hydrothermal Conditions, and Extrapolations to Supercritical Conditions.

13:30 PCC/PCAS Joint WG Meeting
– ICRNs: ICRNs 17, 21, 22, 25, and ICRN on Aluminum, …
– Workshop on "Solution/Interface Chemistry and Engineering"??
- Many Talks Other than Those Listed below
- Andre Anderko. Thermodynamic Modeling of High-Temperature Aqueous Chemistry.
- Masaru Nakahara. Carbon Dioxide Fixation and Hydrogen Storage and Transportation in the Form of Formic Acid.

15:30 PCAS WG Meeting
- ICRNs 17, 21, and 22 (approved)
- ICRN 25: Corrosion mechanisms that are related to the presence of contaminants in steam/water circuits, particularly in boiler-water.

ICRN 26: **Behavior of Aluminum in the Steam Water Cycle of Power Plants**

Wed 21 09:00-17:00 IAPWS Symposium

Thu 22 08:30 TPWS/SCSW/PCAS Joint WG Meeting
– Revision of ICRN-14 on Thermophysical Properties of Humid Air and Combustion-Gas Mixtures (M. Wendland, R. Span, A. H. Harvey)
– Contributed from the Molecular Simulation Task Group

1) Soohaeng Yoo, Pacific Northwest National Laboratory (USA). The Phase Diagram of Water with Various Models
2) Kenji Yasuoka, Keio University (Japan). Surface Tension of Water with Rigid Models
– Properties of Sea Water: Task Group Report "Transport Properties"

- Many Talks Planned Other than Those Listed below
- Andrei Anderko. Development of a Model for Calculating Thermal Conductivity of Seawater.
– Self-Diffusion of Water
- Masaru Nakahara. Scaled Formulation of Self-Diffusion Coefficients for Water over a Wide Range of Density and Temperature Including the Supercritical.

13:30 PCAS WG Meeting Summary
15:30 PCAS Report to Executive Committee

18:30 IAPWS Banquet