2011 IAPWS Annual Meeting
Plzen, Czech Republic
September 5-9, 2011

PCAS WG Minutes

Present:

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Monday, September 5, morning

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

2. **Minutes of the 2010 Meeting** in Niagara Falls were adopted as written.

3. **General policy regarding PCAS meetings.** Masaru Nakahara summarized the group's future policy with regard to meetings. PCAS will meet for internal discussions in separate meetings whereas most technical presentations and discussions will be carried out in joint meetings with other working groups.

4. **Mission statement.** Last year, we prepared a draft of a mission statement, which was subsequently distributed. Masaru Nakahara opened the mission statement for discussion. Frantisek Marsik proposed expanding the mission statement to incorporate items pertaining to the hydrogen economy. Also, it was questioned whether it is appropriate to focus on high-temperature systems considering that a substantial amount of work within PCAS pertains to low-temperature systems. Consensus has been reached that green technologies (such as hydrogen chemistry) should be included but the focus on high-temperature systems should remain to differentiate PCAS from other bodies that deal with aqueous chemistry. David Guzonas prepared a modified mission statement. The revised (in italics) mission statement reads:

   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, *developers of green technologies*, and other industrial applications.

2) To develop new experimental techniques and modeling methods needed to obtain key thermodynamic and transport property data for high temperature aqueous solutions and interfaces relevant to the IAPWS mission.

5. **PCAS output.** Possible forms of output from PCAS were discussed. It has been concluded that the project on hydration properties should result in a guideline or release.

6. Membership. Masaru Nakahara proposed to extend invitations to younger scientists to join PCAS and raised the topic of inactive members. It has been generally agreed that the PCAS chair will send out e-mails to inactive members to ask them whether they intend to participate. If they respond positively, they will be retained on the member list. If they respond negatively, they will be removed. If they do not respond after repeated attempts to contact them, they will be also removed.

Monday, September 5, afternoon

7. Topics for ICPWS 16 (London, UK). The group analyzed the draft program for ICPWS 16. The group went through the 14 topics that have been included in Jeff Cooper's draft. The following conclusions have been reached:

It is suggested to rename Symposium 5 "Reactions in Hydrothermal Systems" to differentiate it from Symposium 2, which deals with thermodynamics of aqueous systems in general.

For Symposium 3 ("Molecular Simulation & Spectroscopy in Aqueous Systems"), it may be beneficial to separate molecular simulation from spectroscopy, especially if the number of submissions warrants having separate symposia.

It is recommended to combine Symposium 8 ("Power Cycle Chemistry, IAPWS Technical Guidance Documents") and 9 ("Power Cycle Chemistry in Nuclear Plant, Safety and New Build") because of the closeness of topics.

Symposium 10 ("Water Purification & Other Auxiliary Systems") may be eliminated because of the narrowness of the topic.

The group suggested possible people to organize or co-organize the sessions that pertain to PCAS activities. Peter Tremaine would be willing to chair Symposia 2 or 5 or 12. Andre Anderko could do the same for Symposium 2. It has been suggested that Kenji Yasuoka and/or Igor Svishchev could chair Symposium 3 (or its molecular simulation component). Somebody may be considered in the area of hydrogen production.

8. Unesco letter. Masaru Nakahara has received a letter from UNESCO that explores the possibility of collaboration to disseminate knowledge in the area of aqueous chemistry. Masaru Nakahara will show the letter to the group and consider a response.

Tuesday, September 6, morning

9. PCAS Workshop "Transport, Hydration and Reactions in Hot Water"

Three presentations were given:

J. Sedlbauer, Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Solutes and Gases

This talk was delivered in relation to the hydration project supported jointly by IAPWS and IUPAC. The chair has continuously encouraged the publication of some papers on the hydration for the past few years. The group reviewed the complicated history of this project. The IAPWS financial support (8,000 euro) was expended before Josef Sedlbauer took over the project. He emphasized that model development was not part of the project. The data collection had been completed but no papers as yet. A summary paper is still in preparation. It may be submitted to the Journal of Physical and Chemical Reference Data. After the paper is finalized, a guideline or a release will be prepared.

M. Ueno, T. Matsui, T. Hoshino, Transport Properties of Tetraalkylammonium Ions in water and alcohols

Transport processes of Ionic mobility and association have been determined as functions of the concentration, temperature, and pressure by using a reliable conductivity equation. The behaviors of alkaline metal, halide, and a variety of tetraalkylammonium ions are investigated and compared from the viewpoint of the dynamic hydration. The experimental results were discussed in terms of the Hubbard-Onsager dielectric friction theory.

Y. Tsujino and M. Nakahara, Noncatalytic Hydrothermal Reaction of Carbon Dioxide with Hydrogen to Form Formic Acid

The kinetics and thermodynamics of the new version of the Water-Gas-Shift Reaction (formic acid discovered as the reaction intermediate) were investigated. It was emphasized that formic acid is useful for the green applications, such as the CO_2 sequestration and the H_2 chemical tank for fuel cells etc.

Tuesday, September 6, afternoon

10. TPWS/PCC/PCAS Joint WG Meeting and Workshop

The following presentation was given:

A. Anderko, P. Wang, M.M. Lencka, R.D. Springer and J.J. Kosinski, Thermodynamic Modeling of Processes Related to Carbon Dioxide Capture and Sequestration

The thermodynamic equilibrium data where carbon dioxide and amines are involved were collected and formulated. The formulation of the equilibrium of the neutralization reactions is studied for the applications.

Thursday, September 8, morning

11. TPWS/PCAS Joint Meeting

The following presentations were given:

N. Okita, Dew Point for Flue Gas in Power Plant Exhaust: Status of Dew Point Equations (in relation to ICRN 23)

R. Span, Thermodynamic Properties of Humid Gases and CO_2 – Rich Mixtures (in relation to closing ICRN 14 and formulating a new ICRN)

J. Hruby, Thermodynamic Properties of Metastable Steam (in relation to closing ICRN 15 and proposing a new ICRN on Thermophysical Properties of Metastable Steam and Homogeneous Nucleation)

V. Holten, C. Bertrand, J. Kalova, D. Fuentavilla, M. Anisimov, J. Sengers, Peculiar Thermodynamics of Supercooled Water

O. Marsalek, Structure, Dynamics and Reactivity of Hydrated Electron

N. Matubayasi, Molecular Study of Hydration Over a Wide Range of Thermodynamic Conditions (PCAS contribution)

Hydration free energies computed for H_2, CO, CO_2, CH_4, HCOOH, CH_3OH, etc. as a function of temperature and density of water were reviewed. Molecular interpretation of the hydration mechanism was given for hydrophobic and hydrophilic solutes.

R. Sakamaki and K. Yasuoka, Molecular Dynamic Simulation of Vapor-Liquid Coexistence for Water and Methane-Water

Thursday, September 8, afternoon

12. Membership. The issues of dealing with inactive members have been revisited. The group went through the membership list and decided to remove the members who cannot be contacted. For the remaining inactive members, an attempt will be made to contact them by e-mail and clarify their intentions to continue their membership.

13. ICRNs. ICRN 10 (pH Measurements and Potentiometric Studies of Supercritical Aqueous Solutions) will be closed. Frantisek Marsik will prepare a new version of this ICRN. Also, Masaru Nakahara indicated that there will be a joint ICRN with PCC on electrochemical potential sensors.

14. Gibbs Award Committee. Andre (Vice-chair)

15. International collaboration. No international collaboration is currently planned.

Adjournment. The meeting adjourned at 2:30 pm.

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

Physical Chemistry of Aqueous Systems Working Group (PCAS WG)

Preliminary Schedule

Pilzen, Czech Republic, 4 – 9 September, 2011

Sun 4, Sept.		Informal Get-together, Cocktails and Registration
Mon 5	08:30	Opening Plenary Session - Executive Committee
	10:00	PCAS Meeting
	13:30	PCAS Meeting
Tue 6	08:30	PCAS Workshop on "Transport, Hydration, and Reactions in Hot Water" 1. Josef Sedlbauer: Progress Report on the IAPWS Project on High-temperature Hydration Thermodynamics of Some Organic Compounds and Gases 2. Masakatsu Ueno: Transport Processes of Tetraalkylammonium Ions in Water and Alcohols at High Temperatures 3. Yasuo Tsujino and Masaru Nakahara: Noncatalytic Hydrothermal Reaction of Carbon Dioxide with Hydrogen to Form Formic Acid
	10:30	PCAS Joint (TPWS/IRS/SCSW/PCC) Meeting
	13:30	PCAS/TPWS/IRS/SCSW/PCC Joint Meeting and Workshop From PCAS, Andre Anderko talks on: Thermodynamic Modeling of Processes Related to Carbon Dioxide Capture and Sequestration
	15:30	PCAS/TPWS/IRS/SCSW/PCC Joint Meeting
Wed 7	09:00-17:00	IAPWS Symposium "Water and Aqueous Mixtures: Research for Future Energy Technologies"
Thu 8	08:30	PCAS/TPWS Joint Meeting From PCAS, Nobuyuki Matubayasi talks on: Molecular study of hydration over a wide range of thermodynamic conditions
	11:00	PCAS Meeting
	13:30	PCAS Meeting (Summary, Report for EC)
		IAPWS Dinner/Banquet
Fri 9	08:30	EC Meeting (8:30-13:00)
	13:30-15:30	Technical Visit to SKODA JS

Agenda for PCAS WG

1. Opening
2. Appointment of Clerk for Minutes
3. Adoption of Schedule and Agenda
4. PCAS Missions and Activity Style
5. Progress Report and Future perspective on The Hydration Project by Josef
6. Possibility of International Collaboration Project
7. Possibility of Release
8. Possibility of ICRN
9. Membership
10. Others