

2012 IAPWS Annual Meeting
Boulder, CO, USA
September 30 – October 5, 2012

PCAS WG Minutes

Present:

Masaru Nakahara (*chair*)

Andre Anderko (*vice chair, clerk of minutes*)

Jana Ehlerova

Maxim Federov

Frantisek Marsik

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Monday, October 1

1. **Opening remarks.** Masaru Nakahara presented the meeting agenda (PCAS Attachment A). Andre Anderko was appointed clerk of minutes.
2. **PCAS mission and activities.** Masaru Nakahara summarized the group's organizational policy. 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. The members have summarized their research interests and current activities. Water and aqueous solution interfacial and hydration phenomena were focused on. Light and heavy metal ions and organics like formic acid as well as simple gases were taken as solutes in terms of free energies, equilibrium constants to seek for likely outputs.
3. **Membership.** The group welcomed Maxim Fedorov (Strathclyde University, Glasgow, UK) as a new member of PCAS.

Masaru Nakahara addressed the issue of deleting inactive members from the PCAS membership list. For this purpose, three criteria have been proposed and accepted by the group. An inactive member will be deleted from the list if (1) they have not participated in the activities of PCAS for a long time (substantially longer than the previously used 3-year period of inactivity), (2) their past contributions (such as creation of releases, guidelines or organizational leadership) cannot be reasonably used to justify their retention or (3) their lack of continued participation is coupled with the associate member status of their home countries. Based on these criteria, seven inactive members have been identified and they are listed in the Appendix. They will be welcome to rejoin the group if they choose to do it.

4. **Progress of the PCAS-sponsored project “Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Solutes and Gases”.** Jana Ehlerova gave the following update:

Over 150 organic solutes and 11 inorganic gases were studied in this work. Data retrieval from literature sources has been finished and hydration properties (in most cases

recalculated from their original format) were entered into the databases. Data processing has been performed. At this point, a paper is being prepared for the Journal of Physical Chemistry Reference Data, to be submitted in November 2012.

There have been no expenditures of IUPAC or IAPWS funds since the last report.

5. **Presentation:**

Maxim Fedorov, Ions and Interfaces: Understanding of Interfacial Behavior of Inorganic and Organic Ions by a Combination of Molecular Simulation and Experiments

Tuesday, October 2, morning

6. **Joint PCC/PCAS workshop on water and energy chemistry.** The following presentations were given:

David Addison, Areas of key interest for the New Zealand National Committee

Frantisek Marsik, Enhancement of hydrogen fuel cell efficiency by the water surface tension control

Hiroshi Takano, Characterization of oxide films formed on welded surfaces of carbon steel for boiler tubes

Andre Anderko, Modeling the effects of solution chemistry on the localized corrosion of engineering alloys

David Addison, Geothermal power – in brief

Masaru Nakahara, Conversion of carbon dioxide and hydrogen into formic acid for CCS: in ambient water without catalyst

Tuesday, October 2, afternoon

7. **Joint PCAS/TPWS/IRS/SCSW Workshop.** The following presentations were given:

Vincent Holten, Mikhail Anisimov, Jan Sengers, Towards a guideline for the thermodynamic properties of supercooled water

Jana Kalova, Surface tension of supercooled water

Radim Mares, Measurement of surface tension of supercooled water

Vaclav Vins, Measurement of surface tension of supercooled water

Olaf Hellmuth, Atmospheric ice formation: Questions of interest to IAPWS

Daphne Fuentavilla, Revised guideline on the critical locus of aqueous solutions of sodium chloride

Further, the following brief communications about recent developments were given:

Andre Anderko, Progress in the development of thermal conductivity guideline for seawater

Richard Pawlowicz, Definition of salinity

Rainer Feistel, Cooperation with BIPM (CCQM, CCT)

CCQM – Consultative Committee on the Amount of Substance

CCT – Consultative Committee on Thermometry

A task group will be appointed for the evaluation of the anticipated guideline for the thermal conductivity of seawater. Allan Harvey suggested that Kiyoshi Miyagawa could check the guideline. Hans-Joachim Kretschmar suggested Andrew Blanghetti. Allan Harvey will check their availability. Andre Anderko has stated that his target for preparing the guideline is Q1 2013.

Thursday, October 4, morning

8. Joint PCAS/TPWS/IRS/SCSW Workshop. The following presentations were given:

Amadeu Sum, The structuring of water in the nucleation of clathrate hydrates

Valeria Molinero, Structural transformations in supercooled water

R. Sakamaki, A. Sum, T. Narumi, K. Yasuoka, melting and freezing point of rigid water models

Subsequently, reports were given on three collaborative projects that were performed under the auspices of IAPWS:

Vaclav Vins, Progress in modeling H₂O - CO₂ mixtures with gas hydrate formation (collaboration between the Institute of Thermomechanics, Prague, Czech Republic, and Ruhr University, Bochum, Germany)

Ilmutdin Abdulagatov, E.N. Shamsetdinov, Experimental study of thermal conductivity of ammonia – water refrigerant mixtures from 278 K to 356 K and pressures up to 20 MPa.

Jan Hruby and Allan Harvey, New data for thermodynamic properties of water in the ideal gas state.

The following announcements were made:

Olaf Hellmuth presented plans for establishing a working group on interfacial properties in aqueous solutions, including supercooled solutions. A secondary objective of the group is the study of properties that control deliquescence and efflorescence.

Maxim Fedorov announced a “satellite” International Workshop on Molecular Solvation to be held in Glasgow in August or September 2013. A discussion ensued whether it would be worthwhile to hold this workshop before, after, or in conjunction with the 2013 IAPWS conference in London. This remains to be determined.

Thursday, October 4, afternoon

Closing session of PCAS

9. Transition in chairmanship. It is expected that a transition in chairmanship will take place at next year’s IAPWS conference. Masaru Nakahara and Andre Anderko will step down as chair and vice-chair, respectively. Masaru Nakahara has proposed Andre Anderko as the new chairman and Josef Sedlbauer Frantisek For vice-chair. Marsik nominated Jana Ehlerova. Josef Sedlbauer accepted the nomination via e-mail and Jana Ehlerova indicated that she would not be available in the near future.

10. Presentations. The following presentations were given:

Tomas Nemeč, Classical nucleation theory – cavitation in binary systems

Andre Anderko, Thermodynamic modeling of actinide solution chemistry

11. Mission and focus areas of PCAS. A discussion was held to specify the topics that are of particular interest to PCAS.

In accordance with the PCAS mission, which states:

- 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.

The following topics are considered to be at the core of PCAS activities:

- Hydration of inorganic and organic species
- Surface and interfacial tension in electrolyte and nonelectrolyte systems in various regions including supercooled and supercritical conditions

- Reactions of organic molecules in solutions – their mechanisms and applications to green technologies
- Speciation and phase equilibria of electrolyte solutions
- Reactions at metal – solution interfaces and their relevance to corrosion phenomena
- Nucleation phenomena
- Interfaces of biomolecules with solutions

Adjournment. The meeting adjourned at 3:30 pm.

Appendix. PCAS members whose membership is not continued

Professor Arthur K. Covington

Dr. Vladimir Majer

Dr. Martin Neumann

Dr. G. Perboni

Dr. A. Regazzoni

Professor N.A. Smirnova

Dr. Dominique You

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

Boulder, USA, 30 September – 5 October, 2012

Sun 30 Sept.		Informal Get-together, Cocktails and Registration
Mon 1 Oct.	08:30	Opening Plenary Session - Executive Committee
	10:00	PCAS Meeting
	13:30	PCAS Meeting
Tue 2	08:30	PCAS & PCC Joint Workshop on "Water and Energy Chemistry" Presentations by PCAS after PCC WG members. 1) Thermodynamical Analysis of the Enhancement of Hydrogen Fuel Cell Efficiency by the Water Surface Tension Control František Maršík, Tomáš Němec, Michal Pavelka 2) Modeling the effects of solution chemistry on the localized corrosion of engineering alloys Andre Anderko 3) Conversion of carbon dioxide and hydrogen into formic acid for CCS: In ambient water without catalyst Masaru Nakahara
	10:30	PCAS Joint (TPWS/IRS/SCSW/PCC) Meeting
	13:30	PCAS/TPWS/IRS/SCSW/PCC Joint Meeting and Workshop
	15:30	PCAS/TPWS/IRS/SCSW/PCC Joint Meeting
Wed 3	09:00-17:00	IAPWS Symposium
Thu 4	08:30	PCAS/TPWS Joint Meeting
	11:00	PCAS Meeting "Classical nucleation theory - cavitation of binary systems" by Tomas Nemece "Thermodynamic modeling of actinide solution chemistry" by Andre Anderko
	13:30	PCAS Meeting (Summary, Report for EC)
		IAPWS Dinner/Banquet
Fri 5	08:30	EC Meeting (8:30-13:00)
	13:30-15:30	Technical Visit

Agenda

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

TPWS Agenda for PCAS and TPWS Joint Meeting

13. Properties of Supercooled Water, joint with PCAS and SC SW
 - 13.1 Towards a Guideline for the thermodynamic properties of supercooled water (V. Holten (speaker), M. Anisimov, J. Sengers)
 - 13.2 Surface tension of supercooled water (J. Kalova, R. Mareš, V. Vinš)
 - 13.3 Atmospheric freezing processes: Questions of interest for IAPWS (O. Hellmuth)
14. Molecular Simulation and Modeling, joint with PCAS
15. Critical locus of aqueous solutions of sodium chloride, joint with PCAS
 - Report (D. Fuentesvilla (speaker), J. Sengers, M. Anisimov)
 - Test Report (K. Miyagawa, A. Harvey)
 - Formal consideration of the Guideline

Masaru Nakahara
10 September, 2012