

**2009 IAPWS Annual Meeting  
Doorwerth, the Netherlands**

**PCAS WG Minutes**

**Monday, September 7, morning**

*Present: Masaru Nakahara (chair), Andre Anderko (vice chair, clerk of minutes), Jana Ehlerova, Anneke Levelt-Sengers, Frantisek Marsik, Pavel Safarik, Milan Sedlar, Josef Sedlbauer*

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 (PCAS Attachment A). The agenda has been adopted unchanged.
2. **Minutes of the 2008 Meeting** in Berlin were adopted as written.
3. **IAPWS Interntional Collaboration.** Josef Sedlbauer presented an update on the collaborative project between Canada (Peter Tremaine) and Czech Republic (Josef Sedlbauer). This project has been finished and report has been sent to the Executive Committee.
4. **Existing ICRNs.** The group discussed the ICRNs that were associated with previous activities.

**ICRN no. 10 (pH).** Masaru Nakahara informed that this project expired. Since both principal investigators, Donald Palmer and Serguei Lvov, are absent, Masaru Nakahara will ask them whether they wish to continue. It has been noted that a guideline on the ionization constant of water has been published and accepted. Anenke Levelt-Sengers noted that pH of seawater is currently being investigated by the Subcommittee on Seawater, which offers an opportunity for cross-linking.

**ICRN no. 13** (surface tension). Frantisek Marsik informed that the project has been closed. An application paper has been published in the Journal of Solution Chemistry. Frantisek Marsik prepared a closing statement, which is attached as PCAS Attachment B.

**ICRN no. 17** (amines). This ICRN is to be reviewed jointly with PCC

**ICRN no. 21** (ultrasupercritical plant chemistry). Masaru Nakahara will inquire about the status of this ICRN with Don Palmer and Barry Dooley.

**ICRN no. 22** (nucleation in steam turbines). Frantisek Marsik has indicated that this ICRN is coordinated by Dr. Stastny and really belongs in PCC.

5. **Task groups, future directions, and future ICRNs.** Masaru Nakahara opened discussion on future research directions that may result in new ICRNs and guidelines. The following possible thrust areas have been discussed:

***Cavitation*** – Frantisek Marsik indicated his interest in a new ICRN on cavitation. He prepared a statement of interest and project outline on this topic. This document is attached as PCAS Attachment C. The group unanimously approved the idea of proposing the new ICRN on cavitation.

***Viscosity and thermal conductivity of seawater*** – Masaru Nakahara indicated that these topics are being studied within the framework of the Subcommittee on Seawater

***Electrolyte thermodynamic modeling of multicomponent solutions*** – Andre Anderko proposed investigating models for complex electrolyte systems with a particular focus on applications in hydrometallurgy and power generation.

***Hydration properties*** – Josef Sedlbauer indicated that guidelines on hydration properties will be closed next year; he also expressed interest in electrolyte modeling

***Application for power generation*** – Masaru Nakahara indicated that he is conducting discussions with Japanese power generation companies on their needs.

***Fuel cell electrochemistry*** – Frantisek Marsik indicated that this may be an appropriate area of research for PCAS.

***CO<sub>2</sub> emission reduction*** – Masaru Nakahara indicated that this may be another area of interest for PCAS.

### **Monday, September 7, afternoon**

*Present: Masaru Nakahara (chair), Andre Anderko (vice chair, clerk of minutes), Jana Ehlerova, Anneke Levelt-Sengers, Frantisek Marsik, Pavel Safarik, Milan Sedlar, Josef Sedlbauer*

5. **Task groups, future directions, and future ICRNs – continued**

***Cavitation*** – Frantisek Marsik gave a presentation on cavitation in pure water and water solution. This topic is intended to be the subject of a new ICRN (see Attachment C). A discussion followed. Andre Anderko asked about the anticipated final product of this research. Frantisek Marsik indicated that focus will be put on publishing algorithms and integrating them with CFD codes. Milan Sedlar will take the lead on the implementation tasks. Masaru Nakahara asked about the theoretical fundamentals. Frantisek Marsik answered that the model will be based on nonequilibrium thermodynamics. Josef Sedlbauer inquired about the main anticipated novelty of the method. Frantisek Marsik responded that the main novelty will lie in taking into account the concentration dependence. A further question related to the effects of gravity. This effect is unimportant.

***Electrolyte thermodynamic modeling of multicomponent solutions*** – Andre Anderko gave an impromptu presentation on the recent work at OLI System on modeling systems of hydrometallurgical importance. Masaru Nakahara inquired about the fundamental nature of the thermodynamic model. Andre Anderko responded that the model is a combination of a formulation for standard-state properties and the excess Gibbs energy. The fundamentals of the model have been already published (P. Wang, A. Anderko and R.D. Young, *Fluid Phase Equilibria*, 203 (2002) 141-176, P. Wang, A. Anderko, R. D. Springer, and R. D. Young, *J. Molec. Liquids*, 125 (2006) 37-44). The work on developing model parameters is carried out in collaboration with Professor Papangelakis of the University of Toronto.

**Tuesday, September 8, morning**

*Present: Masaru Nakahara (chair), Andre Anderko (vice chair, clerk of minutes), Jana Ehlerova, Frantisek Marsik, Milan Sedlar, Josef Sedlbauer*

**PCAS Workshop**

Three presentations were given in the PCAS workshop:

“Standard Partial Molar Properties of Solutes” by Josef Sedlbauer. This work is nearing completion. Publication of the results is planned in the near future. The main medium for disseminating the results of this project will be a database.

“Formic Acid as a Chemical Tank for Hydrogen” by Masaru Nakahara. Recent research in this area has been reviewed. A discussion followed on the fate of carbon dioxide that is associated with this process.

“Equilibrium Constants and Speciation of Aqueous Transition Metal Chlorocomplexes Over a Wide Range of Temperature and Pressure” by Jana Ehlerova (speaker) and Josef Sedlbauer. A summary of this project was given. This work was performed on a collaborative basis between the University of Liberec (Czech Republic) and Guelph University (Canada).

**Tuesday, September 8, afternoon**

**Joint Meeting of PCAS and PCC**

The following presentations were given at workshop:

“The Efficiency of the Coupled Electrode Membrane Processes” by Frantisek Marsik

“Electrophoretic Mobility and Zeta Potential of Magnetite at Temperatures Corresponding to Power Plant Operating Conditions” by Sonja Vidojkovic

“Generator Water Chemistry – Behavior of Copper Oxide” by Robert Svoboda

“Equilibrium Constants and Speciation of Copper Chloride” by Jana Ehlerova

The second part of the joint meeting was devoted to the discussion of ICRNs:

ICRN 17: “Research on Amines in the Power Industry” by Jim Bellows. This topic encompasses (1) degradation of amines, mechanisms and products; (2) what does it do in terms of corrosion and (3) implication of the degradation in plants.

ICRN 20: “Steam Chemistry in Turbine Phase Transition Zone” by Miroslav Stastny. This topic includes (1) formation of substances that act as precursors to nucleation; (2) chemistry of first condensate; (3) additives that influence nucleation; (4) theory for mathematical simulation of heterogeneous condensation processes; (5) chemical and mechanical structure of deposits on turbine blades.

ICRN 21: “Interfacial Situation in Advanced Ultra-Supercritical Plants”. This ICRN had been proposed by Peter Tremaine and was discussed in his absence by Robert Svoboda.

ICRN 25: “Corrosion Mechanisms in the Presence of Contaminants in Steam/Water Circuits, Particularly in Boiler Water”. This ICRN encompasses the study of local corrosive environments that are formed by various cation and anions as a result of condensation and it seeks to relate the local environments to the observed corrosion rates.

**Thursday, September 10, morning**

**Joint Meeting of TPWS, PCAS, SCSW, and IRC (8:30am – 10:30am)**

The following presentations were given at the joint meeting:

“Towards Models for Viscosity and Thermal Conductivity of Seawater: Model Fundamentals” by Andre Anderko

“Critical Locus of Salt Water” by Daphne Fuentevilla

“A New Scheme of Hydrogen Technology Based on Hydrothermal Chemistry of Formic Acid” by Masaru Nakahara

**Thursday, September 10, morning (10:45am – 12:15am)**

*Present: Masaru Nakahara (chair), Andre Anderko (vice chair, clerk of minutes), Jana Ehlerova, Frantisek Marsik, Milan Sedlar*

Milan Sedlar gave a presentation “Numerical and Experimental Investigation of Cavitation in Water”. This presentation was related to the proposed new ICRN.

The group discussed how the declining number of participants should be addressed in the future. It has been agreed that the size of the group dropped below the “critical mass” for effective work. Andre Anderko proposed shifting all presentations to joint sessions with TPWS/SCSW or PCC, depending on the topic. Frantisek Marsik supported the idea. Masaru Nakahara expressed a concern that such an approach is drastic and could make the further existence of the group questionable. Frantisek Marsik and Andre Anderko expressed the opinion that PCAS meetings would be still desirable and would be focused on discussions of present and future activities.

Physical Chemistry of Aqueous Systems Working Group (PCAS WG)

Agenda

Arnhem, The Netherlands, 6 – 11 September 2009  
(Hotel Golden Tulip, Doorwerth)

1. Agenda

- 1.1 Amendments / Adoption of Agenda
- 1.2 Week program: split up of PCAS for joint workshops and task groups

2. Appointment of Clerk of Minutes

3. Approval of Minutes of PCAS WG in Berlin, Germany, 2008

4. Progress Reports on PCAS Activities 2008 / 2009

- ◇ Activities 2008: from minutes of EC, 2008; 8. PCAS, full minutes can be found in Attachment 4.
- ◇ 8.1 International Collaboration on “The aqueous copper (II) complexation as a function of T”  
By Peter Tremaine (Canada) and Josef Sedlbauer (Czech Republic); Ms. Jana Ehlerova (Cz. Pep.)
- ◇ 8.2 The joint symposium with the Electrochemical Society in Washington, DC in 2007.
- ◇ 8.3 New PCAS WG members: D. Guzonas, AECL, Canada; Professor Nobuyuki Matubayasi
- ◇ 8.4 New Chairman and Vice Chairman: Masaru Nakahara and Andre Anderko, respectively.  
(gradual transition from Serguei Lvov between September, 2008 and 1<sup>st</sup> January, 2009)
- ◇ 8.5 Reported on the discussions (joint with PCC) about icrns 17, 21, and 22  
(minutes 9.2)  
ICRN 17 (amines); reviewed jointly  
ICRN 21 (ultrasupercritical plant chemistry); reviewed jointly  
ICRN 22 (nucleation in steam turbines); still under review by PCC, Comments by Hruby, Cz.Rep.

4.1 **The Joint IUPAC/IAPWS Project “Standard Partial Molal Properties of Solutes” to be reported by Professor Josef Sedlbauer: Berlin EC Minute 8.7.**

4.2 **International Collaboration**

08EC8.1 International Collaboration on “The aqueous copper (II) complexation as a function of T” **By Josef Sedlbauer (Czech Republic) and Jana Ehlerova (Cz. Pep.)**

4.3 **ICRN**

Reported on the discussions (joint with PCC) about icrns 17, 21, and 22 (minutes 9.2)  
ICRN 17 (amines, Maughan); reviewed jointly  
ICRN 21 (ultrasupercritical plant chemistry, Don Palmer and Serguei Luvov); reviewed jointly  
ICRN 22 (nucleation in steam turbines); still under review by PCC, Comments by Hruby, Cz.Rep.

**4.4 PCAS Task Groups**

- Hydrometallurgy: Complex Ions, Complex formation, Solubility
- Hydrogen Energy
- EOS of aq nacl; Peter Tremaine, Allan Harvey (Anneke Sengers)
- Self-diffusion coefficients for H<sub>2</sub>O
- Viscosity coefficients for aq solutions
- What outputs can be made by PCAS?
- Changes in PCAS Task Groups, Priority List

**5 New icrns?**

5.1 ICRN #30 “Cavitation...”

**6. Proposals for International Collaboration?**

**7. Other Business**

**8. Changes in Membership, Election of Officers**

**9. Preparation of Action List 2009 / 2010, Task Distribution, Next Year's Agenda**

**10. Preparation of PCAS WG Report for Executive Meeting**

**11. Miscellaneous and Adjournment**

### **IAPWS Certified Research Need 13**

Surface Tension of Aqueous Solutions. Issued September 1998. Expires July 2005. IAPWS Contacts: F. Sigon and F. Gabrielli

### **Closure Document**

In consideration that the sponsor is not longer active in IAPWS, and the subject is covered in an IAPWS book, the Working Group on Physical Chemistry of Water and Steam recommended a closing statement.

### **Background**

This ICRN was first issued in 1998 by researchers from ENEL (Italy) in cooperation with Alstom Power. Studies were continued under grants from the Czech Republic and the Czech Academy of Sciences.

### **Results Achieved**

This subject has been covered by the paper written by: František Maršík, Tomáš Němec, Jan Hrubý, Pavel Demo, Zdeněk Kožíšek, Václav Petr, Michal Kolovratník:

**Binary Homogeneous Nucleation in Selected Aqueous Vapor Mixtures**, J Solution Chem (2008) 37: 1671–1708, DOI 10.1007/s10953-008-9337-4



## **Proposed IAPWS Certified Research Need – ICRN**

### **Cavitation in Pure Water and Water Solutions**

Tomas Nemec, Milan Sedlar, Frantisek Marsik, C. F. Delale (external collaborator)

The reliability, efficiency and life time of hydro-machine performance is strongly affected by cavitation. Classical theory of cavitation, which is based on the surface tension of pure water fails by 5 orders in cavitation rates prediction. It causes the application of empirical formulas for prediction of primary bubbles population in the real fluid (water). These formulas depend not only on a chemical composition of admixtures but on an amount of diluted gases. This is a main reason why applied empirical formulas have to be fitted for each actual working conditions.

The goal of this project is to elaborate better physico-chemical description of the cavitation theory, which would be applicable for the design or optimization of hydro-machines, especially for utilization in current computer codes.