

IAPWS Annual Meeting 2008, Berlin PCAS WG Minutes

Sunday Sept. 7th, Morning

Present: Serguei Lvov (Chair); Peter Tremaine (Clerk of Minutes); Anneke Levelt Sengers; Bill Marshall; Masaru Nakahara; Josef Sedlbauer; Milan Sedlar; Pavel Safarik; Masakatsu Uneo; Vladimir Valyashko.

1. **Opening Remarks** were made by Serguei Lvov (Chair) and Peter Tremaine. Members introduced themselves with a short description of their research interests. Peter Tremaine was appointed Clerk of Minutes. Serguei Lvov proposed a meeting agenda (PCAS Attachment A).
2. **Minutes from 2007 meeting (Lucerne)** were approved as written.

Actions Arising: Three outstanding actions from 2007 remain. (i) Horacio Corti has expressed concern about the difficulties he is having in attending meetings as co-chair. The question will be discussed today. (ii) The delay in the IAPWS/IUPAC project associated with Vladimir Majer's departure must be resolved. (iii) An ICRN on the need for a new equation of state for NaCl(aq) was to be prepared.

Tremaine presented a verbal summary of the need to a new equation of state for NaCl, compatible with the current IAPWS formulations for the PVT properties. He noted that the current equation of state for NaCl(aq) by Don Archer, is based on the Hill (1991) equation for water and Archer's dielectric constant model.

ACTION: (Tremaine, Levelt Sengers): To develop a draft ICRN for 2009 in collaboration with NIST (Levelt Sengers will be replaced by A. Harvey)

3. **IAPWS International Collaboration:** Peter Tremaine presented the progress on the international collaboration between Canada (Tremaine) and the Czech Republic (Sedlbauer), budgeted with an IAPWS contribution of \$14,000 for living expenses of PhD student Jana Ehlerova. The project is for measurements on copper (II) complexation vs. temperature as part of an International Generation IV Forum research project on hydrogen co-generation. Dr. Tremaine and Dr. Trevani will supervise the experimental portion of the project at Guelph; Dr. Sedlbauer will supervise fitting the available models to the new data. Ms. Ehlerova started at Guelph in July, 2008, and returned to Europe for this ICPWS conference. A completely new UV-visible system, flow cell, and automated injection system have been constructed and commissioned. The first results (100 °C) were obtained just before she left Guelph.

MOTION(Lvov): To approve the progress report project. Unanimous approval (Tremaine: abstained).

4. Task Groups and Committees:

4.1. Joint Electrochemical Society IAWS Symposium Topics (Washington, 2007): Serguei Lvov presented a status report on the Joint IAPWS/ECS Symposium (PCAS Attachment B). It was two-day symposium with 25 papers. The financial support of IAPWS and other organizations were used to support seven invited speakers, organize and conduct the symposium, and print out a few copies of the symposium proceedings (in print). Full manuscripts of the submitted for publishing papers will be shortly available in ECS Transactions (<http://www.ecsdl.org/ECST>), an online journal of the ECS (<http://www.ecsdl.org/ECST>).

IT WAS AGREED: PCAS members compliment Serguei on this very successful initiative.

5. New Members: The following new members were suggested.

- (i) Dave Guzonas (Chalk River National Laboratories, Canada);
 - (ii) Nobuyuki Matubayasi (Institute of Chemical Research, Kyoto University, Japan)
- Moved (Serguei Lvov) that both be approved as PCAS members. Both were approved unanimously.

6. Election of new Chair and Vice-Chair

Possible candidates for chair and vice chair were identified and discussed their willingness to serve.

MOTION: Masakatsu Ueno nominated Masaru Nakahara chair of PCAS by e-mail. The nomination was supported by a number of PCAS members and acclaimed.

MOTION: Peter Tremaine nominated Andre Anderko vice-chair of PCAS. The nomination was supported by a number of PCAS members and acclaimed.

Sunday Sept. 7th, Afternoon

Present: Serguei Lvov (Chair); Peter Tremaine (Clerk of Minutes); Anneke Levelt Sengers; Bill Marshall; Masaru Nakahara; Josef Sedlbauer; Milan Sedlar; Pavel Safarik; Masakatsu Ueno; Vladimir Valyashko, Dave Guzonas (for Item 8).

7. ICRNs and Releases (Joint with PCC): The working groups met together to discuss three PCC ICRNs that could require PCAS input.

7.1 ICRN Number 17 (Amines): Jim Bellows presented modifications to ICRN on needs for thermochemical and kinetic data for thermal power station boilers. Temperature range up to

850 F, key areas are 150 °C (nuclear PWR transition point) and 850 F (thermal station turbines). Lower alloys and carbon steels are priority.

7.2 ICRN Number 21 (Steam Chemistry in the Turbine Phase-Transition Region): No discussion. Draft is awaiting PCAS input.

ACTION (Svoboda): To circulate draft to PCAS (to Lvov and Nakahara) for distribution and discussion.

7.3 ICRN Number 22 (Chemistry in Ultra-supercritical Steam): No discussion. Draft had comments from Don Palmer, mostly minor. It was agreed that Don would be asked to indicate whether these need further input, or whether they can be regarded as editorial.

ACTION (Dooley) To contact Don today.

7.4 ICRN (No Number) (NaCl Eqn of State)....See Item 2.

4. Task Groups and Committees (CONTINUED):

4.2. Data Book Project: Prof. Valyashko (editor) presented an update on his data book project “*Hydrothermal Properties of Materials*”. The project started in 2003. Chapter 7 on calorimetric properties of hydrothermal solutions by Dr. Majer has been withdrawn and was written in more limited form by Dr. Valyashko. The draft manuscript is complete and has been reviewed by the publisher (Wiley). It is expected to be published by December, 2008.

IT WAS AGREED: PCAS members compliment Vladimir on this very successful, major project.

4.3: Joint IUPAC/IAPWS Project on Standard Partial Molar Properties of Solutes Serguei Lvov presented a report from Vladimir Majer (PCAS Attachment C) outlining his withdraw from the project and summarizing its status. After discussion, Dr. Josef Sedlbauer was invited to prepare a proposal for continuing the project, possibly with a more focused set of objectives and a new budget. Issues to be resolved are the state of IUPAC involvement, and whether funds can be released before the next IAPWS meeting by the executive subject to receiving a suitable proposal.

IT WAS AGREED: To request from the EC that the project funding remain in place for one year, or until the proposal from Dr. Sedlbauer has been received.

8. Research Presentations:

8.1 Andrei Anderko: OLI Software Andrei presented the underlying models for standard state properties, activity coefficients, transport properties and the capabilities of the OLI Electrolyte Simulation Package, and other OLI systems.

Serguei Lvov and Anneke Levelt Sengers noted that PCAS should be more involved in modeling of aqueous solutions.

8.2 Masuru Nakahara: Masuru presented an overview of NMR methods for hydrothermal studies, and examples of applications from his laboratory including the self-diffusion of water, ionic solvation, speciation in SCW and a new probe design (up to 420 °C).

8.3 Josef Sedlbauer: Josef presented his research on functional group additivity models for organics in high-temperature water. Software is available Majer, Sedlbauer, Begin (2008) Fluid Phase Equil, in press. Gibbs energy of hydration extrapolates well for const C_p° .

8.4 Bill Marshall: Bill presented density-temperature correlations for the dielectric constant of water and dioxane-water mixtures, which yield simple predictive correlations over a wide range of temperature and pressure.

9. Wrap-up: Serguei Lvov led a brief discussion of future directions in PCAS activities. The need to include practical simulation and ab initio methods where they can lead to practically applicable results was noted.

10. The meeting adjourned at 5:40 pm.

Working Group on Physical Chemistry of Aqueous Systems (PCAS WG)

Meeting Schedule

Berlin, Germany, September 7th, 2008
Radisson SAS Hotel

Chair: Serguei Lvov, lvov@psu.edu
Pennsylvania State University, University Park, PA, USA
Vice-Chair: Horacio Corti, hrcorti@cnea.gov.ar
CNEA, Buenos Aires, Argentina

11:00 - 12:30 (Aquamarin Room)

- Opening remarks
- Approval of agenda
- Appointment of clerk of minutes
- Approval of minutes of PCAS WG in Lucerne, Switzerland, 2007
- Reports on IAPWS International Collaborations
- Reports on ICRNs, Releases etc.
- Reports of task groups and committees
- Proposals for membership
- Other business

12:30 - 13:30 Lunch (Conference Foyer)

13:30 - 15:00 (Aquamarin Room)

- Proposals on new IAPWS International Collaborations
- Proposals for new ICRNs, Releases etc.
- Proposals on new task groups and committees
- Research presentations

15:00 – 15:30 Coffee Break

15:30 – 17:00 (Aquamarin Room)

- Research presentations
- Preparation of PCAS WG Report to Executive Committee

Confirmed Research Presentations:

- Peter Tremaine: Equilibrium Constants and Speciation of Aqueous Transition Metal Chloro-complexes over a Wide Range of Temperatures and Pressures
- Masaru Nakahara: The Self-diffusion Coefficient for Supercritical Water
- Andre Anderko: Thermophysical Property Research at OLI Systems
- Josef Sedlbauer: Thermodynamic Modeling of Aqueous Organics in a Wide Range of Conditions
- Bill Marshall: Density-Temperature Correlations for the Dielectric Constant of Water and Dioxane-Water Mixtures

ECS/IAPWS Joint Symposium

212th ECS Meeting - Washington, DC

October 7 - October 12, 2007

**Symposium B4 - Interfacial Electrochemistry and Chemistry
in High Temperature Media**

Symposium Organizers:

S. N. Lvov, Department of Energy and Geo-Environmental Engineering, The Pennsylvania State University, University Park, PA 16802, USA, tel: 814.863.8377, fax: 814.865.3248, e-mail: lvov@psu.edu; **S. R. Narayanan**, NASA-Jet Propulsion Laboratory, 4800 Oak Grove Drive, Mail Stop 277-207, Pasadena, CA 91109, USA, tel: 818.354.0013, fax: 818.393.6951, e-mail: s.r.narayanan@jpl.nasa.gov; **D. D. Macdonald**, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA, tel: 814.863.7772, fax: 814.863.4718, e-mail: ddm2@psu.edu; **R. B. Dooley**, Electric Power Research Institute, 1300 West W.T. Harris Blvd., Charlotte, NC 28262, USA, tel: 650.855.2458, fax: 650.855.1026, e-mail: bdooley@epri.com; **D. J. Wesolowski**, Chemical Sciences Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, USA, tel: 865.574.6903, fax: 865.574.4961, e-mail: wesolowskid@ornl.gov

**Sponsors: ECS Energy Technology Division/ECS Corrosion
Division/IAPWS/ASME Steam Properties Subcommittee**

Tuesday, October 9, 2007

Exhibit Hall, Concourse Level

Co-Chairs: Poster Session

Time Abs#

Title and Authors

- o 229 The Development of Monolithic Design for Methanol Micro-Reformer and CO Clean-Up O. Jeong Hoon, C. Chung (Sungkyunkwan University), S. Haam and J. Park (Yonsei University)
- o 230 Novel Cathode Catalyst for Use in DMFC: The Role of Carbon Support and Promoter M. Lo, Y. Lee and Y. Chen (ITRI)

Wednesday, October 10, 2007

Edison Room, Terrace Level

Co-Chairs: J. Payer and D. Macdonald

Time	Abs#	Title and Authors
08:00		Introductory Remarks (20 Minutes)
08:20	231	Applied and Theoretical Aspects of Interfacial Electrochemistry vs. Room/Near Room Temperature Measurements A. Wieckowski (University of Illinois at Urbana-Champaign)
09:00	232	Kinetics of the Hydrogen Electrode Reaction on Platinum in Alkaline Solutions at Elevated Temperatures J. Bao and D. Macdonald (Pennsylvania State University)
09:20	233	Chemistry in Surface Boundary Layers Related to Flow Accelerated Corrosion of Carbon Steel in High Temperature Water S. Uchida, M. Naitoh, Y. Uehara, H. Okada (Nuclear Power Engineering Corporation) and S. Koshizuka (University of Tokyo)
09:40		Intermission (20 Minutes)
10:00	234	Experimental System for Studying Interfacial Electrochemistry at Temperatures Above 300oC V. Balashov, M. Fedkin, S. Lvov (Penn State University) and R. Dooley (EPRI)
10:20	235	Crevice Corrosion Damage Evolution in High Temperature Brines J. H. Payer, X. Shan, A. S. Agarwal (Case Western Reserve University) and U. Landau (CWRU)
11:00	236	Corrosion of Combustion Turbine Blades M. Caldwell and R. Viswanathan (EPRI)
11:20	237	High Temperature Corrosion of Materials in Supercritical Water and Liquid Lead Environments K. Sridharan, Y. Chen, L. Tan, M. Machut, A. Kruizenga, X. Ren and T. Allen (University of Wisconsin-Madison)
11:40	238	Influence of Temperature and pH on the Identities and Electronic Properties of Surface Films Formed on Chromium and Alloy C22 T. Cohen-Hyams, S. Harrington, M. Miyagusuku, F. Wang and T. Devine (University of California, Berkeley)

Co-Chairs: D. J. Wesolowski and S. Paddison

Time	Abs#	Title and Authors
14:00	239	Structure of and Transport in the Interfaces of Solid Oxide Fuel Cells S. Singhal and X. Zhou (Pacific Northwest National Laboratory)
14:40	240	A Mechanistic Understanding of Solid Oxide Fuel Cell Chemistry Through In-Situ Raman Spectroscopy M. Pomfret (University of Maryland, Naval Research Laboratory), J. Owrutsky (Naval Research Laboratory) and R. Walker (University of Maryland)
15:00	241	Interfacial Resistivity of Yttria Stabilized Zirconia in Operating Solid Oxide Fuel Cells M. Pomfret (University of Maryland, Naval Research Laboratory), E. Bryan and R. Walker (University of Maryland)
15:20	242	Computational and Experimental Analysis of Solid Oxide Fuel Cell Anodes in the Presence of H ₂ S D. A. Daramola, M. Muthuvel, A. Marquez and G. Botte (Ohio University)
15:40		Intermission (20 Minutes)

- 16:00 243 Thin Film Electrochemical Deposition at Temperatures up to 180 {degree sign}C for Photovoltaic Applications C. Levy-Clement (CNRS)
- 16:40 244 Applicability of the Ytria-Stabilized Zirconia pH Sensor on Concentrated Acidic Metal Sulphate Solutions Z. Jankovic, V. Papangelakis (University of Toronto) and S. Lvov (Penn State University)
- 17:00 245 Study of the Electrochemical Step of Novel Active Metal Alloy Thermochemical Cycles for Hydrogen Production V. Rodriguez-Santiago, M. Fedkin and S. Lvov (Penn State University)

Thursday, October 11, 2007

Edison Room, Terrace Level

Co-Chairs: S. N. Lvov and S. R. Narayanan

- | Time | Abs# | Title and Authors |
|-------------|-------------|--|
| 08:00 | 246 | Direct Observations of Mineral-Water Interface Reactivity at Elevated Temperatures with Interfacial X-ray Scattering P. Fenter (Argonne National Laboratory) and N. Sturchio (University of Illinois at Chicago) |
| 08:20 | 247 | The Protonation Behavior of Metal Oxide Surfaces to Hydrothermal Conditions M. L. Machesky (Illinois State Water Survey), D. Wesolowski (Oak Ridge National Laboratory), M. Ridley (Texas Tech University), D. Palmer, J. Rosenqvist (Oak Ridge National Laboratory), S. Lvov, M. Fedkin (Penn State University), M. Predota (University of South Bohemia), L. Vlcek and P. Cummings (Vanderbilt University) |
| 08:40 | 248 | Ion Adsorption on Metal Oxide Surfaces to Hydrothermal Conditions. D. Wesolowski (Oak Ridge National Laboratory), M. L. Machesky (Illinois State Water Survey), M. Ridley (Texas Tech University), D. Palmer, J. Rosenqvist (Oak Ridge National Laboratory), J. Kubicki (Penn State University), M. Predota (University of South Bohemia), L. Vlcek, P. Cummings (Vanderbilt University), Z. Zhang, P. Fenter (Argonne National Laboratory), A. Bandura (Saint Petersburg State University, Russia) and P. Benezeth (CNRS, Toulouse, France) |
| 09:20 | 249 | Interfacial Chemistry of Hydrothermal Deposition of Zirconia on Metal Substrates Z. Zhou, E. Chalkova, V. Balashov and S. Lvov (Penn State University) |
| 09:40 | | Intermission (20 Minutes) |
| 10:00 | 250 | Ab Initio Modeling of Structure, Reactivity, and Transfer at Water/Ionomer and Water/Catalyst Interfaces S. J. Paddison (University of Alabama in Huntsville) |
| 10:40 | 251 | Understanding the Water Retention of Composite PEMs Based on Surface Chemistry of Inorganic Fillers M. Fedkin, E. Chalkova (Penn State University), D. Wesolowski (Oak Ridge National Laboratory) and S. Lvov (Penn State University) |
| 11:00 | 252 | An Overview of Interfacial Processes in Polymer Electrolyte Fuel Cells Operating at Elevated Temperatures S. Sambandam, P. Trogadas and V. Ramani (Illinois Institute of Technology) |
| 11:40 | 253 | The Study of Ethoxy Surface Species on Pt-Sn Surface Alloys by the Decomposition of Chemisorbed Ethyl Nitrite A. Hightower (Occidental College), H. Haibo Zhao (University of Southern California) and B. Koel (Lehigh University, Chemistry Department) |

Number of presented papers: 25 (23 oral and 2 posters)

Invited Speakers:

1. A. Wieckowski (University of Illinois at Urbana-Champaign)
2. J. H. Payer (Case Western Reserve University)
3. S. Singhal (Pacific Northwest National Laboratory)
4. C. Levy-Clement (CNRS, France)
5. D. Wesolowski (Oak Ridge National Laboratory)
6. S. J. Paddison (University of Alabama in Huntsville)
7. V. Ramani (Illinois Institute of Technology)

Physical Chemistry of Aqueous Solutions Working Group (PCAS WG)

Chair: Serguei Lvov, lvov@psu.edu

Pennsylvania State University, University Park, PA, USA

Vice-Chair: Horacio Corti, hrcorti@cnea.gov.ar

CNEA, Buenos Aires, Argentina

Statement regarding the status of the IAPWS / IUPAC project
“Establishing recommended data on thermodynamic properties of hydration
for selected organic solutes and gases”
and the review of the IAPWS costs

August 31, 2008

This short report has been prepared on request of S. Lvov, Chairman of the Physical Chemistry of Aqueous Solutions Working group, in preparation of the 2008 IAPWS EC meeting in Berlin (Germany).

The project was approved by the EC of IAPWS at the 2004 Meeting in Kyoto (Japan) for the period 01/2005 – 06/2007, the total funding allotted to the project by IAPWS was of 12,000 euros (with 5K in 2005, 5K in 2006 and 2K in 2007). These funds were aimed at supporting young scientists from the IAPWS member countries contributing to the Project.

During 2005 and 2006 I have sent to the IAPWS and IUPAC representatives as well as to the Project participants three progress reports describing all the activities carried out in the frame of the project. One Workshop on thermodynamic properties of hydration of nonelectrolytes was organized during the Thermo International held in Boulder, Co (July 30 – August 4, 2006). Most groups participating in the project presented their contributions, this one day workshop attracted a large audience participating in the event.

Unfortunately for the project, I have changed my professional assignment in the fall 2006, named for two years as Director of the Representation of the French National Centre for Scientific Research (CNRS) for Russia and CIS; this Office is attached to the Science Department of the French Embassy in Moscow. Although I had hoped to continue some of my scientific activities while being in the Office, it turned out during the first half of 2007 that my working load did not let me any spare time. I informed about it S. Lvov (IAPWS) and J. Dymond (IUPAC) in the electronic message of May 1, 2007. I discussed with some key participants of the Project the possibility of my replacement in the coordination task but nobody was available for taking over the job. For that reason no progress was made after my departure for Moscow with the exception of the group of R. Fernandez-Prini (Buenos Aires) that has completed an evaluation and correlation work concerning several aqueous gases. I have received their report on March 23, 2007 and after examined it I sent it on May 1, 2007 to both IAPWS and IUPAC as a partial result of the Project.

Moreover, I will very probably extend my mission in Moscow for additional two years (up to the fall 2010), provided there is no major diplomatic crisis between the Western

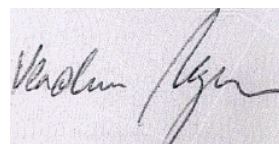
democracies and Russia in future. This will therefore make my involvement in the Project impossible for additional two years or so.

Payments made by IAPWS for the Project are as follows; only a brief survey is given here, more details can be found in the three progress reports; approximately 30 % of the allotted IAWPS funds (12,000 euros) were spent by now:

1. 18th July 2005. Hugues Arcis, PhD student at the Blaise Pascal University, Clermont-Ferrand, France, stipend for data processing during July 2005. \$963.20.
2. 18th July 2005. Martin Slavik, young assistant professor at the University of Liberec, Czech Republic, partial support for travel to Clermont-Ferrand, experimental determination of heat capacities as a function of temperature for several aqueous oxygen containing compounds, (was published in JSC, 2007), September 15 to October 30, 2005. \$1,444.80.
3. 18th July 2005. Pavel Vrbka, young assistant professor at the Institute of Chemical Technology, Prague, Czech Republic, partial support for travel to International Conference on Solution Chemistry in Portoroz, Slovenia, August 21 to 26, 2005. Presentation of a poster directly related to the Project. \$722.40.
4. 19th December 2005. Hugues Arcis, PhD student at the Blaise Pascal University, Clermont-Ferrand, France, stipend for data processing in period September to December, 2005. \$961.12.
5. 14th August 2006. Pavel Vrbka, young assistant professor at the Institute of Chemical Technology, Prague, Czech Republic, partial support for travel to the Thermo International, Boulder, July 30 – August 4, 2006. Presentation of a contribution during the Project workshop. \$1,463.

Enclosures:

1. Progress reports 1 to 3
2. Final report gases (Prini's group)
3. Literature list for the Final report gases



Vladimir MAJER
Project coordinator