MINUTES OF PCAS WG
WITNEY, ENGLAND, SEPTEMBER 3-8, 2006

Members in attendance during the week: *Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Ueno; Frantisek Marsik; Pavel Safarik; Tomas Nemec, Ondrej Mican.*

Monday Morning

1. Opening Remarks were made by Serguei Lvov (Chair). Members introduced themselves with a short description of their research interests. Peter Tremaine was appointed Clerk of Minutes. The Agenda is Attachment A to PCAS Minutes

2. Minutes from 2005 meeting (Santorini) were approved as written.

3. IAPWS International Collaboration: Peter Tremaine presented the proposal by Canada (Tremaine) and the Czech Republic (Sedlbauer). Both national committees support the proposal. The proposal was discussed. Ms. Erhlova is Dr. Sedlbauer's PhD student. Dr. Tremaine and Dr. Trevani will supervise the experimental portion of the project; Dr. Sedbauer will supervise fitting the Sedlbauer-O'Connell-Wood group-additivity model to the new data. The data will form part of a larger project to develop group additivity models for aromatic organic solutes in high temperature water.

Motion (Lvov): To approve the project. Unanimous approval (Tremaine: abstained).

4. ICRNs and Releases: The following were discussed:

ICRN Number 10 (pH Measurements). Don Palmer had formulated this ICRN, and follow-up action/report has not yet been received. ***ACTION: (Lvov)*** to contact Don Palmer and offer a 3 year extension if needed.

ICRN Number 13 (Surface Tension of Aqueous Solutions. Issued September 1998**):** ***ACTION (PCAS):*** Members agreed to revise the ICRN 13, transfer it from TPWS to PCAS, and to extend for 3 years to July 2006. Contacts: T. Nemec and F. Marsik.

New Release: Ionization Constant of Water. The draft release prepared by Lvov was discussed. The release is approved with the following recommendations. (i) There should be a statement of uncertainties vs T, p and density. (ii) It was agreed that density should be added to the Table of sample values. (iii) Minor notation changes are suggested to be consistent with other IAPWS releases. (iv) An ICRN should be written to highlight the need for measurements and simulations in the low-density super-critical region.

ACTION: (Lvov): To address the recommendations and report at joint PCAS/TPWS Meeting on Thursday morning.

5. New Members: The Czech Committee proposes Tomas Nemec be appointed a member of PCAS. Motion (Lvov) to appoint Tomas Nemec: Approved unanimously.

6. Task Groups and Committees: (Deferred)

7. Approval of Agenda: The agenda was approved as written. Horacio Corti has expressed concern about the difficulties he is having in attending meetings as co-chair. The question of attendance from several counties is under review during this meeting by a special committee.

ACTION (Lvov): To communicate the results of the Executive Committee decision on this point to Horacio after Friday's meeting. If Horacio cannot continue, an e-mail election for co-chair will be held.

Monday Afternoon

8. PCC/PCAS Joint Workshop: See the PCC Minutes for details.

Tuesday Morning

9. IAPWS International Collaboration: Ondrej Mican presented a report entitled Thermodynamics of Fuel Cell Transport by Ondrej Mican, Frantisek Marsík, and Serguei Lvov This is a collaboration between the Faculty of Nuclear Sciences And Physical Engineering, CTU, Prague, CZ; the Institute of Thermomechanics, CAS, Prague, CZ; and the Energy Institute and Department of Energy and the Geo-Environmental Engineering, Pennsylvania State University, University Park, USA

The theme of the project carried out a modeling approach of membrane transport in PEM (proton-exchange membrane) fuel cells from the viewpoint of irreversible thermodynamics. A review of PEM fuel cell modeling was made with the main conclusion that almost all membrane models existing in literature belong to one of two basic classes, namely the single-phase diffusion models and the two-phase hydraulic models. Diffusion type models have been more extensively studied, in some cases using an irreversible thermodynamics approach. Based on this analysis a simple diffusion model was obtained and a relation between material properties and geometrical dimensions of the membrane was derived. As a next step of the project, this relation should be further developed so that its validity could be checked by using of experimental obtained at Penn State University and data from literature. Another object of our analysis was the degree of coupling between water diffusion flux and electric current in the membrane. As a result, an expression for "generalized efficiency" of the membrane transport in terms of the degree of coupling was obtained. Hydraulic models have not been previously studied as often as diffusion models and a fundamental thermodynamic analysis for this type of models is still missing. Similar analysis as we have performed for the diffusion model shall be also carried out for the hydraulic type of model.

ACTION (Lvov): To provide a report consisting of an executive summary, and a manuscript for publication or thesis chapter, to PCAS at or before next year's IAPWS Meeting.

10. PCAS Workshop: See the WG Agenda for list of presentations.

Tuesday Afternoon

11. All WG Meting: Workshop on Properties of Seawater

Thursday Afternoon

12. TPWS/PCAS Joint Workshop: See the TPWS Minutes for details.

Thursday Afternoon

13. Topics for 15th ICPWS (Berlin)

The Committee discussed the symposium topics used at the 14th ICPWS and proposed the following modifications of the topics (shown below in bold) for the 15th ICPWS (Berlin):

Calculation of Water and Steam Properties for Industrial Use
Thermophysical and Transport Properties in Water, Ice, and Steam
Structure and Dynamics in Aqueous Systems: Spectroscopy and Molecular Simulation
Nonequilibrium, Metastable and Critical States
Thermodynamics and Kinetics in Hydrothermal Systems
Electrochemistry, Corrosion, and Interfaces in High-Temperature Water
Fuel cells, Hydrogen Production, and Renewable Energy
Advanced Techniques and Instruments for Basic Research and Power Plant Applications in High-Temperatures/Pressure Water
Low Temperature and Super-Cooled Aqueous Systems
Supercritical Water and Aqueous Systems
Seawater and Geothermal Systems
Power Cycle Chemistry
Steam Chemistry, Condensation and Deposition Processes
High Efficiency Power Cycles and New Technologies
Environmental Issues in Power Generation
Miscellaneous

A list of the suggested organizers was briefly discussed.

ACTION (Lvov): To summarize the discussion and send to the Conference Committee a list of the session's chairmen by November 1st 2006.

14. Joint Electrochemical Society (ECS)-IAPWS Symposium (Washington, 2007)

Dr. Lvov presented the draft call for papers for the Joint ECS/ IAPWS Symposium as follows:

Topic: Interfacial Electrochemistry and Chemistry in High Temperature Media

Sponsors: Energy Technology and Corrosion Divisions of the ECS and The International Association for the Properties of Water and Steam

This symposium will focus on the latest advances and developments leading to understanding of interfacial phenomena in high temperature media, particularly the systems involving high temperature water and other solvents. The aim of the symposium is to provide deeper insight into chemical and electrochemical processes at all kinds of interfaces and to elucidate the significant effects of the interfacial processes on the properties and behavior of materials in high temperature aqueous environments. Of particular interest are the high temperature interfacial processes related to water cycles in current and next-generation fossil fuel and nuclear power plants, fuel cells and batteries, hydrogen production and storage, photovoltaics, hydrothermal/electrochemical synthesis of materials, corrosion and passivation of high-performance alloys, etc. Priority is given to areas of research connecting the interfacial chemical and electrochemical phenomena related to traditional and renewable energy generation systems and radioactive waste disposal. In particular, papers on the mechanisms of charge formation at and transfer through the interfaces, electrical

double layer structure and dynamics, electrical conduction through interfaces and heterogeneous phases, interface adsorption/desorption processes, localized corrosion processes, etc. are welcome.

Acceptance of a paper for presentation obligates the author to submit a full manuscript in camera-ready form to the new online publication, *ECS Transactions*. A hard-cover collection of the papers will also be produced. Instructions for preparing the manuscript will be sent out by the Symposium Organizers to each author upon acceptance of their abstract for oral presentation.

Abstracts should be sent electronically to the ECS headquarters office and suggestions and inquiries should be sent to the 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.

The proceedings of the symposium with have an acknowledgement to IAPWS as was requested at the 2005 IAPWS meeting in Santorini.

S. Lvov invited suggestions for organizing committee members from the nuclear community. Dave Newman (U. Toronto) and Dave Shoesmith (U. Western Ontario) were suggested. The call for papers was approved without revision with compliments to S. Lvov on this initiative.

ACTION (Lvov): To complete the initiative as proposed.

15. Data Book

Dr. Lvov presented a status report on the Data Book Initiative, Dr. V. Valyashko (editor). Chapter 2 has been delayed. Chapter 3 seems to be canceled. All other chapters are on schedule. The draft manuscript is expected to be submitted to the publisher by Dr. V. Valyashko by December.

16. Gibbs Award Committee

The WG reviewed the criteria and process for the Gibbs Award and noted that it is given at four year intervals at the ICPWS meeting.

ACTION (Tremaine): The WG elected Peter Tremaine to serve as a member of the Gibbs Award Committee.

ACTION (Lvov): To distribute a call for nominations to the members of PCAS.

17. The Meeting adjourned at 5:25 p.m.

THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

http://www.iapws.org

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

AGENDA

Witney, England, 3 – 8 September 2006

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

1. PCAS Meeting, Monday, 4 September, 10:30 - 12:15

- Opening Remarks
- Appointment of Clerk of Minutes
- Approval of Minutes of PCAS WG in Santorini, Greece, 2005
- Proposals for new IAPWS International Collaborations
- Proposals for new ICRNs, Releases etc.
- Proposals for Membership
- Task Groups and Committees
- Approval of Agenda

2. PCC/ PCAS Joint Meeting and Workshop, Monday, 4 September, 1:30 – 5:30

- Research Presentations on Physical Chemistry for Power Generation
    - … S.N. Lvov, Z. Zhou, E. Chalkova, V.N. Balashov, and P. Chou: ”Development of Hydrothermal Coating Technology to Mitigate Intergranular Stress Corrosion Cracking in BWRs”
    - … G. Bignold: “Chemical Properties Issues Arising in Recent Power Cycle Chemistry Studies”
    - … M. Stastny, O. Blahova, I. Jiricek, and B. Lorenc: “Effects of Steam Chemistry on the Turbine Blades in Transition Zone”
    - … S. Voidikovich, “Influence of Water Chemistry on the Economizer Inner Wall Condition”
    - … P. Tremaine: “Phosphate titanium interactions under boiler conditions”

3. PCAS Workshop, Tuesday, 5 September, 8:30 - 12:15

- Research Presentations on Physical Chemistry of High Temperature Aqueous Solutions
  - … O. Mičan, S. Lvov, and F. Maršík: "Transport Processes on Electrodes and in Membrane of Polymer Electrolyte Fuel Cells"
  - … M. Nakahara: "Self-Diffusion of Supercritical Water in Extremely Low-Density Region"
  - … M. Ueno: "Temperature and Pressure Effects on the Micelle Formation of Lithium Perfluorooctylsulfonate in Aqueous Solutions"
  - … P.R. Tremaine and E. Bulemela: "Standard Partial Molar Volumes of Aqueous Hydroxy Carboxylic Acids, Amines and Amino Acids at Temperatures up to 335 °C and Functional Group Additivity Effects"
  - … E. Balodis, L.N. Trevani, and P.R. Tremaine: "Isotope Effects on Standard and Partial Molar Volumes of NaCl, HCl and NaOH Measured in Light and Heavy Water at 250 and 300 °C"
  - … S. Lvov: "Thermochemical Cycles for Hydrogen Production"

4. All WG Meeting, Tuesday, 5 September, 1:30 – 5:30

- Workshop on Properties of Seawater

5. TPWS/PCAS Joint Meeting and Workshop, Thursday, 7 September, 8:30 - 12:15

- Release on the Ionization Constant of Water (S.N. Lvov) - Appointing an Evaluation Task Group
- T. Němec, F. Maršík, D. Palmer: "Binary Nucleation of Steam with Admixtures Relevant in Power Industry and Atmosphere"
- Report of the Simulation Task Group (I.M. Svishchev, K. Yasuoka)

6. PCAS Meeting, Thursday, 7 September, 1:30 – 5:00

- Information on the ECS/IAPWS Symposium, "Interfacial Electrochemistry and Chemistry in High Temperature Media", 2007, October 7-12, Washington DC, USA
- Information on the IAPWS Data Book
- Reports on Existing IAPWS International Collaborations
- Finalizing and Initiating ICRNs, Releases, etc.
- Approval of New Membership
- Nominations for the Gibbs Award
- Preparation of PCAS WG Report for Executive Meeting