MINUTES OF PCAS WORKING GROUP
SANTORINI, GREECE, JULY 3-8, 2005

Members in attendance during the week: A. Levelt-Sengers; S. N. Lvov; F. Maršik; V. Molinero (vale@WAG.CALTECH.EDU); M. Nakahara; D. A. Palmer; V. Papangelakes (papange@chem-eng.utoronto.cn); M. Ueno; V. Valyashko

Monday morning meeting: July 4.
Opening remarks were given by the working group chairman, S.L., including the introduction of two guests (V.M. and V.P). It was decided to postpone the invitation to join PCAS until Thursday when they have had time to access their interest in joining the PCAS. The proposed agenda was accepted unanimously (PCAS Attachment A). D.P. accepted the suggestion of S.L. to keep the minutes of the PCAS meeting. Acceptance of the minutes of the PCAS working group from the 2004 ICPWS meeting in Kyoto, Japan was proposed by S.L. and seconded by D.P.

One international collaboration proposal has been submitted by F.M. and S.L. for a PhD student, Ondřej Mičon) from the Czech Republic to spend five months at Penn State University in the spring of 2006 (est. cost $9,000US with some supplemental funding from the student's home institute in Prague). No other proposals were immediately forthcoming.

S.L. informed the working group that the ICRN cosponsored by S.L. and D.P. requires action, namely, renewal, revision or termination.

F.M. informed the group that Jan Hruby (Czech Republic) wishes to transfer from PCAS to TPWS.

V.P. raised the question of funding resources and current financial balance of IAPWS. He was told that Barry Dooley also serves as Treasurer of IAPWS and will present a detailed financial report at the EC on Friday, but this information is also available on the IAPWS Web site. It was also stated that the principal outlays of funds are for international collaborations and for organization of the ICPWS meetings.

S.L. introduced the topic of Task Groups and Committees, in particular the two task groups lead by him. He proposed that these two task groups ("Electrochemical Processes in High-Temperature Aqueous Systems" and "Fuel Cell and H_2 Technologies") be combined into a single task group with more general, less restrictive, title. It was agreed that the present members of both groups meet over lunch to discuss this changes and to develop a strategy for the future of this initiative. In particular, S.L. requested that these members and the PCAS membership as a whole, consider organizing a special symposium on the general topic either as a stand alone symposium or in conjunction with a major international meeting (e.g., IUPAC, Electrochemical Society, or an ACS annual meeting). This would serve to advertise the activities of IAPWS to a wider audience and should also attract a wider audience to the symposium than would normally attend a typical IAPWS annual meeting. S.L. emphasized that our niche should be the application of high temperatures to avoid overlap with the large number of research groups already involved in investigations of fuel cells at near ambient conditions.

The morning session was concluded.

Lunchtime meeting of the members of the task group mentioned above, July 4.
Participants: S. Lvov, F. Masik, E. Maughan, V. Molinero, M. Nakahara, D. Palmer, V. Papangelakis, M. Ueno.

1. V.M. asked what the final product of the task group would be. S.L. replied that it could be an ICRN, an international collaboration or it could lead to a publication, or a combination of these.
2. S.L. invited V.M. to become a member of the new task group due to her activities in the field of fuel cell development. Membership in a task group does not depend on membership in IAPWS. V.M. accepted the invitation.
3. S.L. proposed naming the new combined task group, "Interfacial Electrochemical Phenomena in High-Temperature Solutions". It was immediately agreed to replace "Solutions" with "Fluids".

M.N. proposed to make the title more general and to use this name also for that of the proposed international symposium, "Interfacial Chemistry and Electrochemical Phenomena in High-Temperature Fluids". This title was later put to a vote and was accepted unanimously. The definition of "High Temperature" was given as > 100^{o}C. D.P. proposed that this general title would also allow us to consider developments in ultra super critical fossil fuel power generation technology and that ORNL had prepared a white paper for EPRI on chemistry research needs to conditions of 760^{o}C and 40 MPa.

4. M.N. described the large effort in Japan on the development of fuel cells both at the governmental and industrial levels. S.L. agreed that we therefore need the niche of "high temperature" to give this task group a more unique flavor and possibly position us in a favorable position as research on fuel cells in particular may well move to the higher temperature regimes to gain in efficiency.
5. E.M. mentioned a significant effort started 15 years or more ago in ESKOM, South Africa, on fuel cells, although he was not sure whether this research included high temperature work. He kindly offered to seek out the person responsible for this effort within ESKOM and find out what research had been covered and report his findings to S.L. This offer was gratefully accepted.
6. S.L. suggested inviting experts of fuel cells and water/steam cycle chemistry, including those from the nuclear industry, to attend to proposed international symposium. V.P. responded by asking "Who are we helping by doing so?" S.L. gave the example that we would be helping manufacturers of fuel cells, for example. V.M. warned that competing interests of manufacturers often compromises such group effort as they tend to approach the key people in such a task group to make individual private research contracts with them. This point was generally acknowledged. D.P. agreed that we would like to invite participation from say the nuclear industry, for example known contacts as EPRI, but this should be done discreetly with input from PCC. N.M. asked how do we make contact with small fuel cell manufacturers who may be ultimately be more interested, and perhaps more important than large power generation companies, in the development of fuel cells? He also pointed out the computational contributions to the future of fuel cell development; he currently collaborates with Canadian scientists on electron transport issues, far example. V.P. asked, do we know what are the two or three key issues that the industry needs to have solved; this is a key point is giving industry a tangible goal or product? S.L. replied that he does and is currently working with DuPont on fulfilling these needs. V.M. also responded that she has a similar list of key areas.
7. V.P. asked if there was problem suggesting working with solvents other than water within IAPWS? S.L. replied that this is not a problem and that there are precedents for this.

We returned to the matter of the international symposium. S.L. asked again about whether to combine the special symposium with an IUPAC, etc. meeting. E.M. strongly suggested combining with an international meeting rather than a national one to attract the broadest possible participation. This suggestion was immediately accepted. D.P. asked whether we should combine this symposium with an annual IAPWS meeting so as to attract more participation to IAPWS in general and also to not risk antagonizing the host country for the annual meeting. However, S.L. preferred to link this symposium with a major meeting at attract other than the usual IAPWS members. V.M. agreed. E.M. also cited that annual DEKAMA meeting as being a huge conference that attracted a very large industrial participation. S.L. will first contact experts from the nuclear division of EPRI and other similar organizations to see if they would attend an Electrochemistry Society meeting, for instance, which would surely be more attractive to industry folks than an IUPAC conference. S.L. has organized a special symposium with the former in the past and this society provided financial support directly. S.L. asked for volunteers to help organize such a symposium. Apart from himself the following indicated that they would be willing to do so: E.M., F.M., D.P., M.N. Absent members were also suggested, namely, Peter Tremaine and Horacio Corti. It was decided to suggest 2007 as the year for this planned symposium. S.L. has already composed a list of subtitles for this symposium. These ideas will be presented to the PCAS working group on Thursday and the presented to the EC on Friday. The meeting was then adjourned.

Monday afternoon joint meeting with PCC: July 4.

Four talks were given during this session and the titles are available in the amended PCAS agenda.

Tuesday morning meeting: July 5.
S.L. presented the revised PCAS agenda and this agenda was approved unanimously. A number of scientific presentations were then given by PCAS members.

1. M.N. "Self Diffusion of Light and Heavy Water"
2. V.P. "Chemical Modeling of Concentrated Process Solutions as High Temperatures. An Engineering Approach"
3. M.U. "Electrical Conductance of Tetraalkylammonium Bromides in Methanol and Water along the Liquid – Water Coexistence Curve"
4. S.L. "Synthesis, Structure and Surface Chemistry of New Inorganic-Organic Composite Materials for High-Temperature Proton Exchange Membrane Fuel Cells (PEMFC)"

V.V. detailed progress made with the IAPWS Databook which he initiated and for which he provided the necessary references and abstracts thereof. There are seven chapters proposed for this book at the present time and the general topics are listed below with the names of the contributing authors.

Chapter 1. Phase equilibria.	V.V.
Chapter 2. pVTX.	H.C. and V. Mayer
Chapter 3. Calorimetry.	V.M., K. Ballerat and C. Wormald
Chapter 4. Potentiometry.	D.P. and S.L.
Chapter 5. Electrical conductivity data	H.C.
Chapter 6. Thermal conductivity data	I. Abdulagatov and M. Assael
Chapter 7. Viscosity	I. Abdulagatov and M. Assael

Drafts of chapters 1, 4, 5 and 7 have been submitted by the deadline agreed upon last year at the ICPWS in Kyoto, namely by the beginning of this week. Therefore, three chapters have not met the deadline which has already been postponed on several occasions. The following action items and schedule was compiled during the morning's session and in a follow-on lunchtime meetings between V.V., M.A. and D.P.

1. The project is proceeding with some mixed results, but the feeling is that with mutual collaborations we will meet the ultimate deadline of December 10, 2005, for submission by V.V. of the final drafts of all the chapters to John Wiley.
2. H. Corti and I. Abduladatov have informed V.V. that they will complete the first draft of chapters 2 and 6 during September. So the 1st of October should be the deadline for submission of these chapters. V.M. has communicated to V.V. that he must wait until October for C.W. to send him the database and the associated papers that he used to his part of the text of chapter 3. However, these authors are requested to send V.V. any sections of the text or tables or appendices as they are completed. V.V. is requested to communicate as soon as possible the exact final date of this chapter so as not to jeopardize the project.
3. Authors of each chapter are requested to provide the name of a reviewer for their chapter who will be recommended to John Wiley as potential expert reviewers.
4. V.V. will review each draft and communicate his suggestions to the authors before the December 10 deadline. Hence the sooner you can provide him with your drafts the more carefully V.V. can edit your contribution.
5. V.V. will compose a rough Preface for his book in the meantime and send a copy to each author for this approval. D.P. has agreed to edit the wording of the final draft of the Preface.
6. A.L.-S. and D.P. agreed to edit the English grammar of all the final proofs obtained from John Wiley and to submit their recommendations to V.V.

Thursday morning meeting: July 7.
The revised agenda for this final session was presented by S.L. and accepted by the members present. F.M. first presented an oral interim report on the status of the Task Group which he entitled: ""Metastability, Nucleation, Early Condensate, Droplet Spray and Cavitation". He listed the following names initially as being members of this effort: F. Masik, T. Nemic, P. Zima, M. Műller, I. Zuniga, and J. Hruby. He later noted that Jim Bellows and D.P. are also members of the task group. Jan Hubry delivered the section of this presentation highlighting his work on the surface tension of aqueous solutions and the application of atomization, spray and aerosols, which falls under the part of the project title, "Droplet Spray". S.L. asked for action items for his report to the EC and for future plans of this task group. F.M. commented that the

most recent work in this area by the Czech group is summarized in chapter 7 of the IAPWS Hydrothermal book published in June 2004. T. Menic will submit his PhD thesis later this year and will cover the latest results on nucleation. His thesis will include a computer code which predicts nucleation rates for a number of binary systems (e.g., water- ammonia, sodium chloride, sodium hydroxide, and sulfuric acid). He explained that the interest of the Czech utility company has waned and that they are now focusing more on the environmental impact of industrial emissions on atmospheric chemistry and physics, and that this topic could lead to the preparation of an IAPWS Release in the future. M.N. urged F.M. in the future to more precisely define the scope and goals of this task group so that members could better assess the performance of the group. D.P. suggested that the progress report should be presented at the joint PCAS/TPWS meeting in 2006 because of the expected interest by TPWS in this work. Finally, F.M. presented S.L. with a summary document containing five points defining the activity of the task group for inclusion as an attachment to the minutes.

DP gave a brief outline of the origin and goals of the task group on pH measurements. He explained that little progress had been made in the lat 12 months due to his commitment to the IAPWS Databook. However, a large list of interested participants had been collected. V.P. was very enthusiastic about the importance of this topic even suggesting that the product should be an extensive review article or even a book that could replace the classical text of Roger Bates. S.L. commented that the subject areas should include discussion of: (1) buffers and tables of their thermodynamic dissociation constants; (2) diffusion potential which is common to all but Harned cells which are not suitable for very high temperature measurements anyway. Other contributing potentials should also be discussed. He added that the significance of pH at extreme conditions is restricted by our ability to carry out the measurements where very high impedance meters will be needed, even Wheatstone bridges if the current must be zero to obtain a significant result. He later commented that pH making potential measurements at extreme conditions was only the first step and the pH must then be calculated from complicated equations. V.M. asked about the application of spectroscopic techniques to replace electrochemical methods and was informed about the work in this area by Keith Johnston (Univ. Texas, USA) and more recently by Peter Tremaine (Guelph Univ., Canada). V.P. stated that pH measurements in highly concentrated brines are extremely difficult and that he would like to be included in this task group (his application was immediately accepted). He further mentioned the need for robust rather than highly rigorous pH probes in the hydrothermal processing industry and was informed of a working group that was being created within PCC and that S.L. could serve as a conduit between the two groups. M.N. commented that his new NMR apparatus gave sensitive measurements of the proton shift and could therefore perhaps give a fresh approach to pH measurements at high temperature. He mentioned the names of three Japanese colleagues who have published theoretical papers in this area with about the last five years, namely; Professor F. Hirata (Inst. Of Molecular Sciences, Okazaki); Professor I. Ohmine (Nagoya Univ.) and Professor Takahaski (Osaka Univ.). He offered to contact them on behalf of the task group to see if they might be interested in contributing and perhaps joining the group. This was included in the Action Items for this task to be completed by the 2006 annual meeting. The final action item was accepted by D.P. who will contact task group members again at the end of the year when work on the Databook was complete, including researchers at Sendai in Japan who are active in this field but have not responded to his initial e-mails. He will formulate an outline of the project and circulate it amongst the task group members. He was reminded by S.L. that the ICRN on this subject will expire in August and it was agreed that S.L. would send him with a copy to be edited for an extension and returned to S.L. before the end of July.

S.L. reviewed the discussions of his proposal for an International symposium on Interfacial Electrochemistry and Chemistry, and showed a draft of a report he had prepared to submission to the EC. By way of follow up on Monday's discussion, he determined that the annual meeting of the Electrochemical Society will be held in Washington DC, October 7-12, 2007 and that we could consider this as a favorable vehicle for the symposium, which could simply be a one-day affair on Sunday October 7, or a multi-day symposium if the response warranted. The latter appeared more likely and desirable. He pointed out that this symposium for raise awareness of the activities of IAPWS in the electrochemical community. V.P. commented that this was significant but the ultimate reason for organizing such a symposium was scientific in nature and that we should stress that we would bring together an international audience of the many scientists already working in this area to establish the state-of-the-art of interfacial science. S.L. proposed requesting $5,000US to be spent on attracting 4 or 6 invited speakers to the

meeting. There were other suggestions relating to the rewording and formatting of the draft report. Finally DP requested that S.L. invite David Wesolowski (ORNL, USA) to join the organizing committer and he agreed without reservation.

D.P. requested S.L. as chairman of the PCAS to officially enquire of the EC whether a young scientist from a non-IAPWS member country could be considered for the international collaboration program if he or she were sponsored by two member country delegations. V.M. suggested that the list of members of IAPWS be included on the Web site with adequate protection of their e-mail addresses. Both V.M. and V.P. strongly endorsed making further approaches to younger scientists and engineers to join IAPWS. V.P. suggested raising the registration fee for each meeting to procure funds to support participation by younger people, although he was reminded that costs are now quite high and have prevented some regular members from attending.

F.M. then gave a detailed overview of the international collaboration proposal between his group and that of S.L. presented briefly and accepted by PCAS on Monday.

V.M and V.P. were asked if they would like to become members of IAPWS and both agreed and their names will be submitted to the EC on Friday.

The PCAS working group meeting was concluded at 13:15.

Agenda of PCAS Working Group
Santorini, Greece, July 3 – 8, 2005

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 WG Meeting, Monday, July 4, 10:00 - 12:00 (10:45 – 11:15 coffee break)

- Opening Remarks
- Appointment of Clerk of Minutes
- Approval of Minutes of PCAS WG in Kyoto, 2004
- Proposals for IAPWS International Collaborations
- Proposals for ICRNs
- Proposals for Membership
- Task Groups and Committees
- Approval of Agenda

2. Joint Meeting/Business Lunch of Two PCAS WG Task Groups (Electrochemical Processes in High-Temperature Aqueous Systems & Fuel Cell and H_2 Technologies), Monday, July 4, 12:00 - 1:15

Members of Task Groups: H. Corti, S. Lvov, F. Marsik, E. Maughan, M. Nakahara, D. Palmer, T. Petrova, and S. Uchida

3. Joint Workshop - PCAS/PCC WGs, Monday, July 4, 2:30 - 5:30 (4:00 – 4:30 coffee break)

- Research Presentations on Physical Chemistry for Power Generation

a). D. Palmer - The Solubility of Zinc Oxide with Reference to Mitigation of Cobalt-60 Deposition and SCC in the Primary Circuit of PWRs
b.) S. Lvov - Hydrothermal Deposition of Zirconia Coatings on BWR Materials for IGSCC Protection
c.) M. Stastny - The Effects of Steam Chemistry on Condensation Process
d.) R. Svoboda – Copper Solubility Related Presentation

4. Workshop - PCAS WG, Tuesday, July 5, 8:30 - 13:15 (10:45 – 11:15 coffee break)

- Research Presentations on Physical Chemistry of High Temperature Aqueous Solutions

a). M. Nakahara - Self-diffusion Coefficients for Light and Heavy Water under Sub- and Supercritical Conditions
b). V. Papangelakis - Chemical Modeling of Concentrated Process Solutions at High Temperatures - An Engineering Approach
c.) M. Ueno - Electric Conductivities of Tetraalkylammonium Bromide in Liquid Methanol and Water along the Liquid-Vapor Coexistence Curve

d.) S. Lvov - Synthesis, Structure, and Surface Chemistry of New Inorganic-Organic Composite Materials for High-Temperature Proton Exchange Membrane Fuel Cells

- IAPWS Databook Project

V. Valyashko - IAPWS Project - Hydrothermal Experimental Data - Phase Equilibria and Solution Properties in Binary and Ternary Systems

5. Joint Workshop – TPWS/PCAS WGs, Tuesday, July 5, 2:30 – 5:30 (4:00 – 4:30 coffee break)

- Research Presentations on Physical Chemistry of Water and Steam

a.) K. Yasuoka - Report from the Simulation Task Group
b.) K. Yasuoka - Simulation of Bubble Nucleation of Water
c.) K. Okita - Report from the Task Group on Environmental Issues
d.) G. Ghosh - Physically Based Model for the Refractive Index of Water
e.) A. Harvey, A. Levelt Sengers – Dielectric Constant
f). S. Lvov - The Ionization Constant of Water: New Formulation
g). M. Nakahara – Proposal for a Release/Guideline on Self-diffusion Coefficients for Light and Heavy Water

6. PCAS WG Meeting, Thursday, July 7, 8:30 - 13:15 (10:45 – 11:15 coffee break)

- Presentations on Projects, Task Groups, and Committees

a.) F. Marsik - Metastability, Nucleation, Early condensate, Droplet Sprays and Cavitation
b). V. Majer - Standard-State Thermodynamic Properties of Nonelectrolytes
c). D. Palmer - pH of High-Temperature Aqueous Solutions
d). S. Lvov - Electrochemical Processes in High-Temperature Aqueous Systems
e). S. Lvov - Fuel Cell and H_2 Technologies

7. PCAS WG Meeting, Thursday, July 7, 2:30 – 5:30 (4:00 – 4:30 coffee break)

- Proposals for IAPWS International Collaborations (continuation)
- Reports on Existing IAPWS International Collaborations
- Finalizing and Initiating ICRNs
- Approval of New Membership
- Preparation of PCAS WG Report for Executive Meeting
- Preparation of PCAS WG Minutes
- Databook Project (contin.)

Task Group Report
"Electrochemical Processes in High-Temperature Aqueous Systems"
Santorini, Greece, July 3 – 8, 2005

Members: S. Lvov (Chair), E. Maughan, M. Nakahara, D. Palmer, T. Petrova, and S. Uchida

Past year activities:

(1) Participation in organizing the 2005 Annual IAPWS Seminar (S. Lvov)

(2) Preparation of presentations for the 2005 Annual IAPWS Seminar (E. Maughan, D. Palmer, S. Uchida, and S. Lvov)

(3) Preparation of presentations for the 2005 Annual PCAS WG Meetings (M. Nakahara, D. Palmer, and S. Lvov)

(4) Discussion on combining the currently existing "Electrochemical Processes in High-Temperature Aqueous Systems" and "Fuel Cells and H2 Technologies" task groups to form a new task group on "Interfacial Electrochemistry in High-Temperature Fluids" (all members)

(5) Discussion on organizing an international symposium on "Interfacial Chemistry and Electrochemistry in High-Temperature Fluids" (all members)

Attachment 8

Task Group Report
"Fuel Cell and H2 Technologies"
Santorini, Greece, July 3 – 8, 2005

Members: H. Corti, S. Lvov (Chair), M. Nakahara, and F. Marsik

Past year activities:

(6) Preparation of an international collaboration proposal on "Irreversible Thermodynamics of Fuel Cells Membrane Transport" (F. Maršík and S. Lvov)
(7) Discussion on combining the currently existing "Electrochemical Processes in High-Temperature Aqueous Systems" and "Fuel Cells and H2 Technologies" task groups to form a new task group on "Interfacial Chemistry and Electrochemistry in High-Temperature Fluids" (all members)
(8) Discussion on organizing an international symposium on "Interfacial Chemistry and Electrochemistry in High-Temperature Fluids" (all members)

PCAS WG Proposal to EC

Organization of an International Symposium on "Interfacial Chemistry and Electrochemistry in High-Temperature Fluids"

Motivation:

The PCAS WG proposes to significantly stimulate research activities of IAPWS members (mainly from PCAS and PCC) in a number of crucial IAPWS areas of interests (related to the interfacial electrochemistry in high temperature aqueous fluids) such as:

1. Electrochemical corrosion
2. Electrochemical processes in fuel cells
3. Electrical conductance in composite materials
4. Water electrolysis
5. Electrochemical kinetics of oxidation of fuels and reduction of oxygen
6. Interfacial properties of proton conducting membranes
7. Electrochemical/chemical production of hydrogen using hydrothermal cycles
8. Electrokinetics
9. etc.

Goal:

Thus far, a significant number of studies has been carried out, by IAPWS members and others in the area of "Interfacial Chemistry and Electrochemistry in High-Temperature Fluids" systems. However, there is still a significant deficit in fundamental understanding the processes which occur in these systems. Moreover, the interfacial chemical and electrochemical processes are very important for a verity of IAPWS applications such as:

1. Water cycles of fossil fuel, nuclear, and geothermal power plants
2. High temperature proton exchange and solid oxide fuel cells
3. Hydrogen production using electrochemical cycles
4. Hydrothermal/electrochemical synthesis and extraction of materials
5. Supercritical water oxidation
6. etc.

The proposed symposium will attract additional attention of the entire scientific community, funding agencies, and industrial companies and, therefore, activate new research projects in the above-mentioned research areas. As a result, these research projects will significantly stimulate further development in the IAPWS applications listed above.

Times and Places:

It is proposed to organize the symposium based on the framework of the Electrochemical Society (ECS), an international organization, using one of the upcoming ECS meetings. For example, the following ECS meetings could be the most suitable for organizing the symposium:

1. October 29-November 3, 2006, Cancun, Mexico 210th ECS Meeting
2. October 7-12, 2007, Washington DC, 212th ECS Meeting

Organizer:

The IAPWS Task Group on "Interfacial Chemistry and Electrochemistry in High-Temperature Fluids" (S. Lvov – chairman) will organize the symposium.

Requested from IAPWS Funding:

It is estimated that around $5,000 will be needed to partially support four to six key speakers who will be invited to participate in the symposium.