

**THE INTERNATIONAL ASSOCIATION
FOR THE PROPERTIES OF
WATER AND STEAM**

MEMBERS

Argentina and Brazil
Britain and Ireland
Canada
Czech Republic
Denmark
France
Germany
Greece
Italy
Japan
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**Minutes of the Meetings
of the
Executive Committee
of the
International Association for the Properties of
Water and Steam**

**Santorini, Greece
3 – 8 July 2005**

Prepared by: Barry Dooley



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Minutes of the Meetings
of the
Executive Committee
of the
International Association for the Properties of Water and Steam
held in
Santorini, Greece
3-8 July 2005

Plenary Session. Monday, 4 July 2005. 9:00am

The President of IAPWS, Dr. Frantisek Marsik, welcomed the Executive Committee (EC) and other IAPWS members to Santorini for the EC and Working Group (WG) Meetings of IAPWS. The President officially opened the 2005 EC Meetings by introducing the National Delegates. He made special mention that Greece had become a full member of IAPWS on 1 January 2005. Each of the member countries of IAPWS was in attendance with the exception of Argentina/Brazil, Italy and Russia. There were 46 people in attendance.

The President asked the head of the Greece National Committee to provide some comments. Assael welcomed everybody and introduced the other members of the National Committee.

1. Adoption of Agenda

A provisional agenda had been posted on the IAPWS Website for all IAPWS members by the Executive Secretary in January 2005. The President indicated that there had been a rearrangement of the agenda and asked for any other items. There were no suggestions from the EC. The agenda was then approved by the Heads of all National Delegations and forms Attachment 1 of these minutes.

2. IAPWS Business and Appointment of Committees

2.1 Press Release.

The President asked Bellows and Assael to serve on this Committee. The Press Release is discussed in Minute 16.2 and Attachment 12.

2.2 Evaluation Committee on International Collaboration.

The President indicated that only one proposal had been received by the Executive Secretary prior to the meeting. The President reminded the EC that the Committee to review any proposals received by the end of the day

would consist of the WG Chairmen, with the President and Executive Secretary as ex. officio members. A chairman would be chosen if any suggestions are received. The discussion of this Committee is reported in Minute 14.1 and Attachment 11.

2.3 IAPWS Awards Committees

2.3.1 Helmholtz Award Committee

The President indicated that there was an Helmholtz Awardee this year and that the Award would be presented at the Symposium. He then reminded the EC that the Helmholtz Committee for the 2006 award would consist of a member from Canada, Czech Republic, Denmark, France, and Germany. The President asked the Canada delegate (Svishchev) to organize the committee and to report back to the EC on Friday with the names of the members of this committee (Minute 15.1). The procedures to be followed are delineated in the 1999 EC Canada Minutes.

The President indicated that the US National Committee had raised a concern about the lack of candidates for the Helmholtz Award. He requested the US Delegate (Friend) to make a few comments. Friend emphasized that this Helmholtz award is very important to the future of IAPWS and encouraged National Committees and Working Groups to nominate young persons for the award.

2.3.2 Honorary Fellow Award Committee

The President requested that Fernandez-Prini remain as the Chairman of this committee for 2006. Daucik was also requested to remain as the other member. The IAPWS President would be ex. Officio.

2.4 Host Country for 15th ICPWS

The President reminded the EC that in Japan (Kyoto Minute 2) there was a request to the BIAPWS National Committee to host the 15th ICPWS. The BIAPWS National Committee had informed the Executive Secretary by December 2004 that they would be unable to host the ICPWS in 2008. The Executive Secretary then requested the German National Committee to explore whether they would be able to host the Conference. The President then requested the German Delegate to provide an update. Rukes indicated that the German National Committee would organize the 15th ICPWS in Berlin in 2008. More information would be provided at the EC Meetings in the UK in 2006.

2.5 Other Business Considered to Require Special/Extensive Discussions

There were no other items suggested by the EC

3. EC Mandate to Working Groups and Membership

3.1 IAPWS Restructuring

The President provided a possible view of a future for IAPWS in the biological life sciences. He then reminded the EC of the important restructuring activities during the previous two IAPWS meetings, and indicated that IAPWS EC wanted to ensure that the WGs acted upon the suggested approaches from the four Committees and five Task Groups. He requested the WG Chairmen to provide any contrary indications in their WG presentations at the Friday EC meeting (Minute 16.1).

3.2 Releases, Guidelines and Certified Research Needs.

The President asked the Executive Secretary to review the status of various Releases, Guidelines and ICRNs that would need action by the WGs and the EC during the week. The Executive Secretary indicated that one Supplementary Release had been forwarded to the Heads of National Committees in April (Supplementary Release on Backwards Equations for Specific Volume as a Function of Pressure and Temperature $v(p,T)$ for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam). No comments had been received prior to the meeting so the TPWS WG needed to provide a final review prior to presenting it to the EC on Friday for approval. Cooper (UK) indicated that the approval of this Supplementary Release would require an updating of the Advisory Note.

The Executive Secretary then noted that ICRNs 10, 13, 14 and 15 would need action by the respective WGs during the week.

3.3 Working Group Directions.

The President reminded the WG Chairmen that they should only report to the EC on Friday, those activities that needed approval or discussion by the EC.

4. Preview by WG Chairmen of Weeks Activities

President Marsik requested each WG Chairman to review briefly the main topics which would be covered in their WGs during the week. The details of these WG meetings are covered in detail in Minutes 7, 8, 9 and 10.

Activities During the Week

The first day activities of the WGs and Executive Committee were followed by WG meetings on Monday, Tuesday and Thursday. The Symposium entitled “Applied Water Treatment Processes for Power Plant Cycles” was conducted on Wednesday. The program is shown in Attachment 2.

The full IAPWS program for the week is shown in Attachment 3.

Executive Committee Meeting. Friday, 8 July 2005

President Marsik opened the continuation of the EC Meeting at 8:45am. All members of IAPWS were present except Argentina/Brazil, France, Russia and Italy. He first asked the EC if there were any additional items that should be added to the Agenda. None were suggested.

5. Acceptance of Minutes of Previous Meeting

President Marsik asked for comments and changes to the minutes of the EC meeting held in Kyoto, Japan in August 2004. No changes were noted, thus the 2004 Minutes were accepted.

6. President’s Report

President Marsik provided the following comments. He first reiterated that in January 2005 Greece became a full member of IAPWS. On behalf of IAPWS he wanted to officially thank the Greece National Committee for organizing the 2005 EC and WG Meetings, and the Symposium. It had been an excellent week on Santorini Island. The French National Committee had also undergone some changes and had a new head: Dr. Jean-Marc Dorey. The President next reviewed the current officers of the WGs because there were some changes for the 2005 Meetings. He particularly wanted to mention that most of the restructuring activities of the past two years were now being incorporated into the WGs.

7. Report and Recommendations of Thermophysical Properties of Water and Steam Working Group (TPWS)

Chairman Friend highlighted only those activities from the TPWS working sessions during the week, which needed action by the EC. He indicated that most of the WG activities had been conducted with IRS. Full minutes can be found in Attachment 4.

- 7.1 Friend indicated that he would be stepping down as Chairman of TPWS and that the WG proposes to the EC that the new officers would be Kretzschmar, Chair and Harvey, Vice-Chair, effective from 11 July 2005.

The EC approved these new officers unanimously.

- 7.2 The WG proposed the development of an Advisory Note on Calculating Thermodynamic Derivatives from IAPWS Formulations for formal approval in 2006.
- 7.3 The WG established a Task Group on Properties of Sea Water (Feistel, Wagner, Harvey, Hiegemann), and that this would be a cooperative effort with the International Association for Physical Science of the Oceans (IAPSO). Friend also indicated to the President that this would be an activity within Life Sciences as requested in Minute 3.1.
- 7.4 The Guideline on Fundamental Constants had been revised with minor updates.
- 7.5 The document on obsolete documents has been posted on the IAPWS web site.
- 7.6 The WG was proceeding with the density WG of CCM (Consultative Committee for Mass and Related Quantities) to prepare documents clarifying the roles of IAPWS and CCM density standards for possible EC action in 2006.
- 7.7 The WG approved the Revised Release on D₂O Thermodynamics, which had been changed to account for ITS-90. The WG recommends approval by EC, subject to editorial revisions. Svishchev has been added to the D₂O Task Group.

The EC approved this Revised Release unanimously.

- 7.8 The TPWS and IRS WGs discussed property-related priorities in conjunction with the Environmental TG. Further details will be reported in 2006.

- 7.9 The TPWS and IRS WGs recommend that ICRN Number 14 on Humid Air be extended for 3 years to September 2008. Chairman Friend also indicated that the joint project with the European Union is continuing.

The EC approved the revised date of ICRN 14 unanimously.

- 7.10 The Transport Properties Task Group proposed a Release on viscosity. The Evaluation Task Group consists of Mares (chair), Konas, Alexandrov, Cooper, and Ueno. The intention is to present the release to the EC for adoption in 2006. Mares was added to the Transport Properties Task Group for work on thermal conductivity.
- 7.11 The WG proposes a Release on thermodynamic properties of ice. The Evaluation Task Group will be Hruby (chair) and Harvey. The intention is to present this to the EC for adoption in 2006. Chairman Friend indicated that this is a new area for IAPWS.
- 7.12 Membership. The WG proposes the following new members Feistel (Germany) and Hruby (Czech Republic). The latter is moving from the PCAS WG.

The EC approved these WG membership changes unanimously.

At the end of the WG presentation, the German delegate (Rukes) asked the EC to thank Friend for his leadership of the TPWS WG over the last five years.

8. Report and Recommendations of Industrial Requirements and Solutions Working Group (IRS)

Chairman Parry provided the IRS Report to the EC. Full minutes can be found in Attachment 5. The Chairman indicated that many of the technical items had been covered by Friend in the TPWS report. He then presented the items that needed action by the EC.

- 8.1 The TPWS and IRS WGs unanimously voted to recommend adoption of the Supplementary Release on Backwards Equations for Specific Volume as a Function of Pressure and Temperature $v(p,T)$ for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam.

The EC approved this Supplementary Release unanimously.

Chairman Parry then indicated that following the procedure of previous publications the two working groups recommend to the EC to provide up to US\$2,000 for the page charges of a detailed background paper.

The EC approved this expense unanimously.

- 8.2 With regards to the amendment of the “Revised Supplementary Release on Backward Equations for the Functions $T(p,h)$, $v(p,h)$ and $T(p,s)$ for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam”, the working groups recommend to the EC to authorize the editorial committee to make the necessary changes without further formal acceptance by the EC. Parry indicated that a corrected document will be available for the next EC meeting.

The EC approved this revision unanimously.

- 8.3 Computing time investigations of IAPWS-IF97 Equations. Chairman Parry indicated that Miyagawa has agreed to start the preparation of a paper which will document the significant achievements including all now available backward equations and present it at a suitable occasion.
- 8.4 Advisory Note #2 needs to be updated since the additional supplementary release has been approved. The EC was further requested to authorize the Editorial Committee to revise the Advisory Note as needed in the future without further formal acceptance by the EC.

The EC approved this process unanimously.

- 8.5 For new Industrial Requirements of the Future a new Task Group on “Future Cycles” has been formed with the following people: Parry (chair), Okita, Gachon and Hiegemann (potential). This group will identify new ICRNs
- 8.6 ICRN 15 on Thermodynamic Properties of Metastable Steam. The WG recommends to the EC that this ICRN be extended to September 2008.

The EC approved this extension unanimously.

- 8.7 Membership. The WG recommends that the following people are added to the membership roster: Hiegemann (Alstom Power, Switzerland) and Gachon (EdF, France)

The EC approved these IRS membership changes unanimously.

9. Report and Recommendations of Physical Chemistry of Aqueous Solutions Working Group (PCAS)

Chairman Lvov provided the PCAS Report to the EC. Full minutes can be found in Attachment 6. He covered the following items with the EC:

- 9.1 All existing task groups which affiliated with PCAS WG will continue to function except two - “Electrochemical Processes in High Temperature Aqueous Systems” and “Fuel Cells and H₂ Technologies”. These task groups will be combined into a new one entitled “Interfacial Chemistry and Electrochemistry in High Temperature Fluids”. Lvov will be the Task Group chairman. The two closing task group reports approved at the PCAS WG meetings are provided as Attachments 7 and 8.
- 9.2 As a result of the consolidation mentioned in 9.1 and in an effort to expose this area much more broadly, the WG proposes to organizing an International Symposium entitled “Interfacial Chemistry and Electrochemistry in High Temperature Fluids” (Attachment 9). Chairman Lvov indicated that the WG estimated that around \$5,000 will be needed in 2006 or 2007 to partially support four to six key speakers who will be invited to participate in the symposium. This lead to some discussion by the EC about expenses, the number of participants and whether the Electrochemistry Society would be interested in hosting a joint symposium. Finally the following proposal was put to the EC: “The EC supports the concept of providing up to \$5,000 to support this symposium with the caveat that there must be clear attribution to IAPWS”

The EC approved this proposal unanimously.

- 9.3 Two new members for the PCAS WG were proposed: Molinero (California Institute of Technology) and Papangelakis (University of Toronto). It was also proposed to remove Hruby who has transferred to TPWS. The Chairman also reminded the EC that Franck was deceased.

The EC approved these membership changes unanimously.

- 9.4 The WG decided to continue ICRN 10 on “pH Measurements in High-Temperature Solutions”. A revised copy of the ICRN will be provided to the Executive Secretary by D. Palmer in August 2005.
- 9.5 A draft of an IAPWS Release entitled “The Ionization Constant of Water” will be prepared by Lvov and presented at the 2006 IAPWS meeting. Palmer will review the first draft and report to PCAS WG at the 2006 IAPWS meeting.

10. Report and Recommendations of Plant Cycle Chemistry Working Group (PCC)

Vice Chairman Svoboda highlighted those activities that needed action/approval by the EC. A full written report of the PCC WG activities forms Attachment 10.

10.1 Priority List

The WG revised the Priority List, which provides the research needs as formulated by the PCC. This list will also be of interest to the other IAPWS working groups. PCC will develop future activities (International Collaborations, ICRNs, task forces and presentations) from this Priority List. Currently, this list contains 12 items, including 2 of interest for fossil plant chemistry, 1 for nuclear plant chemistry, and 9 of common interest for both fossil and nuclear chemistry. The list will be discussed and revised at each annual meeting. The revision, discussions and Task Groups will be a major topic of the annual PCC meeting maybe taking up to 40% of the WG time. The revised Priority List is attached to the PCC minutes (PCC Attachment B).

10.2 International Collaboration:

Last year PCC initiated an International Collaboration between Japan and Canada on Flow-Accelerated Corrosion. The project was finished within budget and time schedule, and a full report was given at the PCC WG meeting. The quality of work and of the report was positively appraised by the PCC. This also goes for the organization of this collaboration project.

This year, PCC does not have a collaboration project ready, but at least one will be prepared for approval by the EC in 2006. One will be on Sampling and Analysis Techniques for Low Levels of Iron (and other metals) in Water. The collaboration will have more than 2 hosting partners and possibly include partners from IAPWS as well as non-IAPWS members, and possibly from PCC and other IAPWS WGs. PCC will present this proposal at the 2006 meeting.

10.3 The ICRNs on "Surface Tension of Aqueous Solutions" (active, but expiring) and "Origin and Fate of Organics" (expired, closing statement pending) need to be readdressed after the forthcoming PowerPlant Chemistry/EPRI conference on "Interaction of Organics and Organic Cycle Treatment Chemicals with Water, Steam and Materials" in Stuttgart in October 2005. Reconsideration of these ICRNs will therefore be deferred to the 2006 PCC meeting.

The WG identified four more topics from the Priority List that will be formulated into ICRNs for next year's meeting. Two of them are joint PCC / PCAS projects. It was agreed that the respective task group leader will send the draft of the ICRN to the WG chairman by the end March 2006. This will be forwarded to the National Committees before the EC and WG meetings in the UK.

- 10.4 The WG has identified the need to issue a guidance document on the Measurement of the Mechanical Carryover in Steam Generators.

A task group was established at the Kyoto meeting and is expected to produce a document within the coming year. Thus the WG proposes to issue a new IAPWS document. This suggestion created some discussion with the EC which included a review of the definitions of Guidelines and Advisory Notes in the Bye-Laws. The Vice Chairmen then requested the EC to agree in principle to produce such a document.

The EC approved this request unanimously and that the PCC WG will need to suggest a document name for consideration by the EC at the 2006 meeting.

- 10.5 The WG proposes the following persons as new members of the WG: Lister (University of New Brunswick, Canada), Vidoikovich (Serbian Power Generation, Serbia/Montenegro), de Wispelaere (Laborelec, Belgium), and Stellwag (Framatome / ANP, Germany)

The EC approved these membership additions unanimously

11. Editorial Committee Report

Chairman Harvey reported that the Editorial Committee had reviewed and approved the Supplementary Release on Backwards Equations for Specific Volume as a Function of Pressure and Temperature $v(p,T)$ for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. He also indicated that the Committee had reviewed two other documents.

12. Membership and Associates

12.1 Membership.

The Executive Secretary again mentioned that the Greece National Committee had become a full member of IAPWS on 1 January 2005. No other activity had occurred in the membership area.

12.2 Members Defaulting on Dues.

The Executive Secretary indicated that according to the latest Swiss bank account statement (end of May 2005), the following countries had not paid the 2005 IAPWS dues: Argentina/Brazil, France, Greece, and Russia. In 2004 France and Russia had not paid the dues.

13. Executive Secretary's Report

13.1 Financial, Auditors and Dues

The Executive Secretary reported that IAPWS remained on a sound financial footing with currently over SFrs 96,000 in the Swiss bank account and about \$15,000 in the US account for a total of \$90,797 combined. The status as at 22 June 2005 in the bank accounts had been provided to each National Delegate present at the EC meeting.

The Executive Secretary next reported that the 2004 financial statements had been forwarded to the Auditors in January 2005. Mr. Miyagawa in Japan and VDI in Germany had reviewed and approved them. The financial statements for 2004 and the Auditors reports had also been provided to all the National Delegates present.

The Executive Secretary proposed that these organizations continue to act as auditors.

The EC approved this unanimously.

The Executive Secretary proposed to the EC that the dues structure for member countries remain unchanged for 2006.

The EC unanimously agreed to this proposal.

The Executive Secretary also provided a rough estimate of the income and known planned expenditures for 2005.

13.2 Financial Report on the 14th ICPWS

The Chairman of the 14th ICPWS, Watanabe, provided printed copies of the final financial statement for the 14th ICPWS for all the Delegates. He particularly wanted to mention the support by the Sponsors and the Foundation Donations.

The Sponsors were:

- * Chubu Electric Power Co. Inc.
- * Kansai Electric Power Co. Inc.
- * Tokyo Electric Co.
- * Fuji Electric
- * Hitachi, Ltd.
- * Mitsubishi Heavy Industries
- * IHI (Ishikawajima-Harima Heavy Industries, Ltd.
- * Toshiba Corp.

- * CRIEPI
- * JEOL (Japan Electron Optics Laboratory Co. Ltd.)
- * Aoyama Trading Co. Ltd.
- * Gikenkagaku Ltd.
- * Teramecs Co. Ltd.

The Foundation Donations were supplied by:

- * Commemorative Organization for the Japan World Exposition '70
- * Japan Society for the Promotion of Science

The Chairman of the 14th ICPWS also thanks IAPWS for the IAPWS Fund of \$25,000. He then introduced the Editor of the Proceedings, Nakahara, and thanked him for doing an excellent job in developing the final document within a year of the conference. Nakahara provided an overview of the important processes that the German National Committee will have to consider for the 15th ICPWS in Berlin in 2008.

13.3 Time and Place of the 2006 and 2007 Meetings

The 2006 EC Meetings will be held in the UK. The Executive Secretary asked the delegate from BIAPWS to provide the details. Harries indicated that the next EC and WG meetings would be held at a Hotel/Conference Center at Witney, which is about 10 miles west of Oxford in the UK. The dates are Sunday, 3 September to Friday, 8 September. BIAPWS will develop a website for the meetings. The Japanese delegate, Watanabe, requested the BIAPWS organizing committee for the one day symposium to include a presentation on the new IAPWS areas of involvement as well the Helmholtz Lecture, which will start the symposium.

The Executive Secretary indicated that the location of the 2007 EC Meetings was still under consideration. Initial discussions with the new Chairman of the French National Committee (Dorey) indicate a good possibility of holding the meetings in Paris.

14. Guidelines, Releases, Certified Research Needs, and International Collaborations

The President indicated that the Releases and ICRNs had been discussed and approved within the WG Reports so no further discussion took place.

14.1 International Collaborative Projects.

The President asked the Chair of the Committee (Friend) to report on the discussions during the week. The Chairman indicated that the Committee had considered two topics. The first was with regards to eligibility of the member countries and the young collaborator. Friend indicated that the

Committee suggests that these projects should be as flexible as possible in that one of the two member countries could be supplemented by a non-member country, and that the collaborator could be from a member or non-member country.

The EC approved this unanimously.

Chairman Friend then indicated that only one proposal had been received. The details of this proposal are provided in Attachment 11. As both the IAPWS President and the Chair of PCAS were the supporting sponsors, they were asked to leave the room. The Chairman then summarized the proposal for the EC. The IAPWS Sponsors are Frantisek (Czech Republic) and Lvov (USA). A young Czech investigator will travel to Penn State University in the USA to investigate the Irreversible Thermodynamics of Fuel Cells Membrane Transport. The period of performance will be five months starting in February 2006 at a proposed budget cost of \$9,500 for travel expenses and costs. The Chairman indicated that the Committee approved the technical content and recommends to the EC that this project be funded

The EC approved the project unanimously.

15. IAPWS Awards

The President first of all lead some discussion on developing an “Awards Page” on the IAPWS website. The consensus of the EC was that this would be a good idea and that the page should contain descriptions of the IAPWS Awards and listings of the Gibbs, Honorary Fellow and Helmholtz awardees.

15.1 IAPWS Honorary Fellowships

The President reported that Rukes (Germany) had been elected Honorary IAPWS Fellow, following the established procedures and after unanimous approval through the postal ballot conducted by the Executive Secretary. The Fellowship Award had been presented at the IAPWS Dinner on Thursday evening.

The President reminded the EC of the Awards Committee for 2006 with Fernandez-Prini as Chairman and Daucik as member with the IAPWS President as ex.-officio member. Nominations are due to the Executive Secretary by January 31, 2006.

15.2 IAPWS Helmholtz Award

The President reported that Molinero had been selected as the 2005 Helmholtz Awardee and that she had been presented with the award prior to her Helmholtz Lecture at the Symposium on Wednesday. He then asked the Canadian Delegate for the names of the Helmholtz Award Committee for 2005. In his absence, the Executive Secretary indicated that the 2006 Helmholtz Committee would consist of: Svishchev (Chairman), Mares (Czech Republic), Therkildsen (Denmark), Kretzschmar (Germany) and Gachon (France), Nominations are due to the Executive Secretary by January 31, 2006.

16. New Business

16.1 IAPWS Restructuring

At Monday's EC Meeting (Minute 3.1), the President had reminded the EC of the importance of the follow-on activities that were needed within the WGs during the week. The WGs appeared to have taken action on all the committees and Task Groups with the exception of the Task Group on Education and Outreach. The Executive Secretary had received a note from the Chairman of this Group indicating that there had not been much activity over the last year. This led to much discussion by the EC which culminated in the suggestion that the Task Group continue during the next year under the Chairmanship of Corti, and that it should redefine the Task Group approaches and activities. Three new members volunteered to join this important task group: Kretzschmar (Germany), Safarik (Czech Republic) and Lvov (USA). The President requested that the Task Group will report on status at the 2006 EC Meetings in the UK.

16.2 Press Release

The President requested that the Press Release be projected for review by the EC. Suggestions were provided by the EC and the final version is contained in Attachment 12

16.3 Miscellaneous Items

The US Delegate (Friend) requested that the latest Statutes and Bye-Laws be put on the IAPWS website.

The EC approved this suggestion unanimously.

The Greece Delegate (Assael) requested that the EC consider changing the names of the WG activities during the week into a "program" which could then be used to attract new members. He volunteered to take the 2006 Agendas and develop a Program format. Discussion by the EC resulted in

the suggestion to include this item on the 2006 EC Agenda and to possibly form a committee.

16.4 Review of Progress of Research in Member Countries

Written reports on progress in member countries were not reported to the EC but were distributed to other members and the Executive Secretary during the IAPWS week. They are attached to these minutes as follows:

Britain and Ireland	Attachment 13
Czech Republic	Attachment 14
Germany	Attachment 15
Greece	Attachment 16
Japan	Attachment 17
Russia (Forwarded to Executive Secretary)	Attachment 18
USA	Attachment 19

16.5 Participants

Attachment 20 provides a list of participants at the IAPWS EC and WG Meetings in Santorini, Greece in July 2005.

16.6 List of Members

An up-dated list of members of the Executive Committee, Working Groups, and Honorary Fellows will be developed by the Executive Secretary following the Santorini Meetings. This will be forwarded electronically to the Head of each National Committee.

17. Closing Remarks and Adjournment

The President thanked everybody for participating at this EC meeting. He particularly thanked the Greece National Committee for organizing the 2005 Annual IAPWS Meetings, and then he formally closed the 2005 EC meeting at 12:37pm.

**AGENDA for the EXECUTIVE COMMITTEE
IAPWS
Santorini Island, Greece. 3 – 8 July, 2005**

Monday, 4 July 2005. Opening Session (9:00 – 10:30am)

- Opening Remarks and Welcome
- 1. Adoption of Agenda
- 2. IAPWS Business and Appointment of Committees
 - 2.1 Press Release
 - 2.2 Evaluation Committee on International Collaboration
 - 2.3 IAPWS Awards Committees and Process (Honorary Fellow and Helmholtz)
 - 2.4 Host Country for 15th ICPWS (Kyoto Minute 2)
 - 2.5 Other business requiring special/extensive discussions
- 3. EC Mandate to Working Groups and Membership
 - 3.1 IAPWS Restructuring (Committees and Task Forces. Kyoto Minutes 18.1)
 - 3.2 Releases, Guidelines and Certified Research Needs
 - 3.3 WG Directions
- 4. Preview by WG Chairpersons of Week's Activities

Friday, 8 July 2005. Executive Meeting. (8:30am – 12:00noon)

- 5. Acceptance of Minutes of Previous Meeting
- 6. President's Report
- 7. Report and Recommendations of TPWS
- 8. Report and Recommendations of IRS
- 9. Report and Recommendations of PCAS
- 10. Report and Recommendations of PCC
- 11. Editorial Committee Report
- 12. Membership and Associates
 - 12.1 Report on Membership (Including Members Defaulting on Dues)
- 13. Executive Secretary's Report
 - 13.1 Financial, Auditors and Dues
 - 13.2 Financial Report on the 14th ICPWS
 - 13.3 Time and Place of 2006/2007 Meetings
- 14. Guidelines, Releases, Certified Research Needs
 - 14.1 International Collaborations
- 15. IAPWS Awards
 - 15.1 Helmholtz
 - 15.2 Honorary Fellowship
- 16. New Business
 - 16.1 IAPWS Restructuring. Committees and Task Forces
 - 16.2 Press Release
 - 16.3 Miscellaneous Items
- 17. Adjournment

Wednesday July 6th 2005

**Symposium on
Applied Water Treatment Processes for Power Plant Cycles**

Morning Session

Chairpersons: Prof. M. Assael, *Chemical Engineering Dept., Aristotle University, Greece*
A. Kastanaki, *Public Power Corporation, Greece*

- 09:00 Presentation of the Helmholtz Award by the president of IAPWS
- 09:45 Applied water treatment processes for PPC power plant boilers
A. Kastanaki, *Public Power Corporation, Greece*
- 10:15 Main condensers' corrosion in Agios Dimitrios Power Plant
D. Sotiropoulos *Public Power Corporation, Greece*
- 10:45 *Coffee*
- 11:15 Oxidation & contamination of cationic resin beds
P. Tsiampas, *Public Power Corporation, Greece*
- 11:45 Investigation of the boiler corrosion at the Ptolemais P.S.
S. Vasile, *Public Power Corporation, Greece*
- 12:15 Control of Flow Accelerated Corrosion (FAC) in Conventional Fossil and Combined
Cycle Power Plants
B. Dooley, *EPRI, USA*
- 12:45 *Lunch*

Afternoon Session

Chairpersons: Dr B. Dooley, *EPRI, USA*
Prof. Sergei Lvov, *Penn State University, USA*

- 14:45 Partitioning of Acids, Bases and Salts from Liquid Water to Steam: Laboratory-Scale
Experimental Results
D. Palmer, *Oak Ridge National Laboratory, USA*
- 15:15 Latest Experience with High Temperature Water Chemistry Sensors Related to Nuclear
Industries
S. Uchida, *Tohoku University, Japan*
- 15:45 *Coffee*
- 16:15 High Temperature Water Chemistry Sensors Related to Fossil Fuel Power Stations
Eric Maughan, *Thornton Europe, Germany*
- 16:45 State of the Art in Experimental Studies of Electrochemical Corrosion in High
Temperature Aqueous Systems
S. Lvov, *Penn State University, USA*
- 17:15 *Adjourn*

Schedule
IAPWS Meetings
Santorini, Greece. 3 – 8 July 2005
 (All meetings will be at the Santorini Palace Hotel)

- Sunday 3 July. 8:00pm Informal Get-together and Registration
 (Hosted by Greek National Committee)
- Monday 4 July. 9:00am. Opening Plenary Session - Executive Committee
 11:00am TPWS/IRS Joint Meeting
 (To set agendas for the week and to conduct IAPWS Business, thus allowing remainder of week for technical matters)
 11:00am. PCAS and PCC Separate Meetings
 (To conduct IAPWS Business, thus allowing remainder of week for technical matters)
 2:00pm. TPWS and IRS Joint or Separate Meetings
 2:00pm. PCC/PCAS Joint WG Meeting and Workshop
Joint WG Workshop
- Tuesday 5 July. 8:30am. PCAS Workshop (other WG Members will be welcome)
PCAS Workshop on Priority Topics
 8:30am. TPWS and IRS Joint or Separate Working Groups Meetings.
 8:30am. PCC Separate Meetings
 2:30pm IRS and PCC Separate WG Meetings
 2:30pm TPWS/PCAS Joint Meeting
Topics of Interest to Both WGs
 7:00 pm. IAPWS Wine Tasting. (Santos Winery)
- Wednes. 6 July. 9:00-5:00 **IAPWS Symposium**
"Applied Water Treatment Processes for Power Plant Boilers"
- Thursday 7 July. 8:30am. TPWS/IRS/PCAS/PCC Separate or Joint WG Meetings
 1:30pm. Separate meetings of Working Groups
 (If needed to prepare for Executive meeting)
 7:00 pm. **IAPWS Dinner.**
 (Restaurant 1800 at Oia)
- Friday 8 July. 8:30am. Executive Meeting **(8:30am - 1: 00pm)**
 (Will include at least one member from each National Delegation)

TPWS - Thermophysical Properties of Water and Steam WG
 PCAS - Physical Chemistry of Aqueous Solutions WG
 PCC - Power Cycle Chemistry WG
 IRS - Industrial Requirements and Solutions WG

Barry Dooley
 25 February 2005



Minutes
IAPWS Thermophysical Properties of Water and Steam WG

SANTORINI, GREECE

JULY 4-8, 2005

NOTE: Items are listed according to their order on the agenda, which is attached as Attachment A. **Bold print** denotes significant actions. These minutes include some items (4-10) that were done jointly with the WG IRS and some (11f-h,12-14) with PCAS.

1-3. The meeting was opened on Monday, July 4 by the Chair, Dan Friend. The agenda (Attachment A) was adopted after numerous revisions. **New officers were elected; these will be H.-J. Kretzschmar as Chair and A.H. Harvey as Vice-Chair. If approved by the EC, these will take effect July 11.** Allan Harvey was appointed Clerk of Minutes. The minutes of the 2004 IAPWS TPWS WG meeting in Kyoto were approved.

4. No new collaborative projects were proposed by the WGs TPWS or IRS for this year.

5-7. [These items are reported in the IRS minutes.]

8. Prof. Kretzschmar presented a proposed document on the calculation of thermodynamic derivatives from IAPWS-95 and IAPWS-IF97. There was extensive discussion about whether this information should be an Advisory Note or have some less formal dissemination such as an FAQ on the Website. **A vote was taken with 9 in favor of the Advisory Note and 6 in favor of some alternative. Prof. Kretzschmar was authorized to make a draft of what would be Advisory Note #3, with the intention of having it adopted in 2006.**

9. Dr. Bellows from PCC raised the issue of future power cycles possibly requiring steam thermodynamic properties at temperatures above the upper limit of IAPWS-95 and pressures above the upper limit of IAPWS-IF97 Region 5. It was decided that, for the near term, extrapolated properties from IAPWS-95 were sufficient for exploratory calculations. If these cycles get closer to reality, we can look more closely at extending IAPWS-IF97 Region 5 to a higher pressure such as 30 MPa. Prof. Kretzschmar has already done some preliminary work in this area, and he was encouraged to continue.

10. Mr. Hiegemann presented his perspective on industrial requirements for working fluids. He first presented some small comments on water and steam properties. He then described the need for property standards for seawater to be used in condensers and possibly desalination. He will get input from industry before next year to assess the needs. He also described the need for properties of fuel gas to higher temperatures than those covered by current AGA and GERG formulations. Later Dr. Feistel described that seawater properties would also be needed for oceanography and he was working with the IAPSO (International Association for the Physical Science of the Oceans) on a proposal to work toward a new standard. **Dr. Feistel was appointed as our liaison to this organization. A Task Group on Seawater was appointed consisting of Feistel, Wagner, Harvey, and Hiegemann. A letter will be sent to IAPSO from the TPWS and IRS Chairs expressing our interest in working jointly on this problem.**

11a. Dr. Harvey reported that minor changes were needed to the Fundamental Constants Guideline to update references. **The WG endorsed the revisions.**

11b. Dr. Harvey reported that a document describing obsolete IAPWS documents, which had been requested 2 or 3 years ago, had been completed and placed on the Releases and Guidelines section on the IAPWS website. **Jan Sengers will write a FAQ on thermal conductivity near the critical point for industrial use. The new Seawater Task Group was assigned to write a FAQ on that subject, contingent on the approval of the joint project by the IAPSO.**

11c. There was nothing to report regarding the liaison with the IEC.

11d. Dr. Harvey reported on discussions as authorized by TPWS last year with the Chair of the Density WG of the CCM. The CCM is willing in principle to go forward with a joint clarification on the relative roles of their standard for metrology and the wider-ranging IAPWS standard. **The Task Group appointed last year (Harvey and Span) was authorized to go forward working on a joint paper in Metrologia and preparing an Advisory Note (recommending use of the CCM standard for metrology in its range of applicability and use of IAPWS-95 if it is needed to cover a wider range) to be adopted by IAPWS in 2006 or 2007.**

11e. Mr. Cooper presented a thorough analysis of converting the D₂O thermodynamic property release for the ITS-90 temperature scale, and presented a draft for a revised release. Changing the temperature scale within the current formulation does not adversely affect the accuracy within the uncertainty of the formulation. **The WG endorsed the draft revised release and requested approval by the EC subject to editorial revisions.**

11f. Mr. Okita presented some recommendations from the environmental Task Group regarding new trends in power generation for environmental reasons. This was refined later in the week and made into a priority list. In order, the top 5 priorities are (1) solutions for CO₂ capture (time scale, 2008); (2) properties of high-temperature steam (reliable transport properties needed by 2007, extension to higher temperatures for thermodynamic properties (extension of Region 5 to higher pressures) by 2010); (3) properties of humid air (needed quickly); (4) high-temperature oxidation (time scale 2008); (5) dew point of exhaust gases (needed quickly). The Task Group will continue its work with the goal of drafting some ICRNs addressing these priorities for possible adoption in 2006. Mr. Parry presented some related thoughts on future property needs in power generation; these are described in the IRS minutes.

11g-h. Prof. Yasuoka and Prof. Svishchev reported on the activities of the simulation Task Group over the past year. A definitive description of SPC/E water is being worked on, and future plans were described. Prof. Yasuoka also described his progress in simulating bubble nucleation.

12. Dr. G. Ghosh described his physically based model for the refractive index of water.

13. Dr. Harvey described some issues (both new data and theoretical considerations) suggesting a possible need for revision of the current IAPWS standard for the dielectric constant of water. No immediate action was planned at this time.

14. Prof. Lvov described his work on a new formulation for water's self-ionization constant. **He was authorized to proceed forward toward making this work an IAPWS Release for possible adoption in 2006.** Prof. Nakahara reported new experimental data on the self-diffusion coefficient of water to high temperatures and pressures. He was encouraged to continue this

pioneering work and it was the opinion of the working groups that this would be a good subject for an IAPWS Guideline.

15. Prof. Kretzschmar reported on the work of the EU project on properties of humid air for compressed air energy storage. Work is proceeding forward but is hampered by lack of data.

The WG recommends that the ICRN on the topic of properties of humid air and combustion gases be renewed for an additional 3 years.

16. Prof. Sengers explained the history of IAPWS viscosity standards. Dr. Friend presented the new formulation and a draft Release and expressed appreciation to Dr. Huber of NIST who had done much of the work. The WG decided that there was a need for the Release to say something about extrapolation to higher temperature. With that caveat, the WG **adopted the following schedule with an aim of adoption of the Release at the Annual Meeting in 2006:**

Sept. 30, 2005 Deadline for comments by WG members on draft document

Dec. 31, 2005 Completion of evaluation by evaluation Task Group

Jan. 15, 2006 Evaluation report distributed to Working Group

Feb. 15, 2006 Deadline for input from WG members

March 1, 2006 Finalized draft of Release to Editorial Committee

April 1, 2006 Approval by Editorial Committee

April 15, 2006 Final Release distributed to National Delegates

The Evaluation Task Group for viscosity consists of Mares (chair), Konas, Alexandrov, Cooper, and Ueno.

P. Konas presented work on analysis of the thermal conductivity database and examined extension of the correlation to high pressures and possible reduction in the number of parameters.

Prof. Mares was added to the Transport Property Task Group for its ongoing work on thermal conductivity.

17. Dr. Feistel presented a Gibbs potential that had been derived for ice, along with a draft Release. There was discussion about the content of the Release; it was decided that some of the background material needed to be removed (and just reported in the published paper), that some text about uncertainties needed to be added, and other suggestions were given. **The WG decided to proceed ahead with a release with the following schedule:**

Sept. 30, 2005 Deadline for comments by WG members on draft document

Dec. 31, 2005 Completion of evaluation by evaluation Task Group

Jan. 15, 2006 Evaluation report distributed to Working Group

Feb. 15, 2006 Deadline for input from WG members

March 1, 2006 Finalized draft of Release to Editorial Committee

April 1, 2006 Approval by Editorial Committee

April 15, 2006 Final Release distributed to National Delegates

An evaluation committee for the ice release was appointed consisting of Hruby (chair) and Harvey.

18. The WG recommends to add to TPWS membership Dr. Rainer Feistel (Germany) and Dr. Jan Hruby (Czech Republic).

19. Dr. Harvey distributed an interim report on the work done on the IAPWS Collaborative Grant between the U.S. and Russia. With regard to potential contributions to life sciences, at this point we consider our work on seawater as a first step in that direction. Dr. Friend was thanked for his years of service as TPWS Chair.

20. The Chair and Clerk of Minutes were appointed to prepare the formal motion of the TPWS WG to the EC.

21. The meeting was adjourned at 4:15 PM on Thursday, July 7.

Agenda

IAPWS Thermophysical Properties of Water and Steam WG

SANTORINI, GREECE

JULY 3-8, 2005

Monday:

1. Opening Remarks; Adoption of Agenda
2. Officers; Appointment of Clerk of Minutes
3. Approval of Minutes of TPWS WG in Kyoto, Japan (August/September 2004)
4. *Potential International Collaborative Projects
5. *Supplementary release on $v(p,T)$ backward equations in region 3
 - Report of the Evaluation Task group (Kiyoshi Miyagawa)
 - Formal Consideration of Supplementary Release by WGs TPWS and IRS
6. *Computing time investigations of the IAPWS-IF97 backward equations
7. *Revision of Advisory Note #2

Tuesday AM:

8. *Differential quotients of IAPWS-IF97 and IAPWS-95, preparation of a guideline
9. *Extension of IAPWS-95 Formulation
10. *Requirements for Working Fluids: An Industrial Point of View
11. Reports on Other TPWS Activities
 - (a) Fundamental Constants
 - (b) Website Issues/Obsolete Items
 - (c) Liaison with IEC
 - (d) Liaison with CCM
 - (e) D₂O Properties

Tuesday PM:

- (f) +Report of the Environmental Task Group
- (g) +Simulation Task Group
- (h) +Simulation of Bubble Nucleation in Water
12. +Physically based model for the refractive index of water
13. +Dielectric constant
14. +The ionization constant of water-new formulation, also new data for diffusivity.

Thursday:

15. Properties of humid air; status report of the EU project AA-CAES
16. A new equation of state for ice; proposal for a release
17. Transport properties of water and steam
18. Membership
19. Other Business
 - Report on International Collaborative Projects
 - Renewal of ICRN
 - Potential contribution to life sciences
 - Educational Initiatives
20. Preparation of the Formal Motion to the EC
21. Adjournment

* Joint with WG IRS

⁺ Joint with WG PCAS

June 30, 2005

Minutes of meeting of working group Industrial Requirements & Solutions (IRS)

Santorini, Greece, 3.– 8. July 2005

Note: Items are listed in the order of the agenda (Attachment A), not necessarily in the order they were discussed. Most agenda items were discussed as joint sessions with the TPWS working group (denoted with *). The joint items 4, 8, 9, 10 and 11 of the IRS agenda are covered in the TPWS minutes.

Monday, 4. July 2005

(Item 7 was revisited shortly on Wednesday, 6. July 2005)

1.-3. Opening Remarks, Adoption of Agenda

Chairman Bill Parry welcomed the IRS members. Some revisions were made to the agenda before it was adopted. Ingo Weber was appointed clerk of minutes. The minutes of the Kyoto meeting were approved.

5. *Supplementary release on $v(p,T)$ backward equations in region 3

Kiyoshi Miyagawa outlined the progress of the Evaluation Task Group work since the Kyoto meeting. The supplementary release document was revised and had been approved by the editorial committee during this time frame. The task group tested with regards to reproducibility, accuracy and computing speed and verified that all aspects meet the requirements. The task group recommends that the supplementary release is being accepted by IAPWS. The software code should be handled as the code for the previous supplementary releases, i.e. they will be part of the IAPWS-IF97 authorized code.

The working groups unanimously voted to recommend adoption of the supplementary release to the EC.

Prof. Kretzschmar expressed his thanks for the work of the Evaluation Task Group, especially Kiyoshi Myagawa, not only for this supplementary release but also for all supplementary releases on backwards equations in the past. The backward equations $v(p,T)$ in region 3 complete work on backwards equations since all required backward functions are now available in all regions of IAPWS-IF97 except region 5. The development of these backward equations will be documented in a detailed background paper. Following the procedure of previous publications Prof. Kretzschmar asked if the page charges for the publication would be funded by IAPWS. An estimation for the maximum total charge would be US\$ 2000. **The working groups recommend to the EC to provide coverage for the page charges of this paper.**

6. *Amendment of the “Revised Supplementary Release on Backward Equations for the Functions $T(p,h)$, $v(p,h)$ and $T(p,s)$ for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam”

Katja Knobloch presented a necessary amendment to Tables 12 and 15 of the above mentioned supplementary release document. The tables contain test data for computer program verification. Calculating the temperature with the data listed in the

original document will result in temperatures slightly outside region 3. The proposed corrected tables will contain data which result in temperatures in region 3. The changes are considered editorial changes. **The working groups recommend to the EC to authorize the editorial committee to make the necessary changes without further formal acceptance by the EC.**

A corrected document will be available for the EC meeting. In addition to the corrected tables the top page contains a note stating the date and location of the amendments.

7. ***Computing time investigations of IAPWS-IF97 Equations**

Kiyoshi Miyagawa presented an investigation on computing speed comparisons between IFC-67 and IAPWS-IF97 in its original form (i.e. without additional backwards equations) on different PCs and operating systems. His findings were that based on the original assumptions on the typical distribution of function calls the computing time ratios (CTR) between IFC-67 and IAPWS-IF97 generally increased with more modern computer systems. With the computer system agreed upon for verification that IAPWS-IF97 meets the requirements (PC 486DX (33MHz)) the CTR value is 5.1 while it increases up to 8.6 (Pentium 4 (1.5GHz)) on modern systems. Apparently modern computer systems are optimized for “simple” computational operations which favors the simpler structure of IAPWS-IF97. Usage of different operating systems showed no relevant influence. Re-evaluation of the CTR values for all backward functions on an up-to-date computer system (Pentium 4 (3.0GHz)) emphasize the fact that backwards equations are very useful in reducing the computing time of applications.

During the discussion it was suggested to make comparisons between IFC-67 and IAPWS-IF97 including all backward equations from supplementary releases.

There was agreement that it was desirable to document the achievements by presenting a paper at suitable occasions, e.g. power industry conferences. This would give IAPWS an opportunity to advertise its work. Kiyoshi Miyagawa agreed to start with the preparation of such a paper.

8. ***Revision of Advisory Note #2**

Jeff Cooper stated that Advisory Note #2 has to be updated since now an additional supplementary release will be available. Advisory Note #2 explains the proper usage of the various IAPWS releases. Consensus was reached to make the following recommendation to the EC: **The EC is asked to authorize the editorial committee to revise Advisory Note #2 as needed without further formal acceptance by the EC.**

Tuesday, 5. July 2005

(Items 13 and 15 were revisited shortly on Wednesday, 6. July 2005)

13. New Industrial Requirements of the Future

The discussion of future industrial needs was based on the presentation of the Task Group on Environmental Issues by Nobuo Okita covered under item 11. f. of the TPWS minutes. The following areas of interest were identified:

- i. High temperature requirements – extension of region 5 of IAPWS-IF97 to higher pressures
For conceptual studies an industrial formulation is not required. For these studies also TTSE could be used to provide fast property values. However if products are being developed an industrial standard is required. In order to use the currently available knowledge of developing such equations should not be delayed for long.
- ii. IAPWS release on properties of sea water
- iii. H₂O – CO₂ mixtures, especially steam - CO₂ mixtures
- iv. Renewed interest in nuclear power generation, here especially two-phase-flow phenomena
- v. Metastable steam/water, here especially criteria for existence of the metastable state
- vi. H₂O dissociation at high temperatures, here especially under which conditions (temperatures, pressures) dissociation occurs
- vii. Combustion of H₂ and O₂, here especially conditions of the steam after combustion (mixtures of steam with H₂, O₂ and possible other combinations)
- viii. Properties of humid air and humid combustion gases

A task group “Future Cycles” was formed chaired by Bill Parry with members Nobuo Okita, Francois Gachon and potential member Michael Hiegemann. The task group will report next year on more precise requirements for future cycles for power generation.

Chairman Bill Parry reported on this discussion in a later joint meeting with TPWS (see TPWS minutes).

14. Extension of Metastable ICRN

As part of the above discussion of future industrial requirements further need for investigations in the metastable regions was identified. **The working group therefore recommends to the EC to extend this ICRN.**

15. Membership

The working group recommends to add the following persons to the membership roster:

Dr.-Ing. Michael Hiegemann, Alstom Power, Switzerland
Francois Gachon, Electricite de France, France

16. Other Business

In the initial EC meeting it was suggested to hold a symposium on new developments in power generation at the 2006 IAPWS meeting in Great Britain. In case the local organizing committee in fact chooses to hold such a symposium IRS will support the organizing efforts. **Chairman Bill Parry will contact the Head of Delegation of the Britain and Ireland National Committee.**

17. Preparation of Report to the Executive Committee

The Chairman and Clerk of Minutes will prepare the report to the EC.

18. Adjournment

The Chairman adjourned the meeting of the IRS working group at 16:30.

Agenda
of
Industrial Requirement and Solutions Working Group
Santorini, Greece July 4th to July 8th, 2005

Monday:

1. Opening Remarks, Adoption of Agenda
2. Appointment of Clerk of Minutes
3. Approval of Minutes of Kyoto Meeting, August/September 2004
4. *Potential International Collaborative Projects
22. *Supplementary release on $v(p,T)$ backward equations in region 3
 - Report of the Evaluation Task group -- Kiyoshi Miyagawa
 - Formal Consideration of Supplementary Release by WGs TPWS and IRS
23. *Computing time investigations of IAPWS-IF97 Equations -- Kiyoshi Miyagawa
24. *Amendment of the "Revised Supplementary Release on Backward Equations for the Functions $T(p,h)$, $v(p,h)$ and $T(p,s)$ for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam"
25. *Revision of Advisory Note #2
26. *Differential quotients of IAPWS-IF97 and IAPWS-95 -- Prof. Kretzschmar
27. *Extension of IAPWS-95 Formulation -- Jim Bellows
28. *Requirements for Working Fluids: An Industrial Point of View

Tuesday:

12. *Environmental Task Group Report -- Nobuo Okita
13. *New Industrial Requirements of the Future -- Bill Parry
14. Extension of Metastable ICRN
15. Membership
16. Other Business
17. Preparation of Report to Executive Committee
18. Adjournment

*Note: The items 4 to 13 will be discussed at a joint session with WG TPWS.

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 H₂ 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 $> 100^{\circ}\text{C}$. 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°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, for 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 at 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. Abdulagatov 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. Müller, 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 last 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 Takahashi (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 committee 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 H₂ 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 H₂ 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)

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. Maršik 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.

Working group 'Power Cycle Chemistry' (PCC)

IAPWS PCC WG Meetings in Santorini, Greece

3-8 July, 2005

MINUTES OF MEETING

1. Amendments / Adoption of Agenda

The meeting was chaired by Robert Svoboda. A draft agenda was discussed, amendments agreed and the revised agenda is set out in **PCC Attachment A**.

2. Election of Clerk of Minutes

Geoff Bignold agreed to record the minutes.

3. Approval of Minutes of 2004 Meeting in Kyoto, Japan, action points

The minutes of the 2004 meeting were approved without any corrections.

4. International Collaborations

Progress report by **Tomonori Satoh**:

Summary of FAC work as a result of Canada-Japan Collaboration Program

Professor Ushida introduced the background and key aspects of the project which had benefited from \$5000 funding from IAPWS for Mr Satoh to spend a period at the University of New Brunswick at the outset of the study.

Mr Satoh then gave a detailed presentation of the considerable progress that had been achieved within one year. A report of the study was made available to the PCC. He included information on the fatal accident at Mihama Unit 3, and showed how corrosion rate measurements based on electrical resistance of a tubular specimen could be used to deduce when FAC is actively occurring. Support is being sought from the main sponsors to continue the work for a further two years.

Answering questions, Mr Satoh indicated that the work had been performed in neutral pH conditions as a first step.

Barry Dooley commented that PWR apply reducing agents. Further studies should also include such.

Robert Svoboda summarised that this work was an excellent example of international collaboration and congratulated Mr Satoh on making such rapid progress.

Professor Lister expressed his thanks to IAPWS for their part in support of the work.

Derek Lister:

Water Chemistry Issues and Corrosion Research at University of New Brunswick, Canada

Professor Lister gave a description of his department and of the work in support of CANDU, PWR and BWR systems that is conducted.

The list of CANDU related work was extensive and included cracking of carbon steel outlet feeders, FAC in LiOH dosed systems, deposition under boiling heat transfer conditions, solubility of hydrogen and deuterium in H₂O and D₂O and exchange processes between particulate oxides and surface deposits.

In PWR chemistry there is work on the kinetics of iron and nickel exchange relative to water circulation rate. In the BWR work on the influence of zinc on corrosion and release processes is being undertaken.

Robert Svoboda thanked Derek Lister and asked that further consideration be given to these topics after consideration of the priority list.

One new topic for potential international collaboration in 2006/7 was identified (Priority List item number 4).

5. Priority List Review (see also PCC Attachment B)

The priority list set out in 2004 was reviewed and updated. A number of overlapping topics were merged and some additional topics were introduced after thorough and extensive debate. The agreed revised list is given as PCC attachment B.

Arising out of the discussions the following actions were agreed:

- To develop an ICRN on “Interfacial situation in advanced ultra supercritical plants” in collaboration with PCAS.

Barry Dooley to Liaise with Don Palmer

- To develop an ICRN on “Mechanism of Decomposition of Ion-exchange Resin”

Karol Daucik

- To develop a joint PCAS/PCC ICRN on “Development / Application of Sensors (Ambient and High Temperature Sensors)”

Maughan, Lister, Uchida, Lvov

- To develop an ICRN on “Improved analysis of low concentration of metals (Fe, Cu, Co, etc)”

Derek Lister + Karol Daucik

- To formulate a brief description of the problem of the relationships between the chemistry of the contaminants and their concentration at point of measurement, for presentation to IAPWS executive with the aim of potential introduction of a new ICRN proposal in 2006.

Task group: Bellows + Maughan+ Hughes + Bignold

Draft prepared and presented to PCC on 7 July 2005. **PCC Attachment C.**

- To progress the work on a method to quantify mechanical carry-over by the establishment of a guidance document. Robert Svoboda will propose two alternative approaches to the IAPWS executive:
 - Development of a PCC guidance document
 - or
 - Preparation of a paper for publication in the open literature (e.g. PowerPlant Chemistry) under IAPWS PPC team membership.

Team/task group: F.Gabrielli +J.Bellows, S.E.Therkildsen + M. deWispelaere + R.Svoboda

INTERMEZZO: Joint workshop with PCAS:

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

Don Palmer described work on the solubility of zinc oxide as a function of pH and temperature. The aim was to identify the maximum concentration that can safely be used in PWR primary water to displace active cobalt and reduce radiation fields. Details of zinc speciation had been evaluated from the results which now extended up to 350°C.

- b.) **S. Lvov** - Development of Zirconium Oxide Coating Technology to Mitigate Intergranular Stress Corrosion Cracking in BWRs

Sergei Lvov described work on the hydrothermal deposition of zirconia coatings on BWR materials for protection against IGSCC of stainless steels. He showed that, by careful control of deposition conditions, a 2 to 3 µm coating of high density and very good adhesion could be attained. Such a coating was able to suppress the free corrosion potential into a region where the probability of IGSCC was reduced.

- c.) **Stastny, M.**, Sejna M.: The Effects of Steam Chemistry on Condensation Process

Mr Stastny described an advanced theoretical study of condensation processes in expanding steam flows (modeling conditions in the later stages of LP steam turbines) and showed excellent correlations with the limited supporting experimental data. The work showed that the kinetics of droplet formation are too fast for all non-volatile solutes in the steam to be absorbed in early condensate. He confirmed previous conclusions on the very low solubility of NaCl in LP steam.

- d.) **R Svoboda** : The solubility of copper as a function of temperature

Robert Svoboda made a presentation which questioned the apparent inconsistencies between plant observations and published data on the solubility of copper in power plant circuits. Whereas ammonia corrosion of copper alloys in condensers occurs preferentially at the hotter end of the machine, an interpretation of the published data could suggest that copper oxide solubility falls with temperature. In the case of deposition in stator coils, although the solubility data would suggest a risk of blockages developing at the outlet end, the practical experience shows vulnerability at the inlet.

Don Palmer questioned whether just cuprous or cupric ion solubility was being considered and commented on the temperature dependence of the equilibrium constants for the ammonia complexes of both oxidation states. There was a consensus that, although sufficient data may exist, there is a need for clarification of the various dependencies in order to make the information more useful to the power industry.

Action: Svoboda will submit the references to Palmer, who will respond.

Sergei Lvov announced that PCAS had decided to terminate the work of two of its Working Groups and to replace them with a single new group on Interfacial Chemistry and Electrochemistry in High Temperature Fluids. He invited PCC participation in this working group. One of the issues addressed would be the establishment of an international conference to be held in juxtaposition with a relevant conference of the Electrochemical Society.

Action: Interested PCC members to contact Lvov.

7. IAPWS Certified Research Needs

Active ICRNs:

ICRN 13 on Surface Tension of Aqueous Solutions is due for closure. It was agreed that consideration should be given to results from the forthcoming conference in Stuttgart in October 2005. The ICRN therefore to be extended until September 2006.

Action – F.Gabrielli

Closed ICRNs reconsidered:

The ICRN on Evaluation of Binary Nucleation Models is no longer active but the progress has been covered in the IAPWS book. A closing statement is requested from Dr Marsik.

The ICRN on the Origin and Fate of Organics, which was issued originally in 1993, is likely to need to be readdressed after the forthcoming conference in Stuttgart in October 2005. ICRN reconsideration therefore to be done in the 2006 PCC meeting.

Action - E.Maughan

Proposed new ICRNs (to prepared for approval at the 2006 meeting):

Interfacial situation in advanced ultra supercritical plants

Joint PPC/PCAS ICRN: Palmer, Dooley

Mechanism of Decomposition of Ion-exchange Resin

Daucik

Development / Application of Sensors (Ambient and High Temperature Sensors)

Joint PPC/PCAS ICRN: Maughan, Lister, Uchida, Lvov

Improved analysis of low concentration of metals (Fe, Cu, Co, etc)
Lister, Daucik

New Issues:

Dr Safarik asked that PCC consider the need for support for work on the Thermophysical data on Moist Air at up to 10MPa / 1000°C and Steam at up to 50MPa / 1800-2000°C.

Jim Bellows explained the relevance of this to potential developments in hydrogen burning advanced gas turbines.

PCC concluded that the subject was not sufficiently urgent to introduce a further topic into the priority list at this time. It remains important that the necessary work should be undertaken before the practical hardware is developed.

8. Progress on committee work

Progress on the international collaboration within the nuclear committee had been fully reported by Professors Uchida and Lister. The need for further involvement and interest on nuclear plant topics was debated. This group is providing a strong interaction between fossil and nuclear power cycle chemistry, which is rarely found at other technical venues. Strong arguments in support were set out, with no members expressing any disagreement.

New task groups are indicated in the action list.

8. Focused topic: Nuclear Chemistry:

The following presentations were made:

- **Shunsuke Uchida:** Latest Experience with Water Chemistry in Nuclear Power Systems
- **Bernhard Stellwag:** Injection of Methanol at a Boiling Water Reactor as an Alternative to Hydrogen Injection (with Wilfried Ruehle)
- **Donald Palmer:** Zinc oxide solubility
- **Robert Svoboda:** Amine chemistry: blessing or curse for the steam turbine?

9. Focused topic: Combined cycle and fossil cycle chemistry:

The following presentations were made:

- **Robert Svoboda:** The "baby boom" (1988-2003) of combined cycle power plants is over what were the chemistry related teething troubles?
- **Geoff Bignold:** High iron levels in feedwater derived from steel air cooled condensers
- **Richard Harries:** LP steam carryover during load changes
- **Robert Svoboda:** Consequences of upset chemistry during plant startups, required restrictions
- **Marc deWispelaere:** Boiler tube failures – relation to Aluminium in the cycle?
- **Barry Hughes:** Cycle chemistry control automation while cycling at Teeside
- **Sonja Vidoikovich:** Steam purity control in Serbia power plant Nikola Tesla A
- **Karol Daucik:** Sampling for Iron in power cycles.
- **Svend-Erik Therkildsen:** Laboratory analysis for power plants

10. Update on International Power Cycle Chemistry guidelines

Karol Daucik introduced the new EBA / EPPSA / VGB guidelines on the quality of feedwater, boiler water and steam "Guidelines for Feed Water, Boiler Water and Steam Quality for Power Plants / Industrial Plants".

Differences with previous guidelines include a revised philosophy of action levels.

Alignment with the current EN guidance has been optimized.

Some parameters have no recommended upper action levels.

No endorsement from IAPWS is sought. The material was presented for information. The opportunity for information presentations on new guidelines should be allowed for future meetings.

11. Membership

The PCC unanimously supported the membership of:

Derek Lister
Sonja Vidoikovich:
Marc de Wispelaere
Berhard Stellwag (reinstatement)

Eric Maughan recorded the recent death of Barry Conlin. The PCC expressed its regrets and appreciation for the input to the working group, which Barry had contributed in the past.

12. Preparation of next year's agenda

The Priority List will be promoted to the earliest possible point in the next agenda.

Presentations preferably directed on items on the current priority list, or on items that members wish to advocate for the priority list. Any other technical presentations should be limited to no more than ten minutes each.

Time in the programme is to be allowed for working subgroups to undertake the agreed tasks.

Draft documentation for discussion and potential endorsement at the next meeting to be made available from working group chairmen by March of next year (for consideration by national committees and PCC members in advance of next IAPWS meeting).

13. Election of Officers

No requirement for immediate changes, but consideration of future officers will be required during the next year for discussion in 2006.

14. Preparation of the Report to EC

See IAPWS Minute 10.

15. Miscellaneous and Adjournment

The work of this year's meeting includes the proposal for four new ICRNs, two of which are joint with PCC and PCAS, and the intent for two PCC guidance documents.

Seven of the technical presentations are given consideration for publication.

Robert Svoboda thanked all PCC members for a very positive meeting.

Eric Maughan expressed the thanks of the members to Bobby for the excellence of his chairmanship.

Agenda for Working group 'Power Cycle Chemistry (PCC)

IAPWS PCC WG Meetings in Santorini, Greece
3-8 July, 2005

PCC Starting time 10:00 on Monday July 4. Joint WG topics are still to be decided upon (see general schedule)

1. Amendments/Adoption of Agenda
2. Election of Clerk of Minutes
3. Approval of Minutes of 2004 Meeting in Kyoto, Japan, action points
4. International Collaborations, the process
 - Progress report **Tomonori Satoh**: Summary of FAC work as a result of Canada-Japan Collaboration Program
 - **Derek Lister**: Corrosion research at University of New Brunswick, Canada
5. Priority List Review,
6. Progress on committee work

Intermezzo: joint workshop with PCAS:

- 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** - Development of Zirconium Oxide Coating Technology to Mitigate Intergranular Stress Corrosion Cracking in BWRs
- c.) **M.Stastny**, M.Sejna: The Effects of Steam Chemistry on Condensation Process
- d.) **R.Svoboda** – Opening a discussion on the Solubility of Copper and Copper Oxides in Dependence of Temperature

7. IAPWS Certified Research Needs, Closing statements

8. Focused topic: Nuclear Chemistry:

- **Shunsuke Uchida**: Latest Experience with Water Chemistry in Nuclear Power Systems
- **Bernhard Stellwag**: Injection of Methanol at a Boiling Water Reactor as an Alternative to Hydrogen Injection (with Wilfried Ruehle)
- **Robert Svoboda**: Amine chemistry: blessing or curse for the steam turbine?
- **Barry Dooley**: [discussion on FAC on Thursday, as required]

9. Focused topic: Combined cycle and fossil cycle chemistry:

- **Robert Svoboda**: The "baby boom" (1988-2003) of combined cycle power plants is over what were the chemistry related teething troubles?
- **Geoff Bignold**: High iron levels in feedwater derived from steel air cooled condensers
- **Richard Harries**: LP steam carryover during load changes
- **Robert Svoboda**: Consequences of upset chemistry during plant startups, required restrictions
- **Marc deWispelaere**: Boiler tube failures – relation to Aluminium in the cycle?
- **Barry Hughes**: Cycle chemistry control automation while cycling at Teeside
- **Sonja Vidoikovich**: Steam purity control in subcritical power plant

- **Karol Daucik:** Sampling for Iron in power cycles.
 - **Svend-Erik Therkildsen:** Laboratory analysis for power plants
10. Guidelines from EBA/EPPSA/VGB, status on guideline for boiler water (Daucik)
 11. Membership
 12. Preparation of next year's agenda
 13. Election of Officers
 14. Preparation of the Report to EC
 15. Miscellaneous and Adjournment

For more information:

PCC Chairman

André Zeijseink, andre.zeijseink@kema.com, KEMA, Arnhem, The Netherlands

Vice-Chairmen

Michael Rziha, michael.rziha@erlll.siemens.de, Siemens, Erlangen, Germany

Robert Svoboda, robert.svoboda@power.alstom.com, Alstom, Baden, Switzerland

Working group 'Power Cycle Chemistry (PCC)

*IAPWS PCC WG Meetings in Santorini, Greece
3-8 July, 2005*

PCC Priority List

1. Interfacial situation in advanced ultra supercritical plants

Formation and exfoliation mechanism of scale (oxide films) in steam lines
effects of chemistry (oxygen, ammonia ?)

Corrosion interactions materials / steam, influence / effect of
supercritical parameters, protective layers, radiation

Faster decomposition of chemicals (TOC, ammonia etc)?

Joint PPC/PCAS ICRN (Palmer, Dooley); draft: Mar 06

2*. Mechanism of Decomposition of Ion-exchange Resin

Operating conditions, quality control of resin; leak rates are slow, but sulfate is
one of the products, organic leachables, oxidation

Additional information has to be researched

ICRN Daucik -> PCC guidance document; draft: Mar 06

3*. Development / Application of Sensors (Ambient and High Temperature Sensors)

ECP (nuclear, fossil application), ORP,

problem: abstract parameters, acceptance by plant operators

Joint PPC/PCAS ICRN (Maughan, Lister, Uchida, Lvov) ; draft: Mar 06

4*. Improved analysis of low concentration of metals (Fe, Cu, Co, etc)

Techniques for analysis are known, but problems with implementation

Additional problems with adequate sampling

ICRN: Lister + Daucik; draft: Mar 06

(possibly international collaboration 2006: Lister, Daucik, Svoboda)

5*. Corrosion mechanisms that are related to the presence of contaminants in

steam/water circuits, particularly in boiler-water

Define critical species / quantify critical quantities of steam generator water impurities, synergy
with other species (e.g. oxygen), consideration of the materials

**6*. The relationships between the chemistry of the contaminants and their
concentration at point of measurement**

Detailed definition of the problem

*Task group: Bellows + Maughan + Hughes + Bignold (short document
attached, ICRN proposal 2006?; interim report to PCC: Mar 06)*

7*. The quantification of risk of asset damage

problems of getting background data, important long-term issue
need: tool for operators, design engineers & commercial persons

8*. Method to determine the mechanical carry-over?

Outline established in PPC minutes 2004

Guidance document is needed;

PCC will propose to EC establishing a PCC guidance document.

If positive: task group; if not: publication by IAPWS team in e.g. PPChem. Team/task group: F.Gabrielli, J.Bellows, R. Harries, S.E.Therkildsen, M.DeWispelaere, R.Svoboda; draft PPC guidance document:Feb 06.

9*. Improved understanding of condensation mechanisms

- dropwise vs filmwise condensation in condensers (improve heat transfer)
- heterogenous – homogeneous nucleation models for prediction of condensation in steam turbines (chemistry, electrostatic,...)
- chemistry of the phase transition zone in nuclear turbine systems

To be considered in 2006 for ICRN

10*. Deposition of contaminants and corrosion products in steam and water circuits

- supersaturation,
- mass transfer,
- adsorption,
- crystal nucleation,
- deposit re-dissolution,
- scouring and exfoliation,
- activation and activity transport in reactor systems
- Mechanism and Influence of Cu Deposition :
(essentially a solved problem from a scientific viewpoint)
 - mechanism of deposition on a turbine blade is not understood
 - discrepancies in temperature influence on deposition (?)

To be considered in 2006 for ICRN

11. High pressure / high temperature steam and humid air (24 MPa and up, 2000°C), thermophysical properties and chemistry formulation

Long term interest in power industry, should be included in update of ICRN #14

12*. Radiation chemistry of water

Radiolysis

To be expanded in 2006, together with PCAS?

*** includes input from the nuclear group**

The numbering in the list is made for reference only and does not contain any information on actual priority

**Working group 'Power Cycle Chemistry' (PCC)
IAPWS PCC WG Meetings in Santorini, Greece
3-8 July, 2005**

Proposal for new task group within PCC

Guideline on changes in samples between sampling point and analysis.

Samples can change in two modes between the sample point and the analysis. Samples may change chemically at constant overall composition. One example of this mode is the change of phosphate from a dibasic acid to a tribasic acid as it cools from boiler temperature to analytical temperature of 25°C. Crystal species may change crystalline form, disproportionate or react in other ways. Hydrogen peroxide may decompose in the sample line.

The second mode of change is to alter the sample. Examples of the mode are deposition or and release in sample lines, refluxing in sample lines, reaction of oxygen with sample line deposits, and entry of oxygen through apparently, but not completely, tight compression fittings.

A related issue is non-representative sampling. Blowdown samples collected from a blowdown header that is not flowing may be hours old before they are analyzed.

The task group believes that much, if not all of the issue has been dealt with in the literature, but that it needs to be collected and disseminated.

A collection of sample changes would provide guidance to people less familiar with these issues than PCC. We suggest that this task group collect the available literature and prepare a draft guideline.

Is the Daucik-Lister task group doing similar work and should the work be combined?

Note: "Guideline" is used in a sense somewhat different from the usual IAPWS guideline. It may be that a new type of document if the EC so chooses. It could also be an expansion of the meaning of Guideline.

Jim Bellows Geoff Bignold Eric Maughan Barry Hughes

Proposal for Young Scientist IAPWS project

for the year of 2006 in the course of 5 months.

Applicant: **Ondřej Mičan**, PhD student, Faculty of Nuclear Sciences and
Physical

Engineering, Czech Technical University Prague, CZ,
Email: mican@email.cz

Supervisors: František Maršík, Institute of Thermomechanics CAS,
Department of Thermodynamics, Dolejskova 5, 182 00 Prague,
CZ,
Email: marsik@it.cas.cz

Serguei Lvov, Professor of Energy and Geo-Environmental
Engineering

The Pennsylvania State University, 207 Hosler Building
University Park, PA, 16802, Email: lvov@psu.edu
<http://www.ems.psu.edu/egee/Faculty/lvov.htm>

Irreversible thermodynamics of fuel cells membrane transport

Hydrogen/oxygen fuel cells based on the reactions of oxidation of H_2 and reduction of O_2 ($2H_2 + O_2 = 2H_2O$) represent a prospective alternative to traditional ways of generating electrical energy. Since electrical energy can easily be converted into mechanical energy, the fuel cells are also strong candidates for replacing combustion engines, e.g. in vehicles. The basic principle of a fuel cell has been known for about 150 years and it is sometimes referred to as "reversed electrolysis". In a so-called proton exchange membrane (PEM) fuel cell, two electrodes are separated with an electrolyte, which is a very thin (no more than a few tens of micrometers) membrane made of a proton conductive polymer (e.g. Nafion). At the anode hydrogen is oxidized, producing protons and electrons. The electrons flow through an external circuit, while the protons must pass through the electrolyte membrane. At the cathode the electrons and the protons react with supplied oxygen to form water. The electrodes are attached to the membrane forming the so-called membrane electrode assembly (MEA).

Transport processes occurring in MEA are considered to be a crucial point of the fuel cell operation and efficiency. Several models describing these processes have been developed thus far. Some of them focus only on a selected part of PEM fuel cell, while others attempt to describe the behavior of the whole cell considering it as a black box. In this project we would like to focus on the investigation of a possible influence of the membrane material, membrane geometry, and other parameters such as, pressure, temperature, humidity, etc. Due to strong concentrations of protons and electrical field gradients, the application of the extended non-equilibrium (irreversible) thermodynamics is desirable. In the frame of this theory it is possible to include all relevant processes like

convection, diffusion, heat transfer, ionic conductivity, and electrochemical reactions in a natural way, i.e. based on the entropy production concept.

The expertise of the host, The Pennsylvania State University (Penn State), will be of great advantage for the applicant in selecting and modifying an appropriate model and, especially, to supply necessary experimental data. The research team of The Energy Institute's Electrochemical Laboratory at Penn State under the direction of Dr. Lvov has long-term expertise in PEM fuel cell research and high-temperature electrochemical studies. Current experimental systems cover a complete range of membrane and powder tests, including high-temperature proton conductivity (using Electrochemical Impedance Spectroscopy), water uptake, high-temperature electrophoresis for electrokinetic studies of inorganic particles, membrane casting and membrane-electrode assembly (MEA) preparation, high-temperature membrane permeability, and high-temperature fuel cell performance. Research projects on high-temperature PEM fuel cells are carried out with support of Department of Energy, Oak Ridge National Laboratory, and DuPont.

The aims of the project.

- 1 Prepare a database of existing physico-chemical models describing transport and electrochemical processes which occur at all components of MEA of PEM hydrogen/oxygen fuel cells.
- 2 Formulate an adequate physico-chemical model describing the influence of membrane material, including composite materials on the PEM fuel cell performance.
- 3 Develop a computer program for numerical simulations of the model and investigate the behavior of the model in a series of simulations.
- 4 Compare the results of numerical simulations with available experimental results and possibly improve the original model, so that it yield a better agreement with the experiment.

The stay of Ondřej Mičan at The Pennsylvania State University will be supervised by Dr. Serguei Lvov who is an expert in the field of electrochemistry and PEM fuel cells. O. Mičan will spend the proposed 5 months with Dr. Lvov in his lab at Penn State. It is proposed to start Ondřej Mičan's visit in February 2006.

Budget:

A round trip from Prague to State College: \$2,000

Per month in State College: \$1,500 * 5 = \$7,500

Total: \$9,500

Attachment: Mr. Ondřej Mičan's Curriculum Vitae

CURRICULUM VITAE

Personal Details

Name: Ondřej Mičan
 Address: Kaplická 57
 140 00 Praha 4
 The Czech Republic
 Date of birth: 19th December 1977
 Place of birth: Prague, The Czech Republic
 Title: Ing.
 Marital status: Single
 Nationality: Czech
 Telephone: +420 604 627 004, +420 723 682 691
 Email: omican@email.cz

Education

1984 – 1992 Elementary school in Prague.
 1992 – 1996 Electrotechnical high school in Prague.
 Specialization: Electronical Computer Systems.
 1997 – 2003 Czech Technical University in Prague,
 Faculty of Nuclear Science And Physical Engineering.
 Specialization: Mathematical Modeling.
Diploma thesis: Chaotic Dynamics of Reaction-diffusion Equations.
 Since 2003 PhD. study at Czech Technical University in Prague,
 Faculty of Nuclear Science And Physical Engineering.
 Specialization: Mathematical Modeling.

Work Experience

2001 Mediatel, s. r. o., entering data into a database.
 Since 2002 Unicorn, a. s., programmer, analyst.
 Since 2003 FNSPE, CTU Prague, teaching (calculus, algorithms).

Skills

Foreign languages: English (very good knowledge),
 German (basic knowledge)
 Programming languages: C++, Perl, Java, PL/SQL, JCL,.....
 Driving licence: personal vehicles

Hobbies

Music: playing the guitar, singing.
 Sports: bicycle, rollerskates, volleyball, . . .

PRESS RELEASE FOR IAPWS ANNUAL MEETING ON SANTORINI ISLAND, GREECE

July 2005

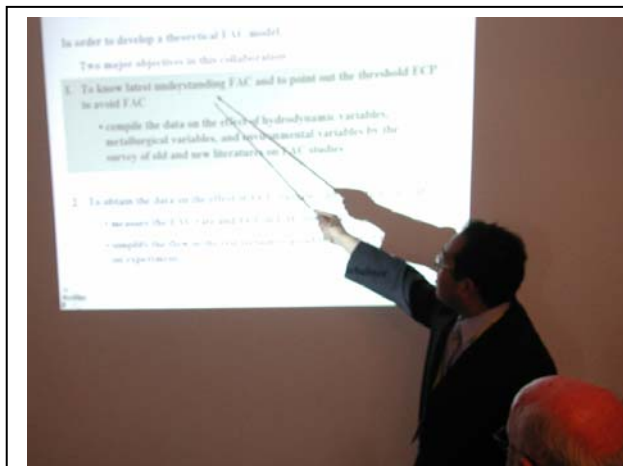
Sixty-two scientists and engineers from twelve countries attended the annual meetings of the International Association for the Properties of Water and Steam (IAPWS), July 3-8, 2005 on Santorini Island, Greece. IAPWS provides standards for steam and water properties and serves as a forum where engineers from the power industry and academic scientists can communicate problems and solutions to each other. IAPWS has traditionally concentrated on the science underlying the thermodynamics and chemistry in steam power plants, but is broadening into other aspects of power generation and high-temperature aqueous systems as well as seawater and ice. Discussions range from puzzling power plant chemistry results to reports on solutions to such problems to practical implications of fundamental theory and molecular modeling of thermodynamic and transport properties.

Highlights of the 2005 meeting include plans to develop guidance notes on water and steam sampling in power plants and on ion exchange resin. These subjects are well known to some of the participants in IAPWS, but the information is disjointed and not widely disseminated. A plan to understand the corrosion and catalysis at metal surfaces related to ultrasupercritical power plants was initiated. It includes a symposium on "Interfacial Chemistry and Electrochemistry in High-Temperature Fluids" to be conducted at an electrochemical conference. (Links will appear on the IAPWS website when the symposium is organized.) Reports on chemistry in nuclear steam cycles included the use of methanol to suppress radiolysis of water in boiling water reactor systems.

Simulation of thermophysical properties of water and aqueous systems continues to be an interest of IAPWS. The IAPWS Helmholtz Award lecture this year, "The Path of Water: A Molecular Perspective of Transport in Membranes and Glasses," by Valeria Molinero of the California Institute of Technology, provided additional insights into ways to understand phenomena that occur in experimentally difficult regions. The IAPWS Helmholtz award is given to a young scientist who is working in a field of interest to IAPWS. It includes a trip to the IAPWS meeting to present a paper.

IAPWS is preparing a Databook, with seven chapters: Phase equilibria, pVTX, Calorimetry, Potentiometry, Electrical conductivity, Thermal conductivity, Viscosity. This book evaluates various high-temperature techniques and collects and summarizes all of the relevant experimental data available in the literature with emphasis on results obtained above 200°C.

This year IAPWS completed the set of supplementary equations associated with the IF-97 standard used worldwide in industrial power generation applications. A supplementary release



Young scientist Dr. Satoh presents his report on an international collaboration on flow assisted corrosion. Dr. Satoh traveled from Japan to Canada to conduct his investigation.

enables the very fast calculation of the specific volume (or density) of water when the pressure and temperature are known, over a broad region around the critical point of water. New documents which will describe the viscosity of water and the thermodynamic properties of ice are now under review for possible adoption as IAPWS standards at its next meeting. Work is also underway or planned on the properties of moist air to assist in technologies related to humid air turbines, and on salt water to meet the needs of the oceanographic community, as well as for applications in power generation cooling systems. A continuing topic is methods of power generation in the future.

A joint project on irreversible thermodynamics of fuel cells membrane transport will send Ondrej Mican, a Czech student from the Institute of Thermomechanics, Prague to the Pennsylvania State University, United States for 5 months.

The next IAPWS meeting will be in Witney, Oxfordshire, United Kingdom, September 3-8, 2006. Details of the meeting will be available through links from the IAPWS website at www.iapws.org. Minutes of the 2005 meeting will appear on the website shortly. The meetings are open to anybody interested in the general topics of IAPWS (see website for registration details). The proceedings from the 14th International Conference on Properties of Water and Steam, *Water, Steam, and Aqueous Solutions for Electric Power*, have been released (see link on Website). The 15th International Conference on Properties of Water and Steam is planned for Berlin, Germany in 2008.

People interested in IAPWS documents and activities should contact the chairman of their IAPWS National Committee (see website) or the IAPWS Executive Secretary, Dr. Barry Dooley, EPRI, 1300 West W.T. Harris Blvd., Charlotte, North Carolina 28262, USA.

To: Professor F Marsik, Chairman of IAPWS
From: Dr R R Harries, Chairman of BIAPWS
Cc: Dr B Dooley, International Secretary, IAPWS

June 2005

A REVIEW OF THE CURRENT STATUS OF BIAPWS IN 2005

Overview

BIAPWS is a joint association within the United Kingdom and the Republic of Ireland. BIAPWS is in healthy position, both financially and with respect to active membership. It has twelve corporate sponsors, one member with academic links, five associate members who are in consultancy or are retired from the power generation industry and three corresponding members (two in academia and one in a professional institution).

BIAPWS has an active role in promoting research and disseminating information within appropriate industries and academic areas. This is achieved through organisation of seminars and workshops and through the BIAPWS Award for final year undergraduate students.

Membership

Since 2004 there has been an increase in corporate sponsors from nine to twelve. Each corporate sponsor is a full member of BIAPWS and the representation is split as follows:

- Power generation companies (8 members),
- Power plant manufacturer (1 member)
- Power plant chemical instrumentation manufacturer (2 members).
- Power plant related research and technical consultancy (1 member)

There are currently two further enquiries about membership from an additional power generation company and power plant research / technical support consultancy.

The academic support has reduced in the last few years. There is now only one active academic member on the committee. Two other universities are currently corresponding members, but are not active on the committee.

There are currently five individual associate members, all of whom have now retired from the power generation industry and have been active within BIAPWS for a number of years. These individual members retain their technical knowledge through part time consultancy and are a key factor in the successful operation of the BIAPWS committee.

It is inevitable, that with all of the sponsors and a high percentage of the membership being drawn from the power generation industry, topics relevant to that industry have a higher priority than academic research. It has proved difficult to determine the level of academic research into topics of interest to BIAPWS / IAPWS, but there is a general feeling that little research of specific interest is currently being conducted within the UK.

All corporate sponsors are required to pay an annual membership fee as a condition of continued membership. These fees allow BIAPWS to pay its IAPWS dues, to fund a delegate to the annual IAPWS international meeting, to organise symposia and workshops within the UK and, more recently, to sponsor the BIAPWS award.

Education and Outreach

BIAPWS sees one of its primary functions to act as a central point of communication and information for matters of steam and water chemistry between the power generation industry, manufacturers of power plant equipment, academia and other interested parties.

This is achieved by regular committee meetings, at which representatives from the major UK and Irish power generation companies can meet and exchange views in a neutral environment. They can also interact with equipment suppliers and with academic institutions.

The second area of education and outreach is the regular organisation of technical symposia. Eight symposia have been held since 1995, initially annually, but latterly at 18 month intervals. The major topic is linked to power plant steam and water chemistry, and BIAPWS provides the only UK and Irish national forum for a regular symposia on power plant chemistry. As such it achieves a very important function and has regularly attracted attendances of 80 people, including speakers and attendees from other European countries. These symposia are a very effective way of raising awareness of BIAPWS and IAPWS within the UK and Ireland.

Following the initiative, in May 2003, of combining workshop sessions with a technical symposia, the pattern was repeated in December 2004, when a one day symposium on Power Plant Chemistry was preceded by a half day workshop on related topics. The workshop was oversubscribed and the increased numbers produced a master class environment rather than a true interactive workshop.

Both the workshop and symposium were well attended with around 30 for the workshop and 75 for the symposium.

The third initiative has been the BIAPWS Award, started in 2002 and first awarded in 2003. Its aim is to raise the awareness of undergraduates about research and careers in areas and industries associated with the properties of water and steam. It offers a prize of £1000 (\$1800US) for a dissertation based on a final year undergraduate project with suitable association to the aims, ideals and topic areas of IAPWS. Despite contact with a large number of Universities the response has been extremely disappointing. The single entry in 2004 was not awarded the prize, for lack of technical merit. In 2005 the response has been similarly disappointing, but entries have not yet been reviewed.

The BIAPWS Award has been discussed at recent committee meetings. The decision whether to reformulate it or abandon it has yet to be taken.

The future

- BIAPWS will aim to continue to expand its membership with appropriate companies and institutions.

- BIAPWS will seek to find further ways of bringing awareness of the topics of steam and water, its scientific properties and its technical applications and challenges to a wider audience.
- BIAPWS will host the 2006 IAPWS International meeting in September 3 – 8th, in Oxfordshire, England.

Richard Harries
Chairman, BIAPWS.

The Czech National Committee
International Association for the Properties of Water and Steam
REPORT on IAPWS related activities – August 2004 / July 2005

Submitted to the EC Meeting of IAPWS, Santorini, Greece – July 2005.

National Committee Contacts:

CZ NC PWS - Institute of Thermomechanics, Dolejskova 5, 182 00 Prague 8, Czech Republic

Fax: + 420 2 858 4695, E-mails: secr.czncpws@it.cas.cz
Prof. R.Mareš, Fax: + 420 19 7429986, E-mail: maresr@kke.zcu.cz

Following Institutions participated in the research into the thermophysical properties and chemical processes:

Institute of Thermomechanics (IT) AS CR, Department of Thermodynamics, Dolejskova 5, CZ-182 00 Prague 8

Czech Technical University in Prague (CTU), Faculty of Mechanical Engineering, Department of Fluid Mechanics and Power Engineering, Technicka 4, CZ-166 07 Prague 6

Technical University Brno (TU), Faculty of Mechanical Engineering, Department of Thermomechanics and Nuclear Energetics, Technicka 2, CZ-616 69 Brno

Institute of Chemical Technology Prague (ICT), Power Engineering Department (ICT-IE) and Department of Physical Chemistry (ICT-IPC), Technicka 5, CZ-166 28 Prague 6

University of West Bohemia (UWB), Faculty of Mechanical Engineering, Department of Power System Engineering, Univerzitní 8, CZ-306 14 Plzen

Application Engineering, SKODA POWER, s.r.o., Tylova 57, CZ-316 00 Plzen

Nuclear Research Institute plc. (NRI), Rez, CZ-250 68 Rez

Technical University of Liberec (TUL), Department of Chemistry, CZ-461 19 Liberec.

SIGMA Research and Development Institute, J. Sigmunda 79, CZ-783 50 Lutín

Activities were sponsored by the Grant Agency of the Academy of Sciences, Grant Agency of the Czech Republic, SKODA POWER-Turbines, Plzen., Ministry of Education, Youth and Physical Training of the Czech Republic, and Ministry of Industry and Trade of the Czech Republic.

- Dr. Sifner (IT) prepared information about history of international cooperation in research of thermophysical properties of water and steam. Ref.[1] and an

information on “Formulations and Steam Tables“ for interested persons from industry (9 pgs).

- Mr. Klomfar issued Molliér $h - s$ diagram of water and steam based on IAPWS - IF97. Diagrams $p - h$, and $t - s$ are enclosed. Ref.[2]
- Prof. Mares (UWB) prepared an information about thermal conductivity of ordinary water. Ref.[3, 4].
- Prof. Mares (UWB) with collaborators prepared an information about surface tension of supercooled water. Ref.[5,6].
- Prof. Marsik (IT) with his research team carried out investigations into metastable state of water and steam, condensation, evaporation, and cavitation. Refs.[7 to 10].
- Prof. Sedlbauer (TUL) collaborated with Profs. Majer (France) and Wood (U.S.A.) and investigated thermodynamic properties of aqueous solutions, Refs. [11 to 16].
- Dr. Hruby (IT) performed tests in the shock tube for atmospheric nucleation studies, experimental studies of water/nonane droplet growth in pressurized methane, constructed an experimental apparatus for measurements of the surface tension in supercooled water, and developed theoretical model for thermodynamic bulk and surface properties of supercooled water. Refs. [17-19].
- The research activities at the CTU in Prague, Department of Fluid Mechanics and Power Engineering, Division of Power Engineering, have continued during the period 8/2004 – 7/2005 in the further improvement of current knowledge on the droplet nucleation in LP steam turbines:
 - ♦ Diagnostics of wet steam i.e. measurement of droplet size spectra and electrostatic charge of the droplets. The tests were carried out in the nozzle (C/D) and in the fossil (210 MW) and nuclear (1000 MW) LP steam turbines with combined optical extinction and charge probe. Refs. [20, 21].
 - ♦ Prediction of initial size and concentration of heterogeneous impurities that could participate in the droplet nucleation process in steam. The measurements were realized in the expansion chamber supplied both with laboratory and with power plant (210MW) steam. Ref. [22].
 - ♦ Improvement of computational model of the droplet nucleation in LP steam turbine employing both mentioned test data. Ref. [20].

Advanced thermal cycles of gas and steam turbines:

- ◆ Mathematical model and thermodynamic analysis of the GT cycle (simple and regenerative) with wet compression i.e. with compressor interstage water injection. Ref. [23].
- ◆ Thermodynamic analysis of evaporative GT cycle (EvGT). Ref. [24].
- ◆ Thermodynamic analysis of hydrogen direct – fired Rankine steam cycle with isothermal HP steam turbine. Ref. [25].

The analysis of all considered cycles suggests considerable increase in thermal efficiency and specific output, thus supporting further development of these promising advanced concepts. In connection with these studies the extension of moist air and steam properties is highly recommended up to (10MPa, 1000°C) and (50 MPa, 1800÷2000°C), respectively.

- In SIGMA Research and Development Institute two types of problems were studied during the last period:
 - ◆ Erosion effects of cavitation bubbles on the blades of water pumps. Ref. [7]. The erosion driving forces were evaluated for multiple collapses of wide spectrum of cavitation bubbles. The effects of flow rate fluctuations as well as the influence of blade surface changes on bubble collapses. Ref. [10].
 - ◆ The problem of head-drop and efficiency-drop of water pumps due to bubble cloud creation inside impeller passages have been studied using means of CFD and then compared with experimental data obtained in SIGMA Research and Development Institute Refs. [26, 27].
- Dr. Jiricek (ICT-IE) with collaborators investigated corrosion processes and chemical effects in water systems of power plants. ICT-IE organized the 5th International Power Cycle Conference (CHEO 5), September 1-3, 2004. Ref.[28 to 54].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles are under Refs [55 to 69].
- Prof. Stastny (SKODA ENERGO) with co-workers studied effects of deposits on the blades in LP part of steam turbine in fossil power plant by chemical analysis; measured degradation of steam turbine blade surfaces by deposits of chemicals; compared numerical models of the steam flow with heterogeneous condensation in nozzles with experiments, and tested numerical model of the steam flow in nozzles with binary nucleation. Refs [70 to 72].
- Zmitko (NRI) collaborated with the nuclear power plants mainly in the fields of water chemistry, corrosion problems and radiation control. Following activities were carried out :

- ◆ investigation of fuel rod cladding materials (e.g. Zircaloy-4 alloy, Zr-1%Nb alloy) corrosion behavior at specific VVER water chemistry conditions, Refs [73, 74]
- ◆ investigation of the effect of water chemistry on radionuclides transport and radioactivity build-up in the VVER reactor primary systems (e.g. effect of different levels of ammonia, hydrogen dosing), Ref. [75]
- ◆ investigation of the effect of water chemistry, stress level and irradiation on irradiation assisted stress corrosion cracking (IASCC) of reactor pressure vessel and in-core structures materials, Refs. [73 to 75]
- ◆ monitoring and evaluation of primary water chemistry and radiation situation at units 1 and 2 of the Temelín Nuclear Power Plant, Ref. [76]
- ◆ data processing technologies and system for diagnostics for water chemistry and corrosion control in Nuclear Power Plants (DAWAC), Ref. [77].

Young Scientists IAPWS Fellowships:

O. Mican submitted his Proposal for Young Scientist IAPWS Project “*Irreversible Thermodynamics of Fuel Cells Membrane Transport*” under supervising Prof.F.Marsik, and Prof.S.Lvov. The project is focused on four areas of interest in the advanced basic research:

- ◆ Preparation of a database of existing physical-chemical models describing transport and electrochemical processes, which occur in all components of MEA of PEM hydrogen/oxygen fuel cells.
- ◆ Formulation of an adequate physical-chemical model describing the influence of membrane material, including composite materials on the PEM fuel cell performance.
- ◆ Development of a computer program for numerical simulations of the model and investigation of the model behavior in a series of simulations.
- ◆ Comparison of the results of numerical simulations with available experimental results and possibly improve the original model, so that it will yield a better agreement with the experiment.

The CZ NC PWS fully recommends this project to the EC IAPWS to support it. The proposal with attached Curriculum Vitae of Mr.O.Mican is in Appendix 1.

• Nomination for 2005 Honorary Fellow of the IAPWS

The US NC IAPWS, CZ NC PWS, and Mr. Ingo Weber collaborated in preparation of the proposal to nomination Dr. Bert Rukes for 2005 Honorary Fellow of the IAPWS.

References:

- [1] Sifner O.: *75 Years of International Cooperation in Research and Standardization of Thermophysical Properties of Water and Steam*, pp. 757-

764. In : *Water, Steam, and Aqueous Solutions for Electric Power*, Advances in Science and Technology, Proceedings of the 14th ICPWS, MARUZEN Co.,Ltd., Kyoto, 2004
- [2] Klomfar J.: *Molliér h-s diagram of water and steam*, Academia, Prague, 2005
- [3] Mares R., Konas P.: *Thermal Conductivity of Ordinary Water Substance in the Ideal-Gas Limit*, pp. 128-131. In : *Water, Steam, and Aqueous Solutions for Electric Power*, Advances in Science and Technology, Proceedings of the 14th ICPWS, MARUZEN Co.,Ltd., Kyoto, 2004
- [4] Konas P., Mares R.: *Thermal Conductivity of Ordinary Water Substance - High Pressure Region*. In : *Proceedings Power System Engineering - 2005*, Pilsen, 2005 (in Czech)
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- [6] Knourek J., Mares R.: *Water Film Separator*. In : *Proceedings Power System Engineering - 2005*, Pilsen, 2005 (in Czech)
- [7] Zima, P., M., Sedlar, M., Marsik, F.: *Bubble Creation in Water with Dissolved Gas: Prediction of Regions Endangered by Cavitation Erosion*, pp. 232-235. In : *Water, Steam, and Aqueous Solutions for Electric Power*, Advances in Science and Technology, Proceedings of the 14th ICPWS, MARUZEN Co.,Ltd., Kyoto, 2004
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German National Committee to IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam Report "Research in Progress 2005"

1. Supplementary backward equations $p(h,s)$ for regions 1 and 2 of IAPWS-IF97
 - The comprehensive article on the backward equations $p(h,s)$ will appear in the "Journal of Engineering for Gas Turbines and Power" in 2005.
2. Supplementary backward equations $T(p,h)$, $v(p,h)$, and $T(p,s)$, $v(p,s)$ for region 3 of IAPWS-IF97
 - The comprehensive article on the backward and boundary equations was prepared and submitted to the "Journal of Engineering for Gas Turbines and Power".
3. Supplementary backward and boundary equations $p(h,s)$ for region 3 of IAPWS-IF97
 - The comprehensive article on the backward and boundary equations for the "Journal of Engineering for Gas Turbines and Power" is being prepared.
4. Supplementary backward equations $v(p,T)$ for region 3 of IAPWS-IF97
 - The evaluation of the "Supplementary Release on Backward Equations for Specific Volume as a Function of Pressure and Temperature $v(p,T)$ for region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was supported.
5. Thermodynamic differential quotients of the Scientific Formulation IAPWS-95 and the Industrial Formulation IAPWS-IF97 for Water and Steam
 - The Proposal for a guideline was prepared.
6. Investigations on thermodynamic properties of humid air - part of the project "Advanced Adiabatic Compressed Air Energy Storage" (AA-CAES) of the European Union
 - The property data base for humid air was completed.
 - Comparison calculations of different models for calculating thermodynamic properties of humid air were carried out.
7. Property libraries for water and steam, humid gases, and aqueous mixtures
 - The property library LibWaLi for water/lithium bromide mixtures was developed.
 - The Add-Ins
 FluidEXL for Excel®
 FluidMAT for Mathcad®
 were extended .
8. Implementation of the industrial formulation IAPWS-IF97 on pocket calculators
 - The program FluidTI for the model TI 84 of Texas Instruments was prepared.

**The Hellenic National Committee
International Association for the Properties of Water and Steam**

REPORT on IAPWS related activities

On the 15th of June 2005, the Greek National IAPWS Committee (GIAPWS) was officially formed by the Hellenic Association of Chemical Engineers, as

Head	Prof. Marc J. Assael	Chemical Engineering Department Aristotle University of Thessaloniki (assael@auth.gr)
Members	Mr Nikos Karnabos	Hellenic Petroleum SA
	Mrs Argyro Kastanaki	Head of Environmental & Chemical Technology Department Division of Power Generation Exploitation Public Power Corporation (rkastan@otenet.gr)
	Mr Panagiotis Tsiambas	Head of Environmental & Chemical Technology Department Megapolis S.E.S., Public Power Corporation (pitsiamp@aias.gr)
	Mr Dimitris Sotiropoulos	Head of Environmental & Chemical Technology Department Agios Dimitrios S.E.S., Public Power Corporation

The first task of GIAPWS was the organization of the Seminar "Applied Water Treatment Processes for Power Plant Cycles" which successfully took place in the 2005 IAPWS Meeting, July 3-8, in Santorini island.

The Head of GIAPWS was responsible for the organization of the 2005 July 3 - 8 IAPWS Meeting in Santorini island in Greece.

Research carried out by GIAPWS during this year, involved

- the completion of the new Viscosity correlation for water. The correlation will be submitted for approval and send to the evaluation group.
- At the same time work for a new correlation for the Thermal Conductivity of water started.

Work on the Chapters of Viscosity and Thermal Conductivity of Aqueous Solutions at high Temperatures and High Pressures has progressed (book edited by V. Valyashko)

The www site of GIAPWS will soon be available in the internet.

It is expected that with the involvement of Greek Public Power Corporation, new areas of research will be activated.

Current Status of Research Activities in Japan
Submitted to the Executive Committee Meeting, IAPWS, Santorini, Greece, July
2005

by

Japanese National Committee
 International Association for the Properties of Water and Steam
 c/o The 139th Committee on Steam Properties
 Japan Society for the Promotion of Science (JSPS)
 6, Ichiban-cho, Chiyoda-ku
 Tokyo 102-8471, Japan

The Japanese National Committee to the IAPWS is playing an active function as the 139th Committee on Steam Properties chaired by Professor Koichi Watanabe, Keio University, at the Japan Society for the Promotion of Science (JSPS), Tokyo. The Committee is pleased to report that the 14th ICPWS held in Kyoto from August 29 through September 3, 2004 was a great success with 267 participants from 19 countries. The Proceedings of the 14th ICPWS, entitled “Water, Steam, and Aqueous Solutions for Electric Power” (Editors: Masaru Nakahara, Nobuyuki Matsumayasi, Masakatsu Ueno, Kenji Yasuoka and Koichi Watanabe, ISBN4-621-07596-9, 770 pp with CD-ROM) was published from Maruzen Publishing, Co., Ltd., Tokyo in March, 2005. Those who wish to purchase any extra copies of the Proceedings are kindly requested to contact Dr. Kenji Yasuoka, one of the editors and the Secretary of the Japanese National Committee for the IAPWS (Assoc. Prof. Kenji Yasuoka, Dept. of Mechanical Engineering, Keio University, 3-14-1, Hiyoshi, Yokohama 223-8522, Japan; phone: +81-45-566-1523, fax: +81-45-566-1495, e-mail: yasuoka@mech.keio.ac.jp). It should be noted that full papers included in the Proceedings of the 14th ICPWS are now downloadable by accessing to the home page of our National Committee (<http://www.iapws.jp>).

The following research projects on the thermophysical and physical-chemical properties of water substances including various aqueous systems of technological importance are currently in progress at several universities and institutions in Japan.

At the Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo, Prof. S. IKAWA and coworkers are engaged in spectroscopic measurements of water and water-hydrocarbon mixtures at high temperatures and pressures. From near-infrared and ultraviolet measurements of water-benzene mixtures in the 373-673 K and 50-400 bar ranges, mutual solubilities were obtained. It has been found that the solubility of benzene in water is an order of magnitude smaller than that of water in benzene throughout the two-phase region, and the effect of pressure on solubilities is opposite between water in benzene and benzene in water. These solubility properties were discussed on the basis of a cavity-based solvation model [*J. Chem. Phys.*, **122**, 024509 (2005)]. In collaboration with Drs. VIGASIN and PAVLYUCHKO, analyses of infrared and near-infrared band shapes of steam at high temperatures and pressures were performed and a state of molecular aggregation in the steam was discussed [*J. Mol. Struct.*, **742**, 173 (2005)].
 [contact: Prof. S. Ikawa; E-mail: sikawa@sci.hokudai.ac.jp].

Prof. S. UCHIDA, who promoted a second phase of the project on water chemistry of BWR at the Department of Quantum Science and Energy Engineering, Graduate School of Engineering, Tohoku University, Sendai, has moved from Tohoku University to Japan Atomic Energy research Institute. The

effects of hydrogen peroxide on corrosion and IGSCC of stainless steel in high temperature pure water have been examined by using the high temperature high pressure hydrogen peroxide water loops with controlled hydrogen peroxide concentrations and lower possible oxygen concentrations at JAERI. By changing concentrations of H_2O_2 and O_2 , in situ measurements of electrochemical corrosion potential (ECP) and frequency dependent complex impedance (FDCI) of test specimens were carried out and then characteristics of oxide film on the specimens were determined by multilateral surface analyses, i.e., laser Raman spectroscopy (LRS), scanning electron microscope (SEM-EDX), secondary ion mass spectroscopy (SIMS), and scanning transmission electron microscope (STEM-EDX) (XPS). As a result of experiments, the following points were confirmed. 1) The ECP and FDCI data of the specimens exposed to 100 ppb H_2O_2 were not affected by co-existing O_2 with the same level oxidant concentration and they were also not affected by pre-exposure to 200 ppb O_2 . From the viewpoint of ECP, this meant that corrosive conditions of hydrogen water chemistry were the same as those of normal water chemistry. 2) Combination of ECP and FDCI sensors might be a hopeful candidate to determine the corrosive conditions in the BWR primary coolant at elevated temperature.

3) The hematite ratio in the oxide films of the specimens exposed to H_2O_2 was expressed as a logarithmic function of $[\text{H}_2\text{O}_2]$. The hematite ratio was measurable for 8 ppm O_2 , but negligibly small for 200 ppb O_2 . 4) H_2O_2 exposure led to thicker oxide layers than O_2 exposure and Cr depletion did. The oxide film thickness first increased as $[\text{H}_2\text{O}_2]$ decreased from 100 ppb to 10 ppb and then it decreased. [Latest publication: (1) N. Yamashiro, et al., *J. Nucl. Sci. Technol.*, **41**, (2004), 890-897, (2) S. Uchida, et al., *J. Nucl. Sci. Technol.*, **41**, (2004), 898-906, (3) J. Sugama, et al., *J. Nucl. Sci. Technol.*, **41**, (2004), 880-889, (4) S. Uchida, et al., *J. Nucl. Sci. Technol.*, **41**, (2005), 66-74 (5) T. Miyazawa, et al., *J. Nucl. Sci. Technol.*, **41**, (2005), 233-241, (6) S. Uchida, et al., *Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology*, 551, Maruzen Co. Ltd. (2005), (7) T. Satoh, et al., *Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology*, 561, Maruzen Co. Ltd. (2005)]

At the Graduate School of Environmental Studies, Tohoku University, Sendai, Profs. N. YAMASAKI, H. ENOMOTO, K. TOHJI, H. ISHIDA, N. TSUCHIYA, and their group are covering wide field related to hydrothermal Material Science, Geofluid Science (Earth Science). Material research group developed several kinds of advanced and functional materials such as synthetic diamond, stratified materials on carbon nano-tube using hydrothermal process (Y. Sato et al., *Chemical Physics Letters*, **385**, (2004), 323-328), and the liquefaction and gasification of heavy oil, the SCWO of rice husk for production of sodium acetate (ICPWS, (2004), 85, 186), the separation and extraction of useful materials from biomass using superheated steam, and the formation of organic materials by the hydrothermal reduction of carbon dioxide (N. Yamasaki et al., *Material Science Letters*, **58**, (2004), 768-771). Geofluid science research group is conducting water-rock interaction under sub- and supercritical condition, including multi-phase and multi-component solutions. (G. Bignall et al., *GEOTHERMICS*, **33**, (2004), 615-635), (Sekine et al., *GEOTHERMICS*, **33**, (2004), 775-793). They organized 1st and 2nd international workshop on WATER DYNAMICS (1st workshop: 17-19th March 2004, 2nd workshop: 11-12th November, 2004), which focused on the role of water in Earth processes, Life science and Material design. The workshop was unique objectives covering very wide range of water and steam properties and utilization. They are planning 3rd workshop of WATER DYNAMICS in 16-17th November 2005 in Sendai International Center. They can provide 1st and 2nd workshop proceedings, please contact N. Tsuchiya (chair of program committee of WATER DYNAMICS) [contact Prof. N. Tsuchiya; tsuchiya@mail.kankyo.tohoku.ac.jp]

At the Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Prof. T. ADSCHIRI and his group are developing a new hybrid nanomaterial from organic, inorganic and bio materials at various reaction conditions. For organic/inorganic nanomaterials, the supercritical hydrothermal synthesis of nanoparticles they invented is advanced, so that metal oxide nanoparticles with a organic monolayer is synthesized in a homogeneous phase of hydrophilic and hydrophobic fluids under the sub/supercritical condition (Tahereh et al. submitted). Hydrophilic or hydrophobic nature of the nanoparticles can be controlled by the organic modification on the surface of the particles, which paves a way to various applications of nanoparticles for materials, electronics, and life science. At room temperature, his group has synthesized ZnO nanoparticles using a peptide with affinity for ZnO (Umetsu et al. submitted). To our knowledge, there have been no reports for room-temperature

synthesis of ZnO nanoparticles. The peptide can also assist in the homogeneous assembly of the ZnO nanoparticles into unique flower-like morphologies. Adschiri's group shows the potential of peptide for fabrication of unique structure. The techniques of patterning and synthesizing ZnO at room temperature are potentially useful for the orientation of ZnO in or on heat-labile or pH-sensitive organic compounds. [contact: Prof. T. Adschiri; e-mail: ajiri@tagen.tohoku.ac.jp]

At the Material Properties and Metrological Statistics Division, National Metrology Institute of Japan (NMIJ, formerly NRLM), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, a section lead by Dr. K. FUJII is working on the density and viscosity standards. Absolute density measurements of silicon crystals for a determination of the Avogadro constant by the X-ray crystal density (XRCD) method are being conducted in this section as an international project organized by the Comité International des Poids et Mesures (CIPM). This project is scheduled to continue through 2004 to 2010 with participants of eight National Metrology Institutes (BIPM, CSIRO, IMGC, IRMM, NIST, NMIJ, NPL, and PTB). The target of this project is to replace the present definition of the kilogram with a new definition based on the Avogadro constant. Most recent situation of this project is given in a paper [K. Fujii, A. Waseda, N. Kuramoto, S. Mizushima, P. Becker, H. Bettin, A. Nicolaus, U. Kuetgens, S. Valkiers, P. Taylor, P. De Bièvre, G. Mana, E. Massa, R. Matyi, E. G. Kessler, Jr., and M. Hanke, "Present state of the Avogadro constant determination from silicon crystals with natural isotopic compositions," *IEEE Trans. Instrum. Meas.*, 2005, 54, 854-859]. The data from the NMIJ and PTB were used for finding the best set of fundamental physical constants most recently recommended by the CODATA Task Group on Fundamental Constants. Using the silicon crystals as a density standard, densities of standard liquids are calibrated by a magnetic suspension density meter developed at the NMIJ [N. Kuramoto, K. Fujii, and A. Waseda, "Accurate density measurements of reference liquids by a magnetic suspension balance," *Metrologia*, 2004, 41, S84-S94]. A relative standard uncertainty of 4×10^{-6} has been achieved in the density measurement of organic liquids used for calibrating the vibrating-tube densimeters. A review article on the density standards is given in a paper [K. Fujii, "Present state of the solid and liquid density standards," *Metrologia*, 2004, 41, S1-S15]. In his group a new absolute viscosity measurement by the falling ball method is in progress. Nano-technologies for measuring the falling distance and diameters of small silicon spheres are developed for providing reference data of transport properties of liquid water with a relative standard uncertainty of 0.01 % [Y. Fujita, N. Kuramoto, Y. Kurano, and K. Fujii, "A new project at NMIJ for an absolute measurement of the viscosity by the falling ball method," *Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology*, 112, Maruzen Co. Ltd. (2005)]. Dr. K. FUJII is working as a chairman of the WG-Density, CCM (Consultative Committee for Mass and Related Quantities) to organize the research activities on the density standards at the National Metrology Institutes. A new density-of-water table having a specified isotopic abundance was recommended by the WG-Density and endorsed by the CCM and CIPM [M. Tanaka, G. Gerard, R. Davis, A. Peuto, and N. Bignel, "Recommended table for the density of water between 0 °C and 40 °C based on recent experimental reports," *Metrologia*, 2001, 38, 301-309]. This new table is recommended as a metrological standard for the density of SMOW. In April 2005, WG-density and CCM meetings were held at the BIPM (Bureau International des Poids et Mesures), where the CCM and IAPWS standards for the density of water were discussed for clarifying their roles, and publishing the clarification in a form of cooperation with the IAPWS was agreed and approved at the meetings. [contact: Dr. K. Fujii, Chief, Fluid Properties Section, NMIJ; E-mail: fujii.kenichi@aist.go.jp].

At the Dept. of Environmental Science & Technology, Faculty of Engineering, Shinshu University, Nagano City, Prof. H. TAKAKU works since Feb. of 2000, and previously worked at Central Research Institute of Electric Power Industry (CRIEPI) in Japan. In the simulated geothermal waters containing the corrosive chemicals such as chlorides, sulfides and others, he and coworkers are studying the corrosion of the steam turbine materials for geothermal power plants and also the corrosion of the Ti-Ni base shape memory alloys for the heat engine actuators. They are also studying on the corrosion behavior of materials for the heat exchanger, and boiler and steam turbine of conventional fossil power plants. [Latest publications: [1] M. Kurashina, H. Takaku, et al, On-line Analysis of ETA and Organic Acids in Secondary Systems of PWR Plants, *Power Plant Chemistry*, 7 (4), p.219, 2005. [2] M. Hirano, H. Takaku, et al, Accelerated Corrosion Behavior due to Alternating Dry-Wet Conditions for LP Steam Turbine Materials of Fossil Power Plants, *ISIJ International*, 45 (3), p.373, 2005. [3] M. Hirano, H. Takaku, et al,

Corrosion Behavior of Boiler Materials during Long-Term Lay-up of a Fossil Unit, *Power Plant Chemistry*, 7 (1), p.16, 2005. [4] H. Takaku, Y. Sakai, et al, Corrosion Behavior of Steam Turbine Materials for Geothermal Power Plants, *Proc. of the 14th International Conference on the Properties of Water and Steam*, p.718, 2004] [Contact: Prof. H. Takaku; E-mail: takakuh@gipwc.shinshu-u.ac.jp]

Mr. K. MIYAGAWA investigated the computing time of equations of the industrial formulation IAPWS-IF97 in the Release and Supplementary Releases adopted one after another from 1997 to 2005. The computing times of each release had been tested on the latest computing platforms at those times. The aim of the investigation was to compare them on the common and state-of-the-art platforms. The test results showed that the today's platforms were more favorable for IAPWS-IF97 than for the previous industrial formulation IFC-67. Test results also showed that the "backward" equations of IAPWS-IF97 were much faster than those of iterative processes to solve inverse equations. The results will be presented at the IAPWS annual meeting in 2005. [contact: Mr. K. Miyagawa; E-mail: miyagawa.kiyoshi@nifty.com]

At the Department of Mechanical Sciences and Engineering, Tokyo Institute of Technology, Tokyo, Prof. A. SAITO, Assoc. Prof. S. OKAWA and their group are studying the effect of various properties of solid surface on nucleation of supercooled water using Molecular Dynamics Method, [See Int. J. of Refrigeration to be published and 14th Int. Conf. on the Properties of Water and Steam, Aug. 29 - Sep. 3, 690-695, (2004).]. They are also studying the effect of loading on fluid permeability and porosity of ice/water mixture, [See IIR Int. Conf. Vicenza (Italy) 2005 to be presented] and the effects of shapes of electrodes on freezing of supercooled water in electric freeze control [See Int. J. of Refrigeration, 28, 389-395, (2005)]. [contact: Dr. S. Okawa; E-mail: sokawa@mech.titech.ac.jp]

At Materials Science Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Kanagawa, Dr. M. DOMAE and his coworkers studies *in situ* Raman spectroscopy, in order to understand corrosion of metals and steels in high temperature water up to 673 K. In air-saturated water at 673 K and 25 MPa, a unique Raman spectrum was observed for a pure titanium sample. They started immersion tests in high temperature water, using metals and steels on which corrosion-resistant metal oxides were coated. [contact: Dr. M. Domae; E-mail: domae@criepi.denken.or.jp]

At the Center for Multiscale Mechanics and Mechanical Systems, Keio University, Yokohama, Prof. M. UEMATSU and his group are measuring the PVT properties of aqueous ammonia mixtures in the range of temperatures from 350 K to 650 K at pressures to 200 MPa. Isobaric specific heat capacities of water + methanol mixtures are being measured for temperatures from 250 K to 400 K at pressures to 20 MPa. The calorimeter was reported at the 14th ICPWS held in Kyoto, 2004. [contact: Prof. M Uematsu; E-mail: uematsu@mech.keio.ac.jp].

At the Department of Mechanical Engineering, Keio University, Yokohama, Dr. K. YASUOKA and his group are studying the molecular dynamics (MD) simulation to clarify the thermodynamic stability of structure-H clathrate hydrate by estimating the free energy difference. [Y. Okano and K. Yasuoka, Proceeding of the Fifth International Conference on Gas Hydrates (ICGH 2005), Trondheim, Norway, June 2005.] They adopt the MD simulation for the adsorption and desorption of ethanol molecules to liquid-vapor water surface. They reported the supercritical phenomena on the 2D of liquid-vapor water surface. [Y. Andoh and K. Yasuoka, Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology, 144, Maruzen Co. Ltd. (2005)] They also evaluated the water model contained in HIV-1 Protease. [T. Aramaki et al., Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology, 208, Maruzen Co. Ltd. (2005)] They estimated the nucleation rate, critical nucleus, and formation free energy for the bubble nucleation process of water. They reported the phenomena of "Nanoscale Hydrophobic Interaction and Nanobubble Nucleation". [T. Koishi et al., *Phys. Rev. Lett*, **93**, 185701 (2004).] [contact: Dr. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.jp].

At the Department of Mechanical Engineering, Kanagawa Institute of Technology, Atsugi, Prof. K. OGUCHI and his group are continuing to measure the PVT_x properties of ammonia + water mixtures. They have measured the PVT_x properties of aqueous dilute solutions of ammonia in the range of temperatures from 265 K to 305 K, pressures up to 16 MPa, densities from 975 kg m^{-3} to 989 kg m^{-3} , and compositions up to 0.10 mole fraction of ammonia including pure water, focusing their attentions on the maximum density phenomena, and also in the range of temperatures from 298 K to 309 K, pressures up to 15.6 MPa, densities from 810 kg m^{-3} to 823 kg m^{-3} , and compositions up to 0.5133 mole fraction and 0.5357 mole fraction of ammonia. Some of their results were presented at the 14th ICPWS. [contact: Prof. K. Oguchi; E-mail: oguchi@kait.jp].

At the Department of Mechanical Systems Engineering, National Defense Academy, Yokosuka, Prof. N. KAGAWA and his group have constructed a twin-cell type adiabatic calorimeter for water + alcohol mixtures. Isochoric heat capacities (c_v) of water, methanol, ethanol, 1-propanol and their aqueous solutions were measured for temperatures from 280 to 420 K and pressures to 30 MPa. Liquid density information was also obtained on the basis of the sample mass and the volume of the calorimetric cell. The experimental results and a theoretical approach to the anomalous behavior of c_v data for the water + alcohol mixtures were presented at the 14th ICPWS. [H. Kitajima, N. Kagawa, and H. Endo, Water, Steam, and Aqueous Solutions for Electric Power -Advanced in Science and Technology-, 107-111 (2005)] [contact: Prof. N. Kagawa; E-mail kagawa@nda.ac.jp]

At the Department of Computational Molecular Science, Institute for Molecular Science, Prof. S. OKAZAKI and his group study quantum-classical molecular dynamics calculation for vibrational relaxation of solute in supercritical fluid of non-polar molecule and in supercritical water. They are interested in understanding relaxation mechanism in the supercritical fluids in terms of the isolated binary collision model popularly used to describe the relaxation in gas phase. [see: M. Sato and S. Okazaki, J. Chem. Phys., (2005), in press and M. Sato and S. Okazaki, J. Chem. Phys., (2005), in press]. [contact: Prof. S. Okazaki; E-mail: okazaki@ims.ac.jp].

At the Department of Applied Chemistry, Ritsumeikan University, Shiga, Prof. S. SAWAMURA studies the solubility of hydrophobic compounds and amino acids under high pressure up to 400 MPa and the viscosity of H_2O and D_2O in the high-pressure and low-temperature region. [See: Seiji Sawamura, AIP Conf. Proc. (Amer. Inst. Phys.) 716, 175-182 (2004)]. At the same department, Prof. Y. TANIGUCHI and Prof. M. KATO are measuring the infrared, Raman, and NMR spectra for biological compounds at high pressures. (contact: Prof. Sawamura, S.; sawamura@se.ritsumei.ac.jp).

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their coworkers study the structure, dynamics, and reactions in super- and subcritical water by means of multinuclear NMR (nuclear magnetic resonance) spectroscopy, computer simulation, and Raman spectroscopy. Their current focus are (1) the thermodynamics, structure, and dynamics of aqueous solutions over a wide range of thermodynamic conditions [“A quantum chemical approach to the free energy calculations in condensed systems: The QM/MM method combined with the theory of energy representation”, H. Takahashi, N. Matubayasi, M. Nakahara, and T. Nitta, *J. Chem. Phys.* **121**, 3989-3999 (2004)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions. [“NMR Spectroscopic Evidence for an Intermediate of Formic Acid in the Water-Gas-Shift Reaction”, K. Yoshida, C. Wakai, N. Matubayasi, and M. Nakahara, *J. Phys. Chem. A* **108**, 7479-7482 (2004)]. [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp]

At the Department of Molecular Science and Technology, Doshisha University, Kyo-Tanabe, Kyoto, Prof. M. UENO, Prof. IBUKI and their group have studied the electric conductivities of KBr and KI in liquid methanol along the liquid-vapor coexistence curve up to the critical temperature to examine the validity of the Hubbard-Onsager dielectric friction theory. The translational friction coefficients ζ of the halide ions (Cl^- , Br^- , I^-) in methanol were well reproduced by the HO theory at the density $\rho > 2.0\rho_c$, where $\rho_c = 0.2756 \text{ g cm}^{-3}$ is the critical density of methanol, compared with those in water [T. Hoshina, K. Tanaka, N. Tsuchihashi, K. Ibuki, and M. Ueno, *J. Chem. Phys.*, **121**, 9517-9525 (2004)]. They have also measured the NMR spin-lattice relaxation times of ^2H of the deuterated solvents (CDCl_3 , C_6D_6 , and C_6D_{12})

at various temperatures under atmospheric pressure, and determined the NMR B coefficients of the solutes (Me_4Si , Et_4Si , Pr_4Sn , Bu_4Sn , and Pen_4Sn) to study the solvent motions in dilute nonaqueous solutions. It has been found that the local effect on the rotation of solvent molecules in nonaqueous nonelectrolyte solutions is much smaller than that in aqueous solutions [K. Yoshida, N. Tsuchihashi, K. Ibuki, and M. Ueno, *J. Mol. Liq.*, **119**, 67-75 (2005)]. Theories for diffusion-controlled reaction dynamics based on the diffusion equation and the Fokker-Planck-Kramers equation have also been reviewed, and the validity of the theories has been examined in the picosecond time region by comparing them with computer simulations in liquid Ar [K. Ibuki and M. Ueno, *Rev. High Press. Sci. Tech.*, **14**, 20-29 (2004)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At the Thermofluid Physics Laboratory, Department of Mechanical Engineering Science, Kyushu University, Fukuoka, Prof. Emeritus T. ITO and Prof. Y. TAKATA have released the 12.1 version of the Computer Program Package for Thermophysical Properties of Fluids, PROPATH. Its new version is now under development and will be released new future. This software consists of 5 subsets. Four programs for light water substances with different formulations and for heavy water substance are available. By using E-PROPATH, one of 5 subsets, one can calculate properties as functions of MS-EXCEL software. [contact: Prof. Y. Takata; E-mail: takata@mech.kyushu-u.ac.jp or <http://gibbs.mech.kyushu-u.ac.jp/propath/index.html>]

At Toshiba Corporation, Isogo Engineering Center, Dr. NARABAYASHI and his coworkers are developing steam injector (SI) system with Dr. MORI and Dr. OHMORI, R&D Center, Tokyo Electric Power Company. SI is a simple, compact and passive pump and also acts as a high-performance direct-contact compact heater. This provides SI with capability to serve also as a direct-contact feedwater heater that heats up feedwater by using extracted steam from the turbine. To develop high performance compact feedwater heater, it is necessary to quantify the characteristics between physical properties of the flow field. Its performance depends on the phenomena of steam condensation onto the water jet surface and heat transfer in the water jet due to turbulence on to the phase-interface. The analysis was conducted by using CFD code embedded separate two-phase flow models and confirmed that the steam has a high-performance direct-contact heater that was suitable for compact feedwater heater. As it is compact equipment, SI is expected to bring about great simplification and materials-saving effects, while its simple structure ensures high reliability of its operation, thereby greatly contributing to the simplification of the power plant by replacing all low-pressure feedwater heaters with the four-stage SI system, having steam extraction pressures equal to those for the existing ABWR system. In a recent paper, development of SI system for simplified nuclear power plant has been reported [13th International Conference on Nuclear Engineering, May 16-20, 2005, Beijing, China] and it was awarded by JSME (Japanese Society of Mechanical Engineering). [Contact: Dr. Narabayashi, tadashi.narabayashi@toshiba.co.jp]

Report of Russian National Committee (2004-2005)

List of Publications

1. L.G. Vasina, V.L. Menshikova, L.s. Krylova, and A.V.Evsyutin, "Effect of Coagulant Base Index and Water Stability in Selection of Optimum Coagulation Mode," Proceedings of the International Conference on Water Treatment "Tekhnovod-2004", Novocherkassk, Russia, 2004, pp. 136-140.
2. A.V. Boglovsky, Yu.V. Balaban-Irmenin, L.G. Vasina, and A.M. Rubashov, "Regularities of Scale Formation in Hot Water Equipment of Heat Supply Systems," Energoberezhenie i Vodopodgotovka, 2004, No. 3, pp. 10-16.
3. A.S. Sedlov, A.V. Boglovsky, K.A. Dunin, and A.A. Zonov, "Corrosion of Steel at Operating Conditions of Evaporation Units," Energoberezhenie i Vodopodgotovka, 2004, No. 1, pp. 86-88.
4. T.I. Petrova and A.V. Furunzhieva, "Use of Helamin and Fossil Power Plants with Drum-Type Boilers," Energoberezhenie i Vodopodgotovka, 2004, No. 1, pp. 3-9.
5. T.I. Petrova, S. Vidojkovic, A.A. Zonov, and A.Y. Petrov, "Effect of Acetic Acid on the Contamination of Saturated Steam by Sulfates and Fluorides," Thermal Engineering, 2004, vol. 51, No. 7, pp. 526-529.
6. D.S. Smetanin, "Evaluation of Water Chemistry Condition at Power Plants with Water Chemistry Quality Index," Novoye v Elektroenergetike, 2004, No. 12.
7. T.I. Petrova, O.A. Povarov, V.N. Semenov, V.I. Kashinsky, A.N. Troitsky, A.Y. Petrov, R.B. Dooley, "Effect of Cycle Chemistry on Corrosion Processes in Steam Turbines," Paper presented at the 14th ICPWS, August 29 – September 03, 2004, Kyoto, Japan.
8. T.I. Petrova and A.V. Furunzhieva, "The Influence of Acetic Acid on Mass Transfer of Copper Corrosion Products in Power Plant Cycle," Paper presented at the 14th ICPWS, August 29 – September 03, 2004, Kyoto, Japan.

U.S. National Committee to IAPWS 2005 Report on Activities of Potential Interest to IAPWS

Communicated from Arizona State University, Tempe, AZ:

- Group concentrated its efforts on evaluation of properties of aqueous organic compounds at 298 K, 0.1 MPa and on development of predictive group contribution schemes. This information is expected to be important for many applications dealing with organic compounds in water, so it may be of interest for IAPWS as well. One of the recent projects concerns the development of methods to estimate activity coefficients of organic compounds in water at room temperatures in the framework of the Savage-Wood model. Several publications, including Plyasunov A.V. and Shock, E.L. Prediction of the Krichevskii parameter for volatile nonelectrolytes in water. *Fluid Phase Equil.*, **222-223C**, 19 (2004)

Communicated from The Pennsylvania State University, University Park, PA:

- *High Temperature Thermodynamics of Aqueous Solutions*
 1. Bandura A. V., and Lvov S.N. The Ionization Constant of Water over Wide Ranges of Temperature and Density, *J. Phys. Chem. Ref. Data*, **34**, 2005, (in press).
- *High Temperature Aqueous Electrochemistry*
 1. Lvov S.N. and Palmer D.A., Electrochemical Studies of High-Temperature Aqueous Systems, Chapter 11, in "*The Physical and Chemical Properties of Aqueous Systems at Elevated Temperatures and Pressures: Water, Steam and Hydrothermal Solutions*" (D.A. Palmer, R. Fernandez-Prini and A.H. Harvey, Eds.), 2004, Wiley, p. 377-408.
 2. Zhou Z.-F., Lvov S.N., Thakur S., Zhou X., Chou P., and Pathania R. Hydrothermal Deposition of Zirconia Coating on BWR Materials for IGSCC Protection. In Proceedings of "International Water Chemistry Conference", San Francisco, October 2004, p. 602-624.
 3. Lvov S.N., Zhou X.Y., Ulyanov S.M., Zhou Z.F., Papangelakis V.G., and Jankovic Z.D. In-situ pH Monitoring of High Concentration Acidified Geothermal Brines and Acidic Sulphate Solutions at Elevated Temperatures, In Proceedings of The Pressure Hydrometallurgy 2004 Conference, Canadian Institute of Mining, Montréal, Quebec, 2004, p. 561-576.
 4. Lvov S.N. Electrochemistry of High Temperature Subcritical and Supercritical Aqueous Systems, Volume 5 (D.D. Macdonald, Vol. Ed.), in "*Encyclopedia of Electrochemistry*" (M. Stratmann and A. Bard, Eds.), 2005, Wiley-VCH, (in press).
- *High Temperature Electrokinetic Studies of Solid Oxide/Water Interface*
 1. Zhang Z., Fenter P., Cheng L., Sturchio N. C., Bedzyk M. J., Predota M., Bandura A., Kubicki J. D., Lvov S.N., Cummings P.T., Chialvo A.A., Ridley M.K., Benezeth, P., Anovitz L, Palmer D.A., Machesky M.L., and Wesolowski D.J. Ion Adsorption at the Rutile-Water Interface: Linking Molecular and Macroscopic Properties, *Langmuir*, **20**, 2004, 4954-4969.
- *Elevated Temperature Proton Exchange Membrane Fuel Cells*

1. Chalkova E., Pague M.B., Fedkin M.V., Wesolowski D.J., and Lvov S.N., Nafion/TiO₂ Proton Conductive Composite Membranes for PEM Fuel Cells Operating at Elevated Temperature and Reduced Relative Humidity, *J. Electrochem. Soc.*, (2005, in press).
 2. Chalkova E., Fedkin M. V., Wesolowski D. J., and Lvov S.L. Effect of TiO₂ Surface Properties on Performance of Nafion-Based Composite Membranes in High Temperature and Low Relative Humidity PEM Fuel Cells, *J. Electrochem. Soc.*, (2004, in press).
 3. Lvov S.N., Fedkin M.V., Chalkova E., Jayabalan D.K., and Wesolowski D.J. Surface Chemistry of Solid Oxides for Developing High Temperature Proton Exchange Membranes, In: The 204th ECS Meeting Proceedings, Orlando, Florida, ECS, (2005, in press).
- *High Temperature Solid Oxide Fuel Cells*
1. Zhou Z.F., Gallo C., Pague M.B., Schobert H., and Lvov S.N., Direct Oxidation of Jet Fuels and Pennsylvania Crude Oil in a Solid Oxide Fuel Cell, *Journal of Power Sources*, **133**, 2004, 181-187.

Communicated from the National Institute of Standards and Technology, Boulder, CO:

- Under IAPWS support, Mr. Magomed Aliev, a PhD candidate in Physics from the Dagestan Scientific Center (Russian Academy of Sciences) visited NIST (Boulder) as a Guest Researcher from October to December, 2004 to work with Drs. Joseph Magee and Ilmutdin Abdulagatov on the project "An Experimental Study of *PVTx* Properties for the System Ammonia + Water at High Temperatures and Pressures." A separate report has been furnished.
- The collaboration of the Thermophysical Division of the Dagestan Scientific Center (Russian Academy of Sciences) and the Experimental Properties of Fluids Group of the Physical and Chemical Properties Division of NIST continues to thrive. In the past year, manuscripts were published on experimental *PVTx* studies of water + methanol mixtures at high temperatures and pressures and also on *PVTx* measurements and an equation of state for the water + hexane binary system.
 - 1) Bazaev, A. R., Abdulagatov, I. M., Magee, J. W., Bazaev, E. A., Ramazanov, A. E., and Abdurashidova, A. A., "*PVTx* Measurements for a H₂O + Methanol Mixture in the Subcritical and Supercritical Regions," *Int. J. Thermophysics* **25**: 805-838 (2004).
 - 2) Abdulagatov, I. M., Bazaev, A. R., Magee, J. W., Kiselev, S. B., and Ely, J. F., "*PVTx* Measurements and a Crossover Equation of State of Pure n-Hexane and Dilute Aqueous n-Hexane Solutions in the Critical and Supercritical Regions," *Ind. Eng. Chem. Res.* **44**: 1967-1984 (2005).
- The Physical and Chemical Properties Division (Boulder and Gaithersburg) of NIST is carrying out experimental studies of room-temperature ionic liquids (liquids composed entirely of ions) that are meant to establish reference systems, methods and data. The ionic liquids studied have both scientific and practical engineering interests. Three manuscripts were published which explore thermophysical behavior of dilute (water + ionic liquid) mixtures.
 - 1) Widegren, J. A., Laesecke, A., and Magee, J. W., "The Effect of Dissolved Water on the Viscosities of Hydrophobic Room-Temperature Ionic Liquids," *Chem. Commun.* 1610-1612 (2005).
 - 2) Widegren, J. A., Saurer, E. M., Marsh, K. N., and Magee, J. W., "Electrolytic Conductivity of Four Imidazolium-Based Room-Temperature Ionic Liquids and the Effect of a Water Impurity," *J. Chem. Thermodynamics* **37**: 569-575 (2005).
 - 3) Archer, D. G., Widegren, J. A., Kirklin, D. R. and Magee, J. W., "Enthalpy of Solution

of 1-Octyl-3-methylimidazolium Tetrafluoroborate in Water and in Aqueous Sodium Fluoride," J. Chem. Eng. Data 50: (published in Web edition, 2005).

- Richard Wheatley, a theoretical chemist at the University of Nottingham, spent part of a sabbatical in Boulder to further the collaborative effort on development of intermolecular pair potentials for aqueous systems and calculation of second virial coefficients that have smaller uncertainties than those obtained by experiment. Work is nearly complete on water with nitrogen, and water with oxygen is underway. Completion of these two systems will allow improved calculations for water with "air" which is essential for humidity standards.
- In collaboration with workers in Greece and Germany and at the University of Maryland, work is continuing on the joint IAPWS and IUPAC efforts to update the formulations for the transport properties of water and steam. The correlating surface for viscosity, including a new form for the critical enhancement, has been completed and is ready for evaluation by IAPWS.
- A model has been developed for the effect of dissolved air on the density and refractive index of liquid water. The density effect is of interest in metrology, and the refractive-index effect is of interest for a technology called immersion lithography, which is being developed for manufacturing computer chips. Collaborators at NIST-Gaithersburg measured the refractive-index effect and obtained good agreement with the model.

Communicated from the Oak Ridge National Laboratories, Oak Ridge, TN

In collaboration with other members of the ORNL High-Temperature Aqueous and Geochemistry group, research work was completed from August 2004 to July 2005 or is ongoing or will begin soon in the following areas.

- Solubility studies of minerals to high temperatures including: lead oxide, dawsonite, zinc ferrite (stoichiometric and nonstoichiometric), zinc silicate, and nickel and zinc oxides in the presence of chloride ions.
- Isopiestic studies of binary aqueous solutions (60 – 170oC) containing combinations of the ions of Na, K, NO₃, Cl, SO₄ to very high concentrations. Isopiestic measurements were completed at 25 and 50 oC on the system: Fe³⁺-Fe²⁺, H⁺, SO₄²⁻.
- Thermodynamic studies of liquid films and the projected solutions existing in actively corroding crevices on canister surfaces containing high-level radioactive waste at the proposed Yucca Mountain repository site in Nevada were begun late last year. These include studies of deliquescent behavior, solute volatility and solution pH and well as modeling and speciation studies.
- Work was initiated on testing certain metal/metal oxide pH sensing electrodes for accurate and reliable measurements to at least 200 oC for use in oxidizing environments where hydrogen electrodes are unsuitable.
- Experimental measurements of designed to follow the dissolution and precipitation kinetics of metal oxide and hydroxide phases in aqueous solutions continued at a modest level with a draft of the first paper being prepared.
- The activities associated with being the editor-in-chief of the Journal of Solution Chemistry and coauthor of a chapter on potentiometry for the IAPWS Databook continued throughout this period.

List of Participants, Santorini, Greece

Lname	Fname	University	Country
BELLOWS	James	Siemens Westinghouse	U.S.A.
BIGNOLD	Geoffrey John	Power Plant Chemistry Consultant	U.K.
COLMAN	Patrick	Electricity Supply Board	Ireland
COOPER	J.R.	Queen Mary, University of London	U.K.
DAUCIK	Karol	Elsam Engineering	Denmark
DOOLEY	Barry	EPRI	USA
FEISTEL	Reiner	IOW	GERMANY
FRIEND	Daniel	National Institute of Standards and Technology	USA
FROHN	M.L.		
GACHON	Francois	EDF/R&D	France
GHOSH	Gorachand	Sujata Ghosh	Australia
HARRIES	Richard	Power Chemistry Consulting & Chairman BIA	U.K.
HARVEY	Allan	National Institute of Standards and Technology	USA
HIEGEMANN	Michael	Alstom (Switzerland) Ltd.	Switzerland
HRUBY	Jan	Institute of Thermomechanics AS CR	Czech Republic
HUGHES	Barry-John	PXLimited	U.K.
KNOBLOCH	Katja	Zittau/Goerlitz University of Applied Sciences	Germany
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MIYAGAWA	Kiyoshi		Japan
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NAKAHARA	Masaru	Kyoto University	Japan
OKITA	Nobuo	Toshiba	Japan
OLAVESSEN	Leonard	Buckman Laboratories International, Inc.	U.S.A.
PALMER	Donald	Oak Ridge National Laboratory	U.S.A.
PAPANGELAKIS	Vladimiro	University of Toronto	Canada
PARRY	William T.	General Electric	U.S.A.
RUKES	Bert	Siemens AG PG	Germany
SAFARIK	Pavel	Czech Technical University in Prague	Czech Republic
SATOH	Tomonori	Tohoku University	Japan
SENGERS	Jan V.	University of Maryland	U.S.A.
SENGERS LEVELT	Johanna	NIST (Retired)	U.S.A.
SIFNER	Oldrich	Institute of Thermomechanics AS CR	Czech Republic
STASTNY	Miroslav		Czech Republic
STELLWAG	Bernhard	Framatome ANP GmbH	Germany
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Attachment 20

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WATANABE	Koichi	Keio University	Japan
WEBER	Ingo	Siemens Westinghouse Power Corporation	USA
YASUOKA	Kenji		Japan
KASTANAKI	Argiro	Public Power Company	Greece
SOTIROPOULOS	Dimitris	Public Power Company	Greece
TSIAMPAS	Panagiotis	Public Power Company	Greece
VASILH	Santa	Public Power Company	Greece
ASSAEL	Markos	Aristotle University of Thessaloniki	Greece
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VAGIA	Katerina	Aristotle University of Thessaloniki	Greece