

**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
Russia
United States of America

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**Minutes of the Meetings
of the
Executive Committee
of the
International Association for the Properties of
Water and Steam**

**Witney, United Kingdom
3 – 8 September 2006**

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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
Witney, United Kingdom
3-8 September 2006

Plenary Session. Monday, 4 September 2006. 8:30am

The President of IAPWS, Dr. Frantisek Marsik, welcomed the Executive Committee (EC) and other IAPWS members to Witney for the EC and Working Group (WG) Meetings of IAPWS. The President officially opened the 2006 EC Meetings by introducing the National Delegates. Each of the member countries of IAPWS was in attendance with the exception of Argentina/Brazil, France, Greece, Italy and Russia.

The President asked the head of the BIAPWS Committee to provide some comments. Harries welcomed everybody and indicated that ABB, British Energy and RWE nPower were sponsoring the 2006 IAPWS meetings.

1. Adoption of Agenda

A provisional agenda had been posted on the IAPWS Website for all IAPWS members by the Executive Secretary in April 2006. The Executive Secretary indicated two additional items relating to the Gibbs Award and Election of Officers for 2007 and 2008. 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 Cooper to serve on this Committee. The Press Release is discussed in Minute 17.1 and Attachment 11.

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 by the Committee. The discussion of this Committee is reported in Minute 14.1 and Attachments 9 and 10.

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 2007 award would consist of a member from Denmark, France, Germany, Greece and Japan. The President asked the Danish delegate (Daucik) 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 President indicated that a number of concerns about the process and procedures for the Helmholtz Award had been raised over the last few years. He suggested that the EC needed to review the procedures developed in 1999 at the Canada EC Meetings through a small committee and report back to the EC on Friday. He requested the US Delegate (Friend) to chair this committee. Cooper and Svishchev were added as members with the President and Executive Secretary as ex officio members.

2.3.2 Honorary Fellow Award Committee

The President requested that Daucik take over as the Chairman of this committee from Fernandez-Prini for 2007. Tremaine was added as the other member. The IAPWS President would be ex. Officio.

2.3.3 Gibbs Award Committee

The President indicated that because of the increased frequency of the ICPWS, it was time to start the process to select the 2008 IAPWS Gibbs Awardee. He then requested each WG to nominate one member for the Gibbs Award Committee at the EC on Friday. At that meeting an EC Member will be selected to Chair the Committee (Minute 15.2).

2.4 Host Country for 15th ICPWS

The President requested the German Delegate to provide an update. Rukes indicated that arrangements are moving along nicely to organize the 15th ICPWS in Berlin in 2008. More information would be provided at the EC Meeting on Friday (Minute 17.2). Rukes indicated that the International Program Committee would meet during the week as well as

the German Organizing Committee. He also indicated that the German National Committee had received a request from the organizers of a Nuclear Water Chemistry Conference to hold the ICPWS in conjunction with it.

2.5 Other Business Considered to Require Special/Extensive Discussions

Vice President Cooper reported that there would be activity during the week on Seawater and that there had already been some association with IAPSO. He proposed that a small group be formed to review the possible IAWPS direction and collaborations. The Heads of the WGs and Tremaine were suggested for membership with Feistel as the Chairman.

The US Delegate, Friend, indicated concern that five IAPWS Member Countries were absent from the 2006 EC Meetings and suggested a small committee to review possible ways of increasing the attendance of members. Friend was nominated to chair the committee with Harries, Watanabe and Cooper as members, together with the President and Executive Secretary as ex officio members

3. EC Mandate to Working Groups and Membership

3.1 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 Draft Release had been forwarded to the Heads of National Committees in March (Draft Release on Ice). 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.

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

3.2 IAPWS Restructuring

The President indicated that there was still one open item from the Restructuring exercise over the last few years. This related to the Task Group on Education and Outreach under the chairmanship of Corti with members Kretzschmar, Safarik and Lvov. The president requested that this Task Group reported back to the EC on Friday on any activities.

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 (Attachments 4, 6, 7, and 8).

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 “Advances in Power Plant Chemistry” 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 September 2006

President Marsik opened the continuation of the EC Meeting at 8:35am. All members of IAPWS were present except Argentina/Brazil, France, Greece, Russia and Italy. In total 26 people were present. Marsik first asked the EC if there were any additional items that should be added to the Agenda. None were suggested. The Executive Secretary showed the latest Agenda with additional items relating to the new activities from the Monday EC Meeting.

5. Acceptance of Minutes of Previous Meeting

President Marsik asked for comments and changes to the minutes of the EC meeting held in Santorini, Greece in July 2005. No changes were noted, thus the 2005 Minutes were accepted.

6. President's Report

President Marsik provided the following comments. He first commented that all four working groups continued to be very active. He indicated that it was very

exciting that a new common task group was being discussed with members of IAPSO/SCOR (Scientific Committee on Oceanic Research). He then noted that there were two proposed International Collaborations to be discussed. He reported that two IAWPS Honorary Fellows had been created and that the Helmholtz Award had been given to a Chinese scientist.

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

Chairman Kretzschmar highlighted only those activities from the TPWS working sessions during the week, which needed action by the EC or which he thought were of interest to the EC. He indicated that most of the WG activities had been conducted with IRS. Full Minutes and the WG Agenda can be found in Attachment 4.

- 7.1 Kretzschmar indicated that the WG had reviewed the Release on the Thermodynamic Properties of Ice. Both TPWS and IRS had approved the release and recommended to the ES that this become an official IAPWS Release

The EC approved this Release unanimously.

- 7.2 Feistel had presented a new equation for the sublimation curve for ice based on the new ice thermodynamic formulation and IAPWS-95. He reported that a Task Group had been formed to develop a supplementary release and that he would form an evaluation task force during the next year if progress was fast enough.
- 7.3 A new release on Viscosity will be proposed to the EC next year and a preliminary formulation on conductivity will be available at the 2007 IAPWS meetings with a final version ready for approval in 2008.
- 7.4 The Chairman indicated that a few editorial corrections to IAPWS-95 and to Advisory Note #1 had been made by the WG. These changes did not affect the formulation. The Editorial Committee had reviewed the changes. The WGs TPWS and IRS recommended that the EC approve these changes.

The EC approved these changes unanimously.

- 7.5 The Chairman indicated that Wagner had prepared a CD with documentation of the experimental data that was used in the development of IAPWS-95 and recommended that the EC approve this information being placed on the IAPWS Website.

The EC approved this unanimously.

- 7.6 Kretzschmar reported that the Workshop on Seawater on Tuesday afternoon had been a big success. He also reported that Feistel had developed an ICRN on Seawater. The Chairman indicated that this would be finalized and forwarded to the Executive Secretary for a Postal Ballot. Tremaine would be added to the IAPWS Task Group on Seawater.
- 7.7 An Evaluation Task Group had been formed to review the draft release on the Ionization Constant of Water prepared by Lvov. It was planned to propose this release to the EC for approval in 2007.
- 7.8 Cooper and Sengers will check the influence of the ITS-90 temperature scale on the current releases for heavy water and possibly suggest a revised release at the 2007 EC Meetings.
- 7.9 A Task Group had been appointed to work on the equations for properties of liquid water at standard atmospheric pressure. The Chairmen indicated that he would form an Evaluation Committee during the year if this work proceeded quickly.
- 7.10 The Chairman requested that the EC authorize spending up to \$3000 to pay page charges for the last 2 of the 4 papers describing supplementary “backward” equations, which will be submitted in 2006 and 2007.

The EC approved this unanimously.

- 7.11 The Chairman next requested that the maintainer of the IAPWS website (Harvey) would develop a location on the website where presentation materials from the WG could be placed so that access could be restricted to members only. Discussion of the EC then focused on whether other WGs would also be interested in such a facility. All WG Chairmen agreed.
- 7.12 The Chairman reported that Sifner would be the TPWS representative on the 2008 Gibbs Award Committee.
- 7.13 On Membership of TPWS, the Chairman proposed M. Nakahara as a new member.

The EC approved this membership change unanimously.

Immediately following the TPWS Report, Feistel made a short report on the activities on Seawater during the week. These are provided in Attachment 5.

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

Chairman Parry provided the IRS Report to the EC. Full Minutes and the Agenda can be found in Attachment 6. The Chairman indicated that many of the technical items had already been covered by Kretzschmar in the TPWS report. He then presented the IRS WG items that needed action by the EC.

8.1 Parry reported on the WG discussions of Region 5 Extension of IAPWS IF-97 to 50 MPa. He indicated that there had been two main points of discussion: a) amending the existing release on IAPWS-IF97 but being careful regarding the naming in order to minimize the impact on the user base, and b) keeping the existing release on IAPWS-IF97 unchanged but creating a supplementary release solely dealing with the new equation for region 5. He then made five recommendations to the EC:

- * Document changes to Region 5 using a Revision of the original Release of IAPWS-IF97.
- * Inclusion of Subheading “The revision only relates to the extension of region 5 up to 50 MPa”.
- * The editorial committee should develop wording to ensure that readers understand that the previous region 5 equation has been replaced by the new equation.
- * Individual national committees should contact their industrial representatives for their opinion on revising IF-97. Any feedback should be channeled to the IRS WG Chairman by 31 December 2006.
- * An evaluation committee has been formed and a timetable established which should allow this revision to be adopted at the annual meeting in 2007.

The EC approved the WG recommendation to revise the Release unanimously.

8.2 Parry reported on Advisory Note No. 3 on Thermodynamic Derivatives from IAPWS Formulations. A draft for an Advisory Note no. 3 on thermodynamic derivatives from IAPWS formulations has been prepared. The draft is based on the presentation given at the IAPWS 2005 meetings in Santorini but extended by guidance for the cases for heavy water and ice. A schedule was established which should allow this Advisory Note to be adopted at next year’s annual meeting (2007).

8.3 The Chairman next reported on “Steam Tables on Pocket Calculators for Students” which could be available on the IAPWS Website. He indicated that at the 2005 Santorini meeting it was decided to make the “Steam Tables on Pocket Calculators” available on the IAPWS website. The

German National Committee verified and accepted the download pages for the pocket calculator steam tables. Since then a link from the IAPWS website to these download pages had been made active. However, the location of the link is somewhat concealed and some discussion developed on how to better present this type of information. Since this is part of the “educational and outreach” efforts it was suggested to add a main topic “educational resources” to the IAPWS website which could contain all the links to available software.

- 8.4 The Chairman reported that Rukes would be the WG representative on the 2008 Gibbs Award Committee.

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

Chairman Lvov provided the PCAS Report to the EC. Full Minutes and Agenda can be found in Attachment 7. He covered the following items with the EC:

- 9.1 The Chairman indicated that the PCAS WG had proposed an International Collaboration project on “Predictive Scheme for Standard Thermodynamic Properties of Aqueous Substitutes Benzenes over a Wide Range of Temperatures and Pressures” by Tremaine (Canada) and Sedlbauer (Czech Republic). Review of this is covered in Minute 14.1.
- 9.2 The Chairman requested a 3-year extension on ICRN Number # 10, Contact: D. Palmer (pH Measurements), and a 3-year extension on ICRN Number # 13, Contact: T. Nemec, F. Marsik (Surface Tension of Aqueous Solutions). This latter ICRN had previously been supported by PCC and would now be transferred to PCAS.

The EC approved these ICRN changes unanimously.

- 9.3 The Chairman indicated that a new IAPWS Release on “Ionization Constant of Water over Wide Ranges of Temperature and Density” would be finalized for the 2007 IAPWS meeting
- 9.4 Lvov proposed that Mr. Tomas Nemec (Czech Republic) become a member of PCAS.

The EC approved this membership addition unanimously.

- 9.5 The Chairman reported that an Interim Report on the IAPWS International Collaboration on “Irreversible Thermodynamics of PEM Fuel Cells” by Ondrej Mican, Frantisek Marsik, and Serguei Lvov had been prepared for this 2006 WG meeting and that a final report will be submitted at the 2007

IAPWS meeting. At this point in the EC Meeting it was suggested that all International Collaboration Reports be placed on the IAPWS Website in future.

- 9.6 Lvov indicated that Tremaine would be the PCAS representative on the 2008 Gibbs Award Committee.

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

Chairman Zeijseink highlighted those activities that needed action/approval by the EC. A full written report of the PCC WG activities forms Attachment 8.

- 10.1 Priority List. The Chairman indicated that the PCC WG had updated its Priority List, which gives the research needs as seen from the power plant chemistry perspective. This list should also be of interest for the other IAPWS working groups.

- 10.2 ICRNs. Zeijseink reported that five ICRNs had been drafted. The first four were new.

10.2.1. “Thermophysical Properties Associated with Ultra-Supercritical Coal-Fired Steam Generators”: in collaboration with PCAS (Dooley/ Palmer)

10.2.2. “Mechanism of Decomposition of Ion-exchange Resin”: (Daucik)

10.2.3 “Development / Application of Sensors (Ambient and High Temperature Sensors)”: in collaboration with PCAS (Maughan, Lister, Uchida/Lvov)

10.2.4. “Improved analysis of low concentration of metals (Fe, Cu, Co, etc)”: (Lister, Daucik)

10.2.5 “Research of Amines for the Power Industry” (Maughan)

A fifth ICRN on organics in the steam cycle was closed, and reopened with a different focus.

A new ICRN covering the presence of contaminants in the steam/water circuits, is being considered, and will be discussed in 2007 (Task group Bellows, Maughan, Hughes, Bignold, January 2007).

The PCC had considered the draft ICRN on dew point quantification in flue gas. It was agreed that this is an important topic and should be supported by PCC.

With respect to ICRN #13 "Surface Tension" a recommendation was made to Gabrielli (*in absentia*) to close this ICRN and to prepare a closure document. However, at the EC meeting the PCAS WG had already reported that this ICRN would remain active with support from PCAS (Minute 9.1)

- 10.3 International Collaboration. The Chairman indicated that the PCC WG had submitted a proposal for an International Collaboration Project on "Improved analysis of low concentrations of particulate oxides in water/steam cycles" which had been prepared by Lister, Daucik and Svoboda. Review of this is covered in Minute 14.1.
- 10.4 Guidance Document on Mechanical Carryover. The PCC Chairman reported that a draft document had been prepared by Gabrielli and had been circulated to WG Members. This will be a new type of document for IAPWS. General discussion on the draft had been favorable. The approach represents good common sense and is a step forward from earlier over simplistic guidance. There are a number of points of detail requiring clarification and amplification and so an *ad hoc* subcommittee has been formed to develop a final document on "Method to determine mechanical carryover". The draft will be presented to the PCC members for review by December 2006. The PCC target is to send it to the Executive Secretary for review within IAPWS by the end of February 2007.
- 10.5 PCC Membership. The Chairman proposed two new members for PCC: Dr. Andy Rudge (British Energy) and Dr. Hideki Takiguchi (Japan Atomic Power Company).

The EC approved these membership additions unanimously.

- 10.6 The Chairman indicated that Bellows will be the PCC Representative on the 2008 Gibbs Award Committee.
- 10.7 Election of PCC Officers. The Chairman indicated that he would be stepping down as chairman of PCC after serving for five years and that the PCC unanimously recommends that Vice Chairman Svoboda takes over immediately.

The EC approved this PCC officer change unanimously.

At the end of the PCC report the EC showed its appreciation for the chairmanship of Zeijseink over the last five years.

11. Editorial Committee Report

Chairman Harvey reported that the Editorial Committee had reviewed the new Release on Ice as well as made a number of revisions to one document approved in Santorini. Harvey also indicated that if anything needs to be changed in the Statutes and By-Laws then it should be done prior to the 2007 EC Meeting. A committee was suggested to review the Statutes and By-Laws prior to the 2007 EC Meetings (Editorial Committee and Watanabe). However before this was consolidated further EC discussion on this item was delayed until later on the agenda (Minute 12.2).

12. Membership and Associates

12.1 Members Defaulting on Dues.

The Executive Secretary indicated that according to the latest Swiss bank account statement (end of August 2006), the following countries had not paid the 2006 IAPWS dues: Argentina/Brazil, Denmark, France, and Russia. A representative of the Danish National Committee (Therkildsen) thought that this was a mistake and would check with the Executive Secretary. The Executive Secretary further reported that in 2005 France Russia and half of the Argentinean/Brazil National Committee had not paid the dues. In 2004 France and Russia had not paid the dues.

12.2 Committee on Non-Participating Members.

The President requested the Chairman to make a report of the Committee which had been formed at the Monday EC (Minute 2.5). Friend made the following recommendations to the EC:

12.2.1 Following the conclusion of this EC meeting, the Executive Secretary should send a letter to the head of each delegation which has not participated. This letter should indicate that participation of the delegation was missed; participation in the EC is one of the obligations of membership; inquiry into how IAPWS can assist in renewing the active participation of this national delegation; and hoping that future participation will be forthcoming. A similar letter should be sent to each participant in the delegation from these member countries.

12.2.2 Participants in this meeting informally contact their colleagues in the non-participating delegations indicating the importance of contributions from each National delegation.

- 12.2.3 The Executive Secretary annually indicates to the organizing committee of the local host country that they would be encouraged to assist heads of each delegation to participate in the meeting; such encouragement might include financial assistance such as reduced/waived registration etc.
- 12.2.4 A committee be formed to investigate the possibility of a re-organization of IAPWS, allowing individual memberships in addition to National memberships. This committee should report back to the EC at the 2007 meeting.

The EC approved these recommendations unanimously.

After this approval, the EC discussed linking this activity with the Statutes and By-Laws discussion (Minute 11) and formed the following Committee to review the continuing participation of member countries and any necessary changes to the Statutes and By-Laws: Watanabe (Chairman), Cooper, Harvey, Hruby, and Svoboda. It was also suggested that people would be invited from the non-participating member countries.

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 SFrs104,000 in the Swiss bank account and about \$7,000 in the US account for a total of \$92,229 combined. The status as at 10 August 2006 in the bank accounts had been provided to each National Delegate present at the EC meeting.

The Executive Secretary next reported that the 2005 financial statements had been forwarded to the Auditors in January 2006. VDI in Germany had reviewed and approved them. Mr. Miyagawa had not yet replied. The financial statements for 2005 and the Auditor's report 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 2007.

The EC unanimously agreed to this proposal.

The Executive Secretary also provided a rough estimate of the income and known planned expenditures for 2006.

13.2 Time and Place of the 2007 and 2008 Meetings

The Executive Secretary explained that the next few member countries in rotation to hold the annual EC and WG meetings had indicated that they would not be able to host the 2007 meetings. He had then asked Svoboda to explore the possibility of hosting the 2007 meetings in Switzerland and asked Svoboda to brief the EC on the status. Svoboda then invited the IAPWS EC and WGs to Switzerland for the 2007 Meetings. Currently there is no Swiss National Committee but he will use the meeting to attract various interested parties. The final dates and location will be available by the end of October 2006. The EC enthusiastically approved holding the 2007 meetings in Switzerland.

The Vice President of IAPWS raised a question about whether a letter of invitation could be sent to IAPWS members.

The Executive Secretary indicated that discussion of the 2008 Meetings (15th ICPWS) would be presented later in the agenda.

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

The President indicated that the Releases and ICRNs had been discussed within the WG Reports so no further action was required by the EC.

14.1 International Collaborative Projects.

The President asked the Chair of the Committee (Lvov) to report on the discussions during the week. The Chairman indicated that the Committee had reviewed two proposals for international collaboration. The details of the two proposals are provided in Attachments 9 and 10. The Chairman then summarized the two proposals for the EC.

“Improved Analysis of Low Concentrations of Particulate Metal Oxides in Water/Steam Cycles”. The IAPWS sponsors are Svoboda (Switzerland), Lister (Canada) and Daucik (Denmark). The young scientist is Piti Srisukvatananan at the University of New Brunswick, Canada. The requested contribution from IAPWS is \$6,500 for travel and subsistence.

“Predictive Scheme for Standard Thermodynamic Properties of Aqueous Substituted Benzenes over a Wide Range of Temperatures and Pressures”. The IAPWS sponsors are Tremaine (Canada) and Sedlbauer (Czech Republic). The young scientist is Jana Ehlerova at the Technical

University of Liberec, Czech Republic. The requested contribution from IAPWS is \$6,000 for subsistence.

The Chairman recommended to the EC that IAPWS support both proposals.

The EC approved both Collaborative Projects unanimously.

15. IAPWS Awards

15.1 IAPWS Helmholtz Award

The President reported that Xiang had been selected as the 2006 Helmholtz Awardee and that he had been presented with the award prior to his Helmholtz Lecture at the Symposium on Wednesday. He then asked the Danish Delegate for the names of the 2007 Helmholtz Award Committee. The 2007 Helmholtz Committee would consist of: Chairman Therkildsen (Denmark), Dorey (France), Wagner (Germany) Assael (Greece) and Nakahara (Japan). Nominations are due to the Executive Secretary by January 31, 2007.

The President next asked the Chairman of the Helmholtz Procedures Committee to review the results of this committee formed at the Monday EC meeting (Minute 2.3.1). Friend indicated that the committee (Cooper and Svishchev) had reviewed the current nomination procedures and made the following recommendations to the EC:

- * Nominations can come from anyone (except self-nominations).
- * Committee-selected candidate(s) should be reviewed by all National Committees prior to further processing.
- * Nominations outside of IAPWS should be sent through the head of National Committee, when possible.
- * Both industrially and academically oriented candidates should be encouraged.
- * Candidate's age limit (40 years old) should be replaced by phrase "10 years from receipt of highest earned degree."

After some discussion ...

The EC approved these recommendations unanimously and requested Friend to provide an updated set of procedures to the Executive Secretary.

15.2 IAPWS Honorary Fellowships

The President reported that Bellows (USA) and Dooley (IAPWS Executive Secretary) had been elected Honorary IAPWS Fellows, following the established procedures and after unanimous approval through the postal ballot conducted by the President. The Fellowship Awards had been presented at the IAPWS Dinner on Thursday evening.

The President reminded the EC of the Awards Committee for 2007 with Daucik as Chairman and Tremaine as member with the IAPWS President as ex.-officio member. Nominations are due to the Executive Secretary by January 31, 2007.

15.2 IAPWS Gibbs Award

The President reminded the EC that the following people had been nominated by the WGs to be members of the 2008 Gibbs Award Committee: Sifner (TPWS), Rukes (IRS), Tremaine (PCAS) and Bellows (PCC). To ensure full member country participation the President suggested that the EC appointed Chairman for this committee should be from Japan. The Japanese Delegate (Watanabe) requested that Nakahara be selected for this important position. Nominations can be provided by National Committees and Working Groups and will be due to the Executive Secretary by 31 May 2007.

16. Election of Officers for 2007 and 2008

The President indicated that he would step down at the end of 2006 and that Vice President Cooper will assume the position of IAPWS President on January 1, 2007. According to the Statutes, the election of the next Vice President should be made at the end of the EC meeting in even years. The President and Executive Secretary had checked the recent history and proposed that the US National Committee should be asked to nominate one of their committee members for the position. The President asked the EC if there were any other suggestions. None were suggested, so he then requested the EC to approve this selection.

The EC unanimously approved this selection.

Action: The US National Committee should inform the Executive Secretary of their nomination for Vice President after the next meeting of their committee, and before the end of 2006.

17. New Business

17.1 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 11.

17.2 15th ICPWS

The President requested the Head of the German National Committee to provide a status report on the 15th ICPWS. Rukes provided the names of the International Program Committee and the German Organizing Committee and indicated that both committees had met during the week. The 15th ICPWS will be held in Berlin on 7-13 September 2008. The title will be “Water, Steam and Aqueous Solutions: Advances in Science and Technology for Power Generation”. Rukes then indicated that each WG had been asked to provide suggestions for the symposia and that the German Organizing Committee would develop an initial list and distribute it to the International Program Committee for final review. The next meetings of the International Program Committee will be during the 2007 IAPWS Annual Meetings and on 16-18 January 2008 in Berlin. In terms of publications there will be no bound proceedings but a CD and hard copy will be provided to attendees. The consensus of the following EC discussion was in agreement with this approach and that each of the symposia could be separately published in a respected technical journal, maybe as a special edition. Each symposia chairperson will be asked to organize this. Rukes finished his presentation by adding that a full financial projection for the 15th ICPWS would be provided at the 2007 EC Meetings.

17.3 IAPWS Restructuring: Education and Outreach

At Monday’s EC Meeting (Minute 3.2), the President had reminded the EC that the WGs had taken action on all the Committees and Task Groups of the IAPWS Restructuring with the exception of the Task Group on Education and Outreach. During the week the Executive Secretary had received a note from the Chairman of this Group (Corti) indicating that there had not been much activity over the last year and that he wished to step down from the Chairmanship. The President asked the new Chairman (Kretzschmar) to report on activities of the committee (Safarik and Lvov) during the week. The Chairman reported on the following four topics:

- * The Members of IAPWS are urged to bring PhD Students or other young scientists with them to the IAPWS annual meetings and to the IAPWS conferences.

- * The committee recommends that the annual meeting and conference fees for students are reduced drastically (to the amount for food). In this way, students from the country where the meeting or conference takes place will get the opportunity to attend the IAPWS annual meetings and IAPWS conferences. For students, rooms in a youth hostel near the meeting place could be offered.
- * The IAPWS Website could be used for educational purposes. The starting point for this will be the Down Load of the CD "Steam Tables on Pocket Calculators". Steam Tables for Excel[®] and Mathcad[®] and other software for students can follow. It is recommended that an item "Education" should be added on the left menu bar. The software for students and substantial papers of the IAPWS meetings can be placed in the related page.
- * For the future, IAPWS Summer Schools (2 or 3 days) in the week before the IAPWS meeting are recommended. The discussion of this matter should begin at the next meeting in 2007.

17.4 Miscellaneous Items

The PCAS Chairman, Lvov, requested that the Agendas for the WG meetings at the IAPWS meetings be prepared as early and distinctly as possible.

Vice President Cooper wished to thank President Marsik for all the work he has accomplished during the last two years of his presidency.

17.5 Review of Progress of Research in Member Countries

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

Britain and Ireland	Attachment 12
Canada	Attachment 13
Czech Republic	Attachment 14
Denmark	Attachment 15
German	Attachment 16
Japan	Attachment 17
USA	Attachment 18

17.6 Participants

Attachments 19 and 20 provide lists of participants at the IAPWS EC and WG Meetings, and those extra BIAPWS Members at the Symposium in Witney, England in September 2006.

17.7 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 Witney Meetings. This will be forwarded electronically to the Head of each National Committee.

18. Closing Remarks and Adjournment

The President thanked everybody for participating at this EC meeting. He particularly thanked BIAPWS for organizing the 2006 Annual IAPWS Meetings, and then he formally closed the 2006 EC meeting at 1:20pm.

AGENDA FOR THE EXECUTIVE COMMITTEE

IAPWS

WITNEY, ENGLAND. 3 – 8 SEPTEMBER, 2006

Monday, 4 September 2006. Opening Session (8:30 – 10:00am)

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, Helmholtz and Gibbs)
 - 2.4 Host Country for 15th ICPWS (Report from German NC)
 - 2.5 Other business requiring special/extensive discussions
3. EC Mandate to Working Groups and Membership
 - 3.1 Releases, Guidelines and Certified Research Needs (New and Expiring)
 - 3.2 IAPWS Restructuring (2005 Minute 16.1)
 - 3.3 WG Directions
4. Preview by WG Chairpersons of Week's Activities

Friday, 8 September 2006. Executive Meeting. (8:30am – 1:00pm)

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)
 - 12.2 Non-participating Member Committee
13. Executive Secretary's Report
 - 13.1 Financial, Auditors and Dues
 - 13.2 Time and Place of 2007/2008 Meetings

14. Guidelines, Releases, Certified Research Needs, and International Collaborations
 - 14.1 International Collaborations
15. IAPWS Awards
 - 15.1 Helmholtz Award and Procedures Committee
 - 15.2 Honorary Fellowship
 - 15.3 Gibbs
16. Election of Officers for 2007 and 2008
17. New Business
 - 17.1 Press Release
 - 17.2 15th ICPWS (German NC Report)
 - 17.3 IAPWS Restructuring (Task Group on Education and Outreach)
 - 17.4 Miscellaneous Items
18. Adjournment

**THE 2006 IAPWS ANNUAL MEETING
FOUR PILLARS HOTEL, WITNEY, UK.
WEDNESDAY SEPTEMBER 5TH 2006**

THE 2006 IAPWS SYMPOSIUM

Programme

SESSION 1 - HELMHOLTZ AWARD LECTURE

- 09:00 Welcome, introduction and presentation of Helmholtz Award.
09:05 Corresponding states: A general theory including aqueous states.
Hong-Wei Xiang, Chinese Academy of Sciences.
09:40 Discussion
09:50 Coffee Break

SESSION 2 - BIAPWS SYMPOSIUM

**ADVANCES IN POWER PLANT CHEMISTRY:
CURRENT TRENDS AND FUTURE DEVELOPMENTS**

- 10:15 Welcome and Introduction - Dr Richard Harries, Chairman BIAPWS.
10:20 Environmental and Water Issues : Current and Future
(Chair Dr Andy Rudge , British Energy)
10:20 The transition to a renewable energy society - A Zeijseink, KEMA.
10:50 Environmental pressures on power plant corrosion control -
E Hobson, RWE npower
11:20 Aqueous chemistry issues in flue gas scrubbing; (Sea water FGD and CO₂
sequestration) - A Howard, E.ON UK
11:50 Control of the Environmental Impact of Phosphate Discharges from Power
Plant. - J Greene, Amec-NNC
12:20 Discussion Session
12:45 Lunch
14:00 Cycle Chemistry and Impurity Transport in Steam Turbines
(Chair Dr Bruce Roberts, Alstom Power)
14.00 The role of CO₂ and organics in cycle chemistry – R Svoboda, Alstom Power.
14.30 Effect of organic matter on steam chemistry and turbine materials -
M Rziha, Siemens Generation
15.00 Mass transfer of impurities in steam turbines -
J Bellows, Siemens Generation
15.30 Discussion Session
16.00 Closing Remarks - Dr Richard Harries

SCHEDULE

IAPWS MEETINGS

Witney, England. 3 – 8 September 2006

(All meetings will be at the Four Pillars Hotel)

Sunday 3 Sept.	6:30pm	Informal Get-together and Registration (Hosted by BIAPWS Committee. Conference Suite, Four Pillars Hotel)
Monday 4 Sept.	8:30am	Opening Plenary Session - Executive Committee
	10:00am	TPWS/IRS Joint Meeting (To set agendas for the week and to conduct IAPWS Business, thus allowing remainder of week for technical matters)
	10:00am	PCAS and PCC Separate Meetings (To conduct IAPWS Business, thus allowing remainder of week for technical matters)
	1:30pm	TPWS and IRS Joint or Separate Meetings
	1:30pm	PCC/PCAS Joint WG Meeting and Workshop Joint WG Workshop
Tuesday 5 Sept.	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
	1:30pm	All WG Meeting (if needed)
	2:30pm	IRS and PCC Separate WG Meetings
	2:30pm	TPWS/PCAS Joint Meeting Topics of Interest to Both WGs
Wednesday 6 Sept.	10:00am - 5:00pm	IAPWS Symposium "Advances in Power Plant Chemistry – Current Trends and Future Developments" (Registration commences at 9.15am, coffee available)
Thursday 7 Sept.	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)
	6:30pm	IAPWS Dinner. (Theme: Water and Steam) (Coaches departs hotel about 5:45pm)
Friday 8 Sept.	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
9 May 2006

MINUTES

IAPWS THERMOPHYSICAL PROPERTIES OF WATER AND STEAM WG WITNEY, UNITED KINGDOM SEPTEMBER 4-7, 2006

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 (5-11, 13-16, 19.6) that were done jointly with the WG IRS and some (18) with PCAS, and also record (item 17) the workshop on seawater held by all 4 Working Groups.

1-3. The meeting was opened at 8:40 AM on Monday, September 4 by the Chair, Hans-Joachim Kretzschmar, who began by informing the WG about two of its members (Prof. Skripov and Dr. Watson) who had died in the previous year. R. Feistel gave a brief appreciation of Prof. Skripov, and J. Sengers gave a brief appreciation of Dr. Watson, followed by a moment of silence. It was announced that WG member J.M.H. Levelt Sengers had won the ASME Touloukian award for outstanding contributions to knowledge in the area of thermophysical properties. The agenda (Attachment A) was adopted after a few revisions. Allan Harvey was appointed Clerk of Minutes. The minutes of the 2005 TPWS WG meeting in Santorini were approved.

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

5. J. Hruby presented the report of the Evaluation Committee on the proposed release for the thermodynamic properties of ice, which was favorable. **The WGs TPWS and IRS voted unanimously to approve the proposed release and recommend its adoption by the EC.**

6. R. Feistel presented a new calculation of the sublimation curve of ice based on the new ice thermodynamic formulation and IAPWS-95, along with some consideration of low-temperature heat capacities. A new melting curve for ice-I can be computed in a similar way, but does not quite meet the (L-I-III) triple point used in the current IAPWS formulation. Issues were discussed such as whether temperature or pressure should be the independent variable in such formulations, and whether correlations for properties (enthalpy, etc.) at saturation, or their differences, would be useful. **A Task Group was appointed to consider these issues and work toward a Supplementary Release, with members Feistel (Chair), Wagner, Harvey, and Hruby. The Chair of TPWS was authorized to appoint an Evaluation Task Group during the year if progress of the work was fast enough for this to be appropriate.**

7. R. Feistel and A. Harvey presented some material on the prospects for achieving an improved description of the ideal-gas heat capacity of water. Better data are available for this computation at high temperature (especially above about 2000 K), and the new formulation might go to lower temperatures than the one currently used (which extends down to 130 K). It was decided that this effort would probably not be an official IAPWS document, but the presenters were encouraged to pursue it and to consult R. Span in the effort. The question was raised of how high in temperature to go with this calculation, and the consensus answer was as high as is feasible. The work mentioned above on a new formulation of the sublimation curve may wait until this new ideal-gas result is available.

8. [This item is reported in the IRS minutes.]

9.1 J. Sengers reported on the development of the new viscosity correlation. It was recognized by all that the Evaluation Task Group had contributed greatly to the improvement of this effort. Prof. Watanabe wished to state for the record the exemplary contributions of the Evaluation Task Group and also his feeling that the earlier effort presented in Santorini had been too rushed. Some discussion ensued about the proposed document, and suggestions for improvement were made. The need was expressed to pay attention to the part of the document describing industrial use of the correlation. R. Mares discussed the work of the Evaluation Task Group, which has not yet finished evaluating the latest version. The following schedule was adopted for further processing of the viscosity release:

Jan. 31, 2007 Completion of evaluation by Evaluation Task Group

Feb. 28, 2007 Revision of draft release if required

Mar. 15, 2007 Evaluation report distributed to Working Group

Apr. 15, 2007 Deadline for input from WG members

Apr. 30, 2007 Finalized draft of Release to Editorial Committee

May 31, 2007 Approval by Editorial Committee and distribution to National Delegates

Mr. Miyagawa was added to the Evaluation Task Group for viscosity and Mr. Cooper withdrew from the TG.

9.2 W. Wagner presented material concerning the differences between the current scientific and industrial formulations for thermal conductivity, and the difficulties the current structure caused for users. D. Friend described the work toward a new thermal conductivity formulation. A complete database has been developed, along with a correlation for the dilute-gas contribution. The goal is to have a preliminary formulation available for our 2007 meeting, and to adopt a final version in 2008. More consideration is needed to decide what to do about industrial use of the thermal conductivity, but it was decided that no “interim” changes would be made to the current formulations.

10. [This item is reported in the IRS minutes.]

11. W. Wagner presented some editorial corrections needed to correct misprints (and update a reference) in the documents for IAPWS-95 and Advisory Note #1. These misprints do not affect the formulation itself. The Editorial Committee provided some improvement of the proposed wording. **The Working Groups TPWS and IRS approved these minor editorial revisions to the documents and recommended their approval by the EC.**

12. W. Wagner reported that he has prepared a CD with documentation of the experimental data that was used in the development of IAPWS-95. **It was decided to recommend to the EC that this information be placed on the IAPWS Website.**

13-16. [These items are reported in the IRS minutes.]

17. The Workshop on Seawater on Tuesday afternoon, was a joint effort of all 4 IAPWS Working Groups. We welcomed B. King from the University of Southampton, who is affiliated with the International Association for the Physical Science of the Oceans (IAPSO). R. Feistel presented an overview of IAPSO and its liaison activities with IAPWS. He described how IAPSO had decided to use IAPWS-95 as their pure-water baseline for a future formulation for the properties of seawater, and that extrapolation below 0 °C was still a question mark. B. King described current seawater property standards and discussed issues regarding conversion to the ITS-90 temperature scale and issues with the definition and scale for salinity. The need for a clearer physical definition of seawater was discussed. R. Feistel described work on new formulations for seawater properties, using IAPWS-95 as a baseline, and work on an extended formulation to cover a wider range of salinity. Material was presented on hydrothermal vents

which can involve water at supercritical conditions; it was pointed out that the composition of the vent fluids is very different than that of normal seawater. B. King briefly discussed measurement needs for the oceanographic community, which included not only thermodynamic properties but also optical properties (refractive index) for possible sensors.

R. Feistel presented a draft ICRN for seawater properties. Further discussion of this was deferred until the TPWS meeting.

The future of cooperation between IAPWS and IAPSO was briefly discussed. Liaison and email communication will continue, and attendance at the other organization's meetings will continue to be encouraged. **P. Tremaine is added to the existing IAPWS Task Group on seawater** (which also includes Feistel (Chair), Wagner, Harvey, and Hiegemann).

The WG returned Thursday to the proposed ICRN on seawater. **The WG recommends that the proposed ICRN be adopted, subject to editorial revisions.**

18. A joint session with PCAS was held on Thursday morning. The topics are listed in the attached Agenda (TPWS attachment A), except that there was no presentation from the Simulation Task Group.

The item requiring WG action was the proposed new release on the ionization constant of water. S. Lvov summarized the formulation and the proposed draft release. Several suggestions for improvement were agreed upon, including the addition of a table of check values, a clear definition of the K_w quantity, and a more complete statement of the uncertainty in various regions (possibly with the aid of a figure). **An Evaluation Task Group (joint between the 2 WGs) was appointed consisting of Harvey (Chair), Nakahara, Palmer, and Tremaine. The following schedule was adopted, anticipating final approval in 2007:**

Oct. 1, 2007 Draft Release (incorporating comments from this meeting) sent to Evaluation TG and WG members, with WG members invited to send comments to Evaluation TG.

Dec. 31, 2006 Completion of evaluation by Evaluation Task Group

Jan. 15, 2007 Evaluation report and revised release distributed to Working Group

Feb. 15, 2007 Deadline for input from WG members

Mar. 1, 2007 Finalized draft of Release to Editorial Committee

April 1, 2007 Approval by Editorial Committee

Apr. 15, 2007 Distribution by Executive Secretary to National Delegates

19. A. Harvey reported that no update was needed this year on the IAPWS Fundamental Constants document.

J. Cooper stated that there was nothing to report concerning liaison with the IEC.

A. Harvey reported that some progress had been made toward producing a joint document with the CCM to guide people about when to use their standard for water density for metrology, and when use of IAPWS-95 is appropriate. However, progress has been delayed due to concerns on the CCM side, which it is hoped can be addressed soon. It is hoped to have something completed before the next IAPWS meeting.

A. Harvey briefly presented some reasons why it might be useful for IAPWS to adopt simple equations for various properties of liquid water at standard atmospheric pressure. It was agreed that this would be useful. **A Task Group was appointed to work on this, consisting of Harvey (Chair), Hruby, and Kretzschmar. The WG Chair was authorized to appoint an Evaluation Committee during the year if work proceeded quickly enough for this to be appropriate.**

J. Cooper reported briefly on the status of heavy water. He pointed out the need to clarify the existence of a comprehensive data collection for future thermodynamic work. J. Sengers reported that the International Association for Transport Properties (IATP) was suspending work on heavy water for the moment. The Chair volunteered to ask the Canadian delegation about current interest in heavy water. **J. Cooper and J. Sengers will check the influence of the ITS-**

90 temperature scale on the current releases for heavy water transport properties, and if all goes well they will bring a proposal for a revised release to the 2007 meeting.

19.6. [This item is reported in the IRS minutes.]

20. **It was voted to accept M. Nakahara for membership in TPWS.** National committees are asked to check the status of inactive members in their home countries before next meeting.

21. For item 21.1, there were no collaborative projects to report on. Item 21.4 is in the IRS minutes. As additional other business, it was decided that the Chair would email TPWS presentations from the meeting to all members of the WG, and that the maintainer of the IAPWS website would be asked to investigate the possibility of putting these documents on the website in a way so that access could be restricted to members only.

21.2 **The WG requests that the EC authorize spending up to \$3000 to pay page charges for the last 2 of the 4 papers describing supplementary “backward” equations, both of which will be submitted in the next year.**

21.3 **O. Sifner was appointed as the TPWS representative to the Gibbs award committee.**

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

23. The meeting was adjourned at 4:50 PM on Thursday, September 7.

Agenda

IAPWS THERMOPHYSICAL PROPERTIES OF WATER AND STEAM WG WITNEY, UK,

SEPTEMBER 3-8, 2006

1. Opening Remarks; Adoption of Agenda
2. Appointment of Clerk of Minutes
3. Approval of Minutes of TPWS WG in Santorini, Greece (July 2005)
4. Potential International Collaborative Projects
5. Release on Ice, joint with WG IRS
 - Report of the Evaluation Committee (J. Hruby and A.H. Harvey)
 - Formal Consideration of the Release by the WGs TPWS and IRS
6. Development of New Equations for Melting Pressure and Sublimation Pressure (R. Feistel)
7. Possibility for Improvement of Ideal-gas Partition Function and Heat Capacity of Water, Especially at Low Temperatures (R. Feistel and A.H. Harvey).
8. Development of a New Basic Equation for Region 5 of IAPWS-IF97 for Pressures up to 50 MPa, joint with WG IRS
 - Proposal for a Revised Release (W. Wagner)
 - Appointment of an Evaluation Task Group
9. Transport Properties of Water and Steam, joint with WG IRS
 - 9.1 Viscosity
 - Report of the Task Group (J.V. Sengers)
 - Report of the Evaluation Task Group (R. Mares)
 - 9.2 Thermal Conductivity
 - Statement on the Differences Between the Equations for Thermal Conductivity for Industrial and Scientific Use (W. Wagner)
 - Report of the Task Group (D.G. Friend)
10. Advisory Note No. 3 on Thermodynamic Derivatives from IAPWS Formulations (H.-J. Kretzschmar), joint with WG IRS
 - Appointment of an Evaluation Task Group
11. Editorial Corrections to IAPWS-95 Release Document and Advisory Note No. 1 (W. Wagner)
12. CD with Experimental Data the IAPWS-95 Formulation is Based on (W. Wagner)

13. Computing Time Investigations of the IAPWS-IF97 Backward Equations, joint with WG IRS
14. Calculation of the Dissociation of Steam - Guidance for Users of the IAPWS Formulations (J. Bellows), joint with WG IRS
15. Requirements on Properties for Working Fluids, joint with WG IRS
 - Power Cycles with CO₂ Sequestration (R. Span)
 - Requests for New Equations of Working Fluids from Industrial Point of View - Environmental Issues Task Group Report (Environmental Task Group, N. Okita)
16. "Steam Tables on Pocket Calculators" for Students Available on the IAPWS Website (H.-J. Kretzschmar, A.H. Harvey, B. Rukes), joint with WG IRS
17. Workshop on Properties of Seawater (R. Feistel), joint with WGs IRS, PCAS, PCC (Tuesday Afternoon)
 - A Brief History and Current Activities of the International Association for the Physical Science of the Oceans (IAPSO) (R. Feistel)
 - Liaison with IAPSO, Letters Between the IAPWS President and the President of IAPSO (R. Feistel)
 - Oceanographic Seawater Standards (B. King, R. Feistel)
 - Unit for the Salinity of Seawater, Conflict with ISO (B. King)
 - Development of an Extended Formulation of the Thermodynamic Properties of Seawater (R. Feistel)
 - Physical Chemistry of Vents, Critical Properties (R. Feistel)
 - Request for Measurements/Instruments (B. King)
 - Formulation of an ICRN on Thermodynamic Properties of Seawater (R. Feistel)
 - Future Cooperation between IAPWS and IAPSO (R. Feistel, B. King)
18. Joint Meeting with PCAS (Thursday Morning)
 - 18.1 Release on the Ionization Constant of Water (S.N. Lvov)
 - Appointment of an Evaluation Task Group
 - 18.2 Binary Nucleation of Steam with Admixtures Relevant in Power Industry and Atmosphere (T. Némec, F. Maršík, D. Palmer)
 - 18.3 Report of the Simulation Task Group (I.M. Svishchev, K. Yasuoka)
 - 18.4 Thermochemical Cycles for Hydrogen Production (S. Lvov)
19. Reports on Other TPWS Activities
 - 19.1 Fundamental Constants (A.H. Harvey)
 - 19.2 Liaison with IEC (J. Cooper), joint with WG IRS
 - 19.3 Liaison with CCM (A.H. Harvey, R. Span)

- 19.4 Discussion of Need for Equations for Properties of Liquid Water at Standard Atmospheric Pressure (A.H. Harvey)
- 19.5 Thermophysical Properties of Heavy Water
- 19.6 Dewpoint Data in Exhaust Gas, joint with WG IRS
 - Measurement of Data status (E. Maughan)
 - ICRN status (N. Okita)
- 20. Membership
- 21. Other Business
 - 21.1 Report on International Collaborative Projects
 - 21.2 Page Charges for Publication of Archival Papers on Supplementary Backward Equations for IAPWS-IF97
 - 21.3 Gibbs Award Committee
 - 21.4 Topics for the 15th ICPWS 2008 in Berlin
- 22. Preparation of the Formal Motion to the EC
- 23. Adjournment

REPORT TO THE IAPWS EXECUTIVE COMMITTEE ON 08 SEPT. 2006, WITNEY, UK

**Witney Committee “Future Cooperation of IAPWS with the SCOR/IAPSO WG127”
(R. Feistel, H.-J. Kretzschmar and J.R. Cooper)**

- The IAPWS Task Group on the Properties of Seawater consisting of R. Feistel (chair), A.H. Harvey, J.R. Cooper, M. Hiegemann and W. Wagner works together with the WG 127 of IAPSO.
- P. Tremaine will be a new member of the IAPWS Task Group on Seawater. He will be proposed to become a corresponding member of WG 127.
- IAPWS-95 experimental background data will be provided to WG127 by W. Wagner with a general permission for its use in oceanographic research.
- The existing IAPWS-95 computation source code will be provided to WG127 by W. Wagner with a general permission for its use in oceanographic research.
- A task group for the investigation of IAPWS-95 properties between the freezing points of pure water and of seawater will be established. At given pressure, the range of freezing temperature lowering due to dissolved salt is between 0 and 8 K. A report on the usability of IAPWS-95 as the pure-water reference for the Gibbs function of seawater in this range will be prepared.
R. Feistel, W. Wagner, M. Anisimov are proposed to participate in this TG.
- The possibility of a modification of the IAPWS-95 computation source code with regard to a relaxation of its low-temperature application limit will be considered by W. Wagner.
- The IAPWS 2006 Release on Ice, consistently extending IAPWS-95 to the solid phase, will be provided as a new standard description usable for the determination of seawater freezing points.
- IAPWS will evaluate the new Gibbs function of seawater valid between 0 and 100 MPa, -17 and +40°C, 0 and 110 g/kg, planned for 2007, to be developed by R. Feistel.
- The IAPWS task group “Seawater” will continue its activity with the members R. Feistel (chair), A. H. Harvey, M. Hiegemann, P. Tremaine
- R. Feistel, appointed as the IAPWS liaison, will report to WG127 about the Witney meeting.
- IAPWS adopts a Certified Research Need (ICRN) on seawater properties over the parameter ranges of interest for industry and oceanography
- P. Tremaine will consider possibilities for measuring standard seawater properties at elevated pressures, in particular density and electrical conductivity
- R. Feistel will examine the conditions required for extending the planned Gibbs function to temperatures higher than 40°C at normal pressure. This range is of particular interest for power station cooling and desalination.
- It is recommended that the IAPWS 2007 meeting considers a suitable form of a repeated seawater workshop and the invitation of one or more members of the WG127, e.g. the specialists in seawater chemistry, F. J. Millero (RSMAS, USA), A. C.-T. Chen (NSYSU, Taiwan), P. Spitzer (PTB, Germany), or G. M. Marion (DRI, USA).

- The ICPWS 2008 Organizing Committee will consider the IAPWS interest a specific seawater topic and will, in case, offer to WG127 the participation of oceanographers. A particular aspect of interest may be the relevance of the IAPWS work for climate research.

A reply letter from IAPWS to WG127 will be formulated by H. J. Kretzschmar, A.H. Harvey and R. Feistel regarding the topics reported above, including the minutes of the Witney meeting.

MINUTES OF MEETING OF WORKING GROUP INDUSTRIAL REQUIREMENTS & SOLUTIONS (IRS)

Witney, UK, 3. – 8. September 2006

Remark: The IRS minutes cover the topics chaired by the IRS working group chairman. All other agenda topics of joint meetings are covered in the TPWS working group minutes.

1. Opening remarks, Adoption of Agenda

Chairman B. Parry welcomed the WG members to Witney. The agenda was adopted with slight adjustments (Attachment A to IRS Minutes)

2. Appointment of Clerk of Minutes

I. Weber was appointed clerk of minutes.

3. Approval of Santorini Meeting Minutes

The minutes of the 2005 IRS WG meeting were approved unchanged.

4. Potential International Collaborative Projects

There were no proposals for International Collaborative Projects from IRS.

5. Release on Ice

See TPWS minutes.

6. Development of New Equations for Melting Pressure and Sublimation Pressure

See TPWS minutes.

7. Possibility for Improvement of Water's Ideal-gas Partition Function and Heat Capacity especially at Low Temperatures

See TPWS minutes.

8. Development of a New Basic Equation for Region 5 of IAPWS-IF97 for Pressures up to 50 MPa

W. Wagner presented the proposal of a new basic equation for region 5 of IAPWS-IF97 for pressures up to 50 MPa:

- Ideal gas part of original equation remains unchanged.
- Number of term for residual part of the equation is increased from 5 to 6.
- Original equation has better consistency with the basic equation of region 2 of IAPWS-IF97, however the consistency requirements are also met by the proposed new equation.

W. Wagner additionally presented a draft of a revised release of the IAPWS-IF97 release. This draft contained changes necessary due to the new equation for region 5 as well as minor editorial corrections.

Extensive discussion developed regarding the impact of the new development. Two major directions established during the discussion:

- Amend the existing release on IAPWS-IF97 but being careful regarding the naming in order to minimize the impact on the user base.
- Keep the existing release on IAPWS-IF97 unchanged but create a supplementary release solely dealing with the new equation for region 5.

No final conclusion could be found on this topic. An ad-hoc committee consisting of N. Okita, B. Parry and B. Rukes was established to make a suggestion on how to handle this issue. They were requested to report back on Thursday.

An evaluation task group will be set up to technically evaluate the proposed new equation; B. Parry will contact K. Miyagawa in order to form this task group.

Revisited on Thursday, 7. September 2006:

The ad-hoc task group recommends a revised release on IAPWS-IF97. Additionally a subtitle "The revision only relates to the extension of region 5 up to 50MPa" should be added. Discussion developed about this topic, the consensus is that it should be called a "revised release" and that the editorial committee develops a proper wording for the subheading making clear that the previous region 5 equation has been replaced by the revised equation. The WGs will recommend this procedure to the EC. Additionally the WGs will recommend to the EC that individual national committees contact their industrial representatives for their opinion on revising IFC-97. Any feedback should be channeled to the IRS WG Chairman by 31 December 2006.

H.-J. Kretzschmar reported that he had contacted K. Miyagawa concerning his participation on the evaluation task group for revised region 5. K. Miyagawa expressed his willingness to chair the evaluation task group. R. Mares volunteered to participate on the task group. Therefore, the evaluation task group will consist of R. Mares and K. Miyagawa; Mr. Miyagawa will be the chairman.

The working groups suggest the following schedule:

- 2006-12-31: completion of evaluation
- 2007-01-15: evaluation report to working groups
- 2007-02-15: deadline for input by the working group members
- 2007-03-01: evaluation report to editorial committee
- 2007-04-01: approval by the editorial committee and handover to Executive Secretary
- 2007-04-15: Executive Secretary distributes to National Committees

K. Miyagawa has agreed to this schedule.

9. Transport Properties of Water and Steam

See TPWS minutes.

10. Advisory Note No. 3 on Thermodynamic Derivatives from IAPWS Formulations

H.-J. Kretzschmar presented a draft for an advisory note no. 3 on thermodynamic derivatives from IAPWS formulations. The draft is based on the presentation given at the IAPWS meeting 2005 in Santorini but extended by guidance for the cases heavy water and ice. H.-J. Kretzschmar has contacted K. Miyagawa prior to the meeting and he is willing to chair an evaluation task group. The task of the evaluation task group is to verify the formulas stated in the advisory note.

The working groups suggest the following schedule:

- 2006-12-31: completion of evaluation
 - 2007-01-15: evaluation report to working groups
 - 2007-02-15: deadline for input by the working group members
 - 2007-03-01: evaluation report to editorial committee
 - 2007-04-01: approval by the editorial committee and handover to Executive Secretary
 - 2007-04-15: Executive Secretary distributes to National Committees
- This schedule requires approval by K. Miyagawa in order to be effective.

11. Editorial Corrections to IAPWS-95 Release Document and Advisory Note No. 1

See TPWS minutes.

12. CD with Experimental Data which form the basis of IAPWS-95 Formulation

See TPWS minutes.

13. Computing Time Investigations of the IAPWS-IF97 Backward Equations

Since K. Miyagawa was not able to attend the meeting H.-J. Kretzschmar presented the results of the computing time investigations. The report is to a large extent based on the material presented 2005 in Santorini. In addition to the previous information also the effects of using the IAPWS-IF97 backward equation as starting point for high accuracy iterative calculations of the IAPWS-IF97 fundamental equations were investigated. Using the backward equation as starting point increases the calculation speed roughly by a factor of 2. This also holds for calculations with IAPWS-95, the speed increase is even somewhat higher in this case.

Meanwhile a paper on this topic has been submitted to the ASME Journal of Engineering for Gas Turbines and Power.

14. Calculation of the Dissociation of Steam - Guidance for Users of the IAPWS

J. Bellows gave a short verbal presentation on the question of dissociation of steam. He pointed out that all steam property formulations describe the properties of H₂O molecules but that there is no model available for the dissociated case or steam with oxygen or hydrogen excess. A first approximation would be to consider an ideal mixture with equilibrium conditions. However the question remains how ideal these mixtures really are. Additionally cases which involve kinetics would have to be considered. Possible questions for steam dissociation could be:

- Amount of dissociated matter
- Changes in properties due to dissociation

Chairman B. Parry pointed out that as long as there is no defined request from industry IAPWS would not become active in this field.

15. Requirements on Properties for Working Fluids

a. Power Cycles with CO₂ Sequestration

R. Span gave a presentation on power cycles with CO₂ capture and CO₂ transportation and storage. He gave an overview about different storage options as well as about the status of projects, i.e. demonstration plants and plans for commercial plants. He presented different approaches for CO₂ capturing and went to somewhat more detail for the so called oxyfuel processes where combustion takes place with pure oxygen. Combustion products are mainly CO₂ and H₂O, i.e. a proper model for the properties of this mixture is required. Not only non-ideal behavior at various conditions has to be covered but also phase equilibria, e.g. for the separation of CO₂ by means of H₂O condensation. Even additional constituents like N₂, Ar, O₂, CO, NO_x and unburned hydrocarbons may have to be considered depending on the application. Additional requirements emerge from the areas of CO₂ compression, transportation and storage. Apparently there is a strong need of accurate data and accurate models but also better interaction is required with the geology / oceanography community to share knowledge and ideas.

During the discussion W. Wagner pointed out that a model exists which is capable of producing property data for the discussed mixture. This model

currently includes 18 constituents and is based on the property data of binary mixtures, however property data for more complex mixtures can be produced almost as good as the experimental uncertainties.

Revisited on Thursday, 7. September 2006:

R. Span pointed out that there is a requirement to fund further research however this cannot come from IAPWS. Therefore he suggests to revise the existing ICRN on humid air and combustion gases to cover also the liquid phases. He agreed to prepare a draft for an updated ICRN to be presented in 2007.

b. Requests for New Equations of Working Fluids from Industrial Point of View

N. Okita gave a presentation on the industrial requirements for new equations of working fluids. He gave a summary of the work of the environmental task group which has been presented in 2005. The areas CO₂ capture and humid combustion gases were addressed before and work is continuing. However another area of urgent need for further investigations is the dew point in combustion gases. There is knowledge about the dew point in air however for combustion gases there is not sufficient data available. From industrial point of view the condensation of sulfuric acid presents severe corrosion issues. Currently industry applies high design margins to cover the impact however better knowledge could help to reduce these margins and therefore power plant efficiencies. He summarizes that there is a need for accurate data and formulation for the dew point of combustion gases. Discussion continued under item 17. b.

16. “Steam Tables on Pocket Calculators” for Students Available on the IAPWS Website

At the 2005 Santorini meeting it was decided to make the “Steam Tables on Pocket Calculators” available on the IAPWS website. H.-J. Kretzschmar gave an update on the status:

The German National Committee verified and accepted the download pages for the pocket calculator steam tables. Since then a link from the IAPWS website to these download pages is active. H.-J. Kretzschmar gave a short online presentation of the download pages. He also expressed that the location of the link is somewhat concealed and some discussion developed on how to better present this type of information. Since this is part of the “educational and outreach” efforts it was suggested to add a main topic “educational resources” to the IAPWS website which could contain e.g. all the links to available software.

17. Dew Point Data in Exhaust Gas

a. Measurement of data status

E. Maughan gave a presentation on the theory of humidity and dew point measurement techniques. The dew point is defined to be the temperature for given pressure where condensation of some liquid matter occurs. He pointed out that the dew point depends on the composition of the gas and additionally that the condensate may possibly be corrosive.

b. ICRN status

N. Okita proposes to prepare an ICRN on the dew point in combustion gases. During the discussion R. Span pointed out that the existing ICRN on humid air

and combustion gases does not cover this issue. Extensive discussion developed about the proposed ICRN. There was concern that it will be very difficult to realize (due to measurement uncertainties for SO₂ and SO₃, liquid formation processes, exact definition of dew point, etc.). It was suggested to first evaluate the existing equations and based on this the need for further equations and research could be derived. Apparently PCC will propose an ICRN on a similar topic, there should be some discussion to reach a common position.

A task group on evaluation of this issue was formed consisting of N. Okita, R. Span and J. Hruby, chaired by N. Okita. The task group is requested to present its findings in 2007 and also contact PCC on this issue.

18. Workshop on Properties of Seawater

See TPWS minutes.

19. Appointment of IRS WG member to serve on Gibbs Award Committee

B. Rukes agreed to serve as a member of the Gibbs Award Committee. If he is unable to serve, Roland Span agreed to serve in this capacity.

20. Membership

There were no membership items to be discussed this year.

21. Other Business

a. Topics for 15th ICPWS 2008

The WGs discussed the list of topics suggested by the German Organizing Committee and made some comments.

22. Preparation of Report to Executive Committee

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

23. Adjournment

The Chairman adjourned the meeting of the IRS working group at 7. September 2006, 3:30pm.

**Agenda
of
Industrial Requirement and Solutions Working Group**

WITNEY, UK, 3 TO 8 SEPTEMBER 2006

1. Opening Remarks, Adoption of Agenda
2. Appointment of Clerk of Minutes
3. Approval of Minutes of Meeting, IRS WG in Santorini, Greece (July 2005)
4. Potential International Collaborative Projects
5. Release on Ice, joint with WG TPWS
 - Report of the Evaluation Committee (J. Hruby and A.H. Harvey)
 - Formal Consideration of the Release by the WGs TPWS and IRS
6. Development of New Equations for Melting Pressure and Sublimation Pressure (R. Feistel)
7. Possibility for Improvement of Water's Ideal-gas Partition Function and Heat Capacity especially at Low Temperatures (R. Feistel and A. H. Harvey)
8. Development of a New Basic Equation for Region 5 of IAPWS-IF97 for Pressures up to 50 MPa, joint with WG TPWS
 - Proposal for a Revised Release (W. Wagner)
 - Appointment of an Evaluation Task Group
9. Transport Properties of Water and Steam, joint with WG TPWS
 - 9.1 Viscosity
 - Report of the Task Group (J.V. Sengers)
 - Report of the Evaluation Task Group (R. Mares)
 - 9.2 Thermal Conductivity
 - Report of the Task Group (D.G. Friend)
 - Statement on the Differences Between the Equations for Thermal Conductivity for Industrial and Scientific Use (W. Wagner)
10. Advisory Note No. 3 on Thermodynamic Derivatives from IAPWS Formulations (H.-J. Kretschmar), joint with WG TPWS
11. Editorial Corrections to IAPWS-95 Release Document and Advisory Note No. 1 (W. Wagner), joint with WG TPWS
12. CD with Experimental Data which form the basis of IAPWS-95 Formulation (W. Wagner), joint with WG TPWS
 13. Computing Time Investigations of the IAPWS-IF97 Backward Equations, joint with WG TPWS
14. Calculation of the Dissociation of Steam - Guidance for Users of the IAPWS Formulations (J. Bellows), joint with WG TPWS
15. Requirements on Properties for Working Fluids, joint with WG TPWS
 - Power Cycles with CO₂ sequestration (R. Span)
 - Requests for New Equations of Working Fluids from Industrial Point of View
Environmental Issues Task Group Report (N. Okita)

16. "Steam Tables on Pocket Calculators" for Students Available on the IAPWS Website (H.-J. Kretzschmar, A.H. Harvey, B. Rukes), joint with WG TPWS
17. Dewpoint Data in Exhaust Gas – joint with WG TPWS
 Measurement of Data status (Eric Maughan)
 ICRN status (N. Okita)
18. Workshop on Properties of Seawater (R. Feistel) – joint with WGs TPWS, PCAS, & PCC
19. Appointment of IRS WG member to serve on Gibbs Award Committee
20. Membership
21. Other Business
22. Preparation of Report to Executive Committee
23. Adjournment

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

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

Monday Morning

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

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

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

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

4. **ICRNs and Releases:** The following were discussed:

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

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

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

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

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

6. **Task Groups and Committees:** (Deferred)

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

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

Monday Afternoon

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

Tuesday Morning

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

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

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

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

Tuesday Afternoon

11. All WG Meeting: Workshop on Properties of Seawater

Thursday Afternoon

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

Thursday Afternoon

13. Topics for 15th ICPWS (Berlin)

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

Calculation of Water and Steam Properties for Industrial Use

Thermophysical and Transport Properties in Water, Ice, and Steam

Structure and Dynamics in Aqueous Systems: Spectroscopy and Molecular Simulation

Nonequilibrium, Metastable and Critical States

Thermodynamics and Kinetics in Hydrothermal Systems

Electrochemistry, Corrosion, and Interfaces in High-Temperature Water

Fuel cells, Hydrogen Production, and Renewable Energy

Advanced Techniques and Instruments for Basic Research and Power Plant Applications in High-Temperatures/Pressure Water

Low Temperature and Super-Cooled Aqueous Systems

Supercritical Water and Aqueous Systems

Seawater and Geothermal Systems

Power Cycle Chemistry

Steam Chemistry, Condensation and Deposition Processes

High Efficiency Power Cycles and New Technologies

Environmental Issues in Power Generation

Miscellaneous

A list of the suggested organizers was briefly discussed.

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

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

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

Topic: Interfacial Electrochemistry and Chemistry in High Temperature Media

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

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

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

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

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

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

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

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

15. Data Book

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

16. Gibbs Award Committee

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

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

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

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

THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

<http://www.iapws.org>

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

AGENDA

Witney, England, 3 – 8 September 2006

*Chair: Serguei Lvov, lvov@psu.edu
Pennsylvania State University, University Park, PA, USA*

*Vice-Chair: Horacio Corti, hrcorti@cnea.gov.ar
CNEA, Buenos Aires, Argentina*

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

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

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

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

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

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

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

- Workshop on Properties of Seawater

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

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

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

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



September, 2006

**The
International
Association for the
Properties of Water
and Steam**

<http://www.iapws.org>

Working group Power Cycle Chemistry (PCC)
MINUTES OF IAPWS PCC WG MEETINGS
Witney, United Kingdom 3-8 September, 2006

Chairman: Andre Zeijseink
Members present See addendum 1

Members attended 3 data presentation sessions covering topics set out under the agenda.

1. Amendments/Adoption of Agenda

Andre Zeijseink welcomed new attendees.
There were no amendments to the main Agenda. Additional presentations and revisions to the order of presentation were agreed – see addendum 2.

Members were asked to consider a nomination to sit on the Gibbs Award Committee.
Jim Bellows was nominated and agreed to undertake this task.

2. ELECTION OF CLERK OF MINUTES

Geoff Bignold agreed to record the minutes.

3. Approval of Minutes of 2005 Meeting in Santorini, Greece,

The minutes were agreed without any corrections or additions.

4. International Collaborations

A proposal for a Project on “Improved analysis of low concentrations of particulate oxides in water/steam cycles” had been prepared by Derek Lister, Karol Daucik and Robert Svoboda and circulated for consideration. (Related to priority list item IV.)

The proposal was described by Derek Lister. It covers aspects of a number of items on the priority list, and is directly relevant to a proposed IRCN. It was agreed that the objectives

needed to be more closely defined, so that it would be clear what systems are being considered (steam sampling, water sampling, particulate oxides, iron corrosion products, etc.). The authors discussed this and subsequently provided a more specific set of objectives which received the support of the PCC. The proposal for International Collaboration was agreed upon by PCC; the Executive Secretary was asked for further processing.

5. Priority List Review - postponed pending discussion of status of committee work.

6. Status report on progress on committee work:

6.1 Priority list item #1. To develop an ICRN on “Interfacial situation in advanced ultra supercritical plants” in collaboration with PCAS: Barry Dooley/Don Palmer

The action to provide a draft ICRN had been completed and Robert Svoboda advocated its adoption.

Barry Dooley indicated that EPRI are sponsoring work on chemistry implications of operation up to 760°C. The EPRI programme is more wide ranging, including work on oxide growth and exfoliation (not currently considered as a chemistry issue).

It was agreed that PCC support for the draft ICRN should be confirmed provisional on the agreement of PCAS. The Executive Secretary was asked for further processing.

6.2 Priority list item #2. To develop an ICRN on “Mechanism of Decomposition of Ion-exchange Resin”: Karol Daucik

The draft ICRN had been circulated and Karol Daucik presented it for consideration.

In answer to the question of whether this is a suitable topic for IAPWS, Jim Bellows stated that, if the PCC WG regarded it as important then it is *de facto* suitable. In view of the increasing use of air cooled condensers in hot climates and the need for condensate polishing on these plants, it was agreed that the need for work in this area patently exists.

PCC support for the draft ICRN was confirmed. The Executive Secretary was asked for further processing.

6.3 Priority list item #3. To develop a joint PCAS/PCC ICRN on “Development / Application of Sensors (Ambient and High Temperature Sensors)” : Eric Maughan, Derek Lister, Sunshuke Uchida, Serguei Lvov)

- 6.4** The difficulty of producing a sufficiently well defined ICRN in this general area caused lack of current agreement on how best to take this issue forward. It was acknowledged that progress had been made on ECP measurements in CANDU sampling systems, and BWR primary circuits.

Barry Dooley's view was that the ICRN in this area could be relatively simple and broad ranging. The aim is to interest researchers to work in this area.

The draft joint PCC / PCAS ICRN (E.Maughan, S.N.Lvov) was reviewed and then accepted by PCC. The Executive Secretary was asked for further processing.

There is also the question on the interpretation of such data. It is suggested that this should be subject for another ICRN ("Database for the interpretation of electrochemical sensors data"). Will be done by the same task group for 2007 (Eric Maughan, Jan 2007)

- 6.5** Priority list item #4. To develop an ICRN on "Improved analysis of low concentration of metals (Fe, Cu, Co, etc)": Derek Lister, Karol Daucik.

A draft ICRN, as well as a draft for International Collaboration was sent to the PCC members, discussed, updated and agreed upon. The Executive Secretary was asked for further processing.

It was also agreed that the objectives for the International Collaboration (see item 4) can be narrower than the ICRN and should be corresponding to the proposed resources (PhD student working for ca. 3 months).

- 6.6** Priority list items #5 and #6. It should be considered to make an ICRN covering the priorities of both topics (Task group Bellows, Maughan, Hughes, Bignold, Jan 2007).

- 6.7** Priority list item #8. A draft document by Frank Gabrielli had been circulated and was introduced by Robert Svoboda. For IAPWS this will be a new type of document. Barry Dooley confirmed that such an initiative could be made by PCC WG (comparable to Advisory Notes from TPWS).

General discussion on the draft was favourable: the approach represents good common sense and is a step forward from earlier over simplistic guidance. There are a number of points of detail requiring clarification and amplification and so an *ad hoc* subcommittee (Team/task group: Frank Gabrielli, Jim Bellows, Sven ErikTherkildsen, Marc DeWispelaere, R.Svoboda and G Bignold) is to be convened and further e-mail discussion is expected to follow before agreement of a final text. #8 "Method to determine the mechanical carry-over". The draft will be presented to the PCC members for review by Dec 2006. Target is to send it to the Executive Secretary for review within IAPWS by end February 2007.

6.8 Potential New Activity on behaviour of Amines:

Jim Bellows announced that ASME is planning research and seeking funding to address the question "Do decomposition products of amines discount the benefits of their use?". The chosen system will be ethanolamine with contamination from acetic acid, hydrochloric acid, etc. Work to be done under Digby MacDonald's supervision at Penn State University using ellipsometry and electrochemical noise. Expressions of interest were invited.

Barry Dooley indicated that this would have represented an opportunity for IAPWS| involvement via an international collaboration, although the current need is for project funding rather than provision of a suitable student.

The existing ICRN #5 shall be closed. The closing document has been prepared by E.Maughan and will be transferred to the Executive Secretary for further processing. A follow-up draft ICRN "Research on Amines for the Power Industry" was prepared by E.Maughan and finalized following discussions within PCC. The Executive Secretary was asked for further processing of the closing document as well as of the new ICRN.

7. Priority List Review

7.1 IAPWS Certified Research Needs, Closing statements

#13 "Surface Tension"

The ICRN was originally started by PCC. As there have been no activities in recent years, a recommendation was made by F.Gabrielli to close this ICRN. The 2006 meeting however revealed a new interest of TPWS, who will take over further processing of this ICRN.

7.2 PRIORITY LIST - OTHER PENDING ISSUES

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

and

#6 "The relationship between the chemistry of the contaminants and their concentration at point of measurement"

Consideration is to be given to making a single ICRN covering the priorities of both topics (Task group Bellows, Maughan, Hughes, Bignold, Jan 2007).

7.3 PRIORITY LIST - OTHER ITEMS

#7 "The quantification of risk of asset damage"

A session on this item will be considered for the 2007 meeting. E. Maughan (coordinator) K. Daucik, J. Bellows, A. Rudge, B. Hughes, M. Rziha, A. Zeijseink,

#9 "Improved understanding of condensation mechanisms"

As part of this item, an ICRN on "Improvement of steam turbine efficiency by chemical additives" shall be developed for 2007. (M. Stastny, Jan 2007)

#10 "Deposition of contaminants and corrosion products in steam and water circuits"

This topic should be kept, although there was no PCC activity this year. It is proposed to be reviewed at the 2007 meeting.

#11 "High pressure/high temperature steam and humid air (24MPa and up to 2000°C), thermo-physical properties and chemistry formulation"

To be coordinated with TPWS. Joint workshop PCC / TPWS in 2007 to exchange information on requirements (PCC chairman). Jim Bellows agreed to define needs from the chemical side and to present it at the workshop.

#12 "Radiation chemistry of water"

To be coordinated with PCAS. Joint workshop PCC / PCAS in 2007 to exchange requirements (PCC chairman). Dr Uchida agreed to define requirements from the PCC side for presentation at the workshop.

Derek Lister contacted Peter Tremaine regarding PCAS contacts for radiolysis issues.

7.4 New Items

PCC had considered the draft PCAS ICRN on dew point quantification in flue gas. It was agreed that this is an important topic and should be supported by PCC.

Andy Rudge indicated that there remain open questions on the possible effect of oxygen on two-phase FAC. This, together with other potential items will be reviewed in 2007.

7.5 OLD ICRNS

#5 "Organics"

Discussed under item 7 above.

8. Nuclear Chemistry Session

Copies of the presentations are available.

9. Tasks Distribution - Planning for 15th ICPWS – 2008

PCC discussed the title and session organisation proposals for the 2008 conference. A number of suggestions for the detailed organisation of the conference and for convenors of sessions relevant to PCC activities were put forwards and noted for consideration by the IAPWS executive. The PCC chairman undertook to present the consensus suggestions to the Executive for consideration.

10. News from other international groups, and new developments

PCC noted relevant conferences on organic materials (Stuttgart – 2005) and power plant chemistry (ESKOM 2005) and forthcoming conference on chemical instrumentation (Zurich Sep 2006).

VGB plan to update their chemistry guideline but had not yet sought to convene a group of appropriate experts. Michael Rziha and Robert Svoboda will ensure that VGB are fully aware of IAPWS interest.

The European Standard, EN12952: Part 12, remains in place and is regarded as mandatory in some countries. Richard Harries reported that BIAPWS were actively seeking to have it updated. BIAPWS is now represented on the relevant British Standards Institute committee and is actively lobbying for reconsideration of this standard by the appropriate CEN committee.

11. Membership

PCC unanimously recommended membership of Dr Andy Rudge and Dr Hideki Takiguchi.

12. Preparation of next year's agenda

In addition to progress on ICRN and priority list items covered above, PCC will plan short joint workshops on radiation chemistry, dew point issues and assessment of risks of damage.

13. Election of Officers

Andre Zeijseink is now standing down as chairman.

Robert Svoboda was unanimously elected to be proposed to the EC as new PCC chairman.

14. Preparation of the Report to EC

Report to be based on these minutes.

15. Miscellaneous and Adjournment

Jim Bellows requested input for the IAPWS Press Release.

Derek Lister proposed the thanks of the membership to Andre Zeijseink for his chairmanship over the last five years.

Robert Svoboda proposed to perform work on PCC action list earlier in the year as has been done in 2006, so the technical discussion will take place to a good part by E-mail, and more time at the annual meeting is left for new issues.

It is to be noted that last year's meeting was followed up by publications on 5 PCC presentations, and 1 further still pending. Acknowledgement is given to the authors.

ADDENDUM 1 – Attendees

Malcolm Ball	U.K.
James Bellows	USA
Geoff Bignold	U.K.
Karol Daucik	Denmark
Barry Dooley	USA
Andreas Drexler	Germany
Roy Fyfield	U.K.
Fionn Griffin	Ireland
Richard Harries	U.K.
Alex Hörig	Germany
Eric Huff	U.K.
J. Barry Hughes	U.K.
Derek Lister	Canada
Eric Maughan	Germany
Han Pflug	Germany
Michael Rziha	Germany
Andy Rudge	U.K.
Michael Sparrey	U.K.
Miroslav Štastný	Czech Republic
Robert Svoboda	Switzerland
Hideki Takiguchi	Japan
Svend-Erik Therkildsen	Denmark
Shunseke Uchida	Japan
Sonia Vidoikovitch	Serbia
Andre Zeijseink	Netherlands

ADDENDUM 2 - Agenda

1. Amendments/Adoption of Agenda
2. ELECTION OF CLERK OF MINUTES
3. Approval of Minutes of 2005 Meeting in Santorini, Greece, action points (see also point 6)
4. International Collaborations
5. Priority List Review
6. Status report on progress on committee work:
 - 1 To develop an ICRN on "Interfacial situation in advanced ultra supercritical plants" in collaboration with PCAS: Barry Dooley/Don Palmer
 - 2 To develop an ICRN on "Mechanism of Decomposition of Ion-exchange Resin": Karol Daucik
 - 3 To develop a joint PCAS/PCC ICRN on "Development / Application of Sensors (Ambient and High Temperature Sensors)" : Eric Maughan, Derek Lister, Sunshuke Uchida, Serguei Lvov
 - 4 To develop an ICRN on "Improved analysis of low concentration of metals (Fe, Cu, Co, etc)": Derek Lister, Karol Daucik
 - 5 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: Jim Bellows, Eric Maughan, Barry Hughes, and Geoff Bignold (Draft prepared and presented to PCC on 7 July 2005)
 - 6 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: Frank Gabrielli, Jim Bellows, Sven Erik Therkildsen, Marc DeWispelaere and R. Svoboda
- 7 New tasks distribution list

Intermezzo 1: joint workshop with PCAS

- Research Presentations on Physical Chemistry for Power Generation
 - **S.N. Lvov**, Z. Zhou, E. Chalkova, V.N. Balashov, and P. Chou, "Development of Hydrothermal Coating Technology to Mitigate Intergranular Stress Corrosion Cracking in BWRs"
 - **G. Bignold**: Chemical Properties Issues arising in recent Power Cycle Chemistry Studies
 - **Stastny M.**, Blahova O., Jiricek I., Lorenc B. " Effects of Steam Chemistry on the Turbine Blades in Transition Zone".
 - **Vidoikovitch, S.**, " Influence of Water Chemistry on the Economizer Inner Wall Condition"

- **P. Tremaine:** "Phosphate titanium interactions under boiler conditions"
 - **A. Rudge:** "Chemistry issues related to control of rippled magnetite development"
6. Progress on committee work (continued)
 7. IAPWS Certified Research Needs, Closing statements and new proposals (joint ICRN of PCC / PCAS on "Development/Application of Sensors (Ambient and High Temperature Sensors))
 8. Nuclear Chemistry Session:
 - **D. Lister:** Flow Accelerated Corrosion in Nuclear Reactor Primary Coolants
 - **A. Drexler:** Experiences with FAC in German PWRs
 - **S. Uchida:** Deposition and Release of Crud and Metallic Ions on Boiling Surfaces and Change in their Chemical Form
 - **H. Takiguchi:** Development of Environmental Remedies against FAC in Secondary System of Tsugura-2 PWR
 - **G. Bignold:** Erosion-corrosion or 'FAC' as it is now known
 - **S. Uchida:** Evaluation Method for Flow Accelerated Corrosion of Components by Corrosion Analysis Coupled with Flow Dynamics Analysis

Intermezzo 2: joint workshop with TPWS, IRS, PCAS:

Properties of Seawater (**R. Feistel**),

- A brief history and current activities of the International Association for the Physical Science of the Oceans (IAPSO)
 - Liaison with IAPSO, Letters between the IAPWS President and the President of IAPSO
 - Oceanographic Seawater Standards
 - Unit for the Salinity of Seawater, Conflict with ISO
 - Development of an Extended Formulation of the Thermodynamic Properties of Seawater
 - Physical Chemistry of Vents, Critical Properties
 - Request for Measurements/Instruments
9. Tasks distribution
 10. News from other international groups, and new developments
 11. Membership
 12. Preparation of next year's agenda
 13. Election of Officers
 14. Preparation of the Report to EC
 15. Miscellaneous and Adjournment

APPENDIX
Working group Power Cycle Chemistry (PCC)
Action List for IAPWS PCC WG Meetings

Participant(s)	Action	Deadline
J. Bellows	To represent PCC on the IAPWS Gibbs Award Committee.	
B. Dooley	To progress the PCC following proposals for approval by IAPWS: 1) draft ICRN Priority List topic #1 2) draft ICRN Priority List topic #2 3) draft ICRN Priority List topic #3 4) draft ICRN and International Collaboration Priority List topic #4 5) closure document for ICRN #5 and the draft follow-up ICRN ("Amines")	8 Sept 2006
<u>E. Maughan</u> , D. Lister, S. Uchida, S. Lvov	To develop an ICRN covering the generation of a database for the interpretation of electrochemical sensors data.	Jan 2007
<u>J. Bellows</u> , E. Maughan, J.B. Hughes, G. Bignold,	To develop an ICRN combining the topics: Corrosion mechanisms that are related to the presence of contaminants in steam/water circuits, particularly in boiler-water and The relationships between the chemistry of the contaminants and their concentration at point of measurement	Jan 2007
<u>F. Gabrielli</u> , J. Bellows, S-E. Therkildsen, M. deWispelaere, R. Svoboda, G. Bignold	To develop further the draft guidance note on method for the determination of mechanical carry-over in boiler drums.	Draft to PCC members for review by Dec 2006.
E. Maughan	To co-ordinate a session at the 2007 IAPWS PCC meeting on the quantification of risk of asset damage.	2007 meeting
M. Stastny	To develop an ICRN on improvement of steam turbine efficiency by chemical additives.	May 2007
PCC chairman	To coordinate with TPWS arrangements for a Joint PCC / TPWS workshop on requirements related to high pressure/high temperature steam and humid air (24MPa and up to 2000°C).	2007 meeting
J. Bellows	To define needs from the chemical side and to present it at the workshop.	
PCC chairman	To coordinate with PCAS arrangements for a joint PCC/ PCAS workshop on radiation chemistry of water	2007 meeting
S. Uchida	Dr Uchida agreed to define requirements from the PCC side for presentation at the workshop.	

Participant(s)	Action	Deadline
A. Zeijseink	To propose that IAPWS Executive approve PCC membership of Dr Andy Rudge and Dr Hideki Takiguchi.	8 Sept 2006
A. Zeijseink	To present to IAPWS Executive a summary of PCC recommendations with regard to the ICPWS to be held in 2008.	8 Sept 2006
PCC Chairman	To approach contributors to PCC workshops 2006 to consider making a manuscript to be published in a technical or engineering magazine to be selected	30 Sep 2006

IAPWS WG PCC

04 September 2006

PROPOSAL FOR IAPWS SUPPORT TO INTERNATIONAL COLLABORATION PROJECT

**Improved analysis of low concentrations of particulate metal oxides in water/steam
cycles**

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YOUNG SCIENTIST

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BACKGROUND

The formation and transport of corrosion products in water/steam cycles has been a major problem since the inception of thermal energy circuits. The determination of corrosion product concentrations has subsequently become a very important method of monitoring the chemical state of an operating unit. Since the solubility of the corrosion products is rather low at the conditions of the water/steam cycle, they appear mainly as particulates. This complicates the sampling, as the heterogeneous character of the system can easily lead to partial separation of phases resulting in non-representative sampling. This problem becomes particularly pronounced at low concentrations of corrosion products.

The subject has received attention in several publications and even specific procedural norms have been issued (1). However, the norms have found little application in practice because of their high cost and inability to achieve reliable results. The only comprehensive work concentrating on steam sampling, where most of the critical parameters are evaluated (2), deals with the design of sampling equipment. Most power utilities analyse the corrosion products at different places in the cycle and have different designs of equipment and use their own procedures. The reliability of the data is poor and outliers occur frequently.

Several members of IAPWS WG PCC are involved in minor investigations verifying the effects of different parameters on the reliability of corrosion product analyses; however, an overall evaluation of

the sampling and analysis of corrosion products in water/steam cycles is missing. A general agreement on system design and operating procedures for sampling would be of great value to industry.

OBJECTIVE

The objective of this project is to assemble the experience within IAPWS WG PCC on the sampling of corrosion products from steam/water cycles, augment it with published information and then provide an assessment of the state of the art. WG PCC will on this basis issue a recommendation for reliable practice.

It is acknowledged that the overall subject of sampling and analysing corrosion products from coolant systems is extensive and complex. The scope of this proposed collaboration therefore concentrates on issues that are of immediate concern to both steam and water systems in operating plants, namely:

- how representative are measurements taken from cooled samples obtained at the end of a (usually) iron-containing-alloy sample line?
- how precise does a measurement of iron corrosion products need to be at the <1ppb and the >1ppb level?
- what is the partition of iron between particles and solubles at those levels?

COMPLETION

The young scientist will visit three members (Canada, Switzerland and Denmark) of the WG PCC, which are in possession of unpublished data and experience related to the sampling of corrosion products. He will on the basis of this material and the published work produce an assessment of the state of the art.

Deliverables

Report on "Assessment of the State of the Art of Sampling of Corrosion Products from Water/Steam Cycles".

TIME SCHEDULE

The work will be done in autumn 2006. The stay in Canada, Switzerland and Denmark will take about one week in each country. The literature study and reporting will take 5 weeks.

Budget

Item	Cost (\$US)	Sponsor
Travelling young scientist	3 500	
Cost of living young scientist	3 000	
Sub sum	6 500	IAPWS
Local costs	1 500	
Time participants	15 000	
Sub sum	16 500	Participants
Total cost	22 000	

Required contribution from IAPWS is \$ 6 500.

References

- 1 Standard Practice for Sampling Steam, ASTM D-1066-97.
- 2 Jonas Inc., Development of a Steam Sampling System, EPRI TR-100196, Dec. 1991.

YOUNG SCIENTIST IAPWS FELLOWSHIP PROJECT

**Predictive Scheme for Standard Thermodynamic Properties of Aqueous
Substituted Benzenes over a Wide Range of Temperatures and
Pressures**

IAPWS Sponsors

Peter R. Tremaine

Professor

Department of Chemistry

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Guelph, Ontario, Canada N1G 2W1

Josef Sedlbauer

Professor

Department of Chemistry

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461 19 Liberec, Czech Republic

Young Scientist

Jana Ehlerova

PhD Student

Department of Chemistry

Technical University of Liberec

46119 Liberec, Czech Republic

August 24, 2006

Background and Scope

This project is aimed at measuring the high-temperature thermodynamic properties of aqueous solutions of organic compounds. The development and application of instruments capable of operating up to and above 300°C at the University of Delaware, Blais Pascal University in Clermont-Ferrand, the CNEA (Argentina), the University of Guelph, the Institute of Chemical Technology in Prague, the University of Lethbridge and other laboratories during the last ten years has made it possible to launch a systematic evaluation and modeling of these systems. Because of the experimental difficulties of such measurements, much attention has been focused on the development of models that are based on a group contribution approximation. Such models are, however, often constrained by an incomplete experimental database and are applied only to the thermodynamic property (or properties) measured in the authors' own laboratories. The only group contribution schemes providing a complete description of standard state thermodynamic properties at high temperatures and pressures for a wide set of aqueous organics have been up to recently those by Amend and Helgeson (*Geochim. Cosmochim. Acta* 1997, **61**, 11-46) and Criss and Wood (*J. Chem. Thermodyn.* 1996, **28**, 723-741). The first method is based on the modified Helgeson-Kirkham-Flowers model for standard partial molar properties; the second is based on the "density" model. Both papers are based on data available in 1996. These are just a small fraction of experimental data available nowadays, leading generally to only semi-quantitative predictions. A new approach, which is based on the Sedlbauer-O'Connell-Wood (SOCW) equation of state, was published by Yezdimer *et al.* (*Chem. Geol.* 2000, **164**, 259-280). This treatment included simultaneous parameterization of the model by most available results on standard molar derivative properties (volumes and heat capacities): no other data were, however, taken into account. A systematic attempt to improve this method was initiated in the last few years, leading to exhaustive data compilation and model parameterization for aqueous aliphatic, aromatic and cyclic hydrocarbons (Sedlbauer *et al.*, *AIChE J.* 2002, **48**, 2936-2959), phenols and anilines (Censky *et al.*, *Cosmochim. Acta*, 2006, in press) and ketones, ethers and esters (Sedlbauer and Slavik, *J. Solution Chem.*, in press.).

The group contribution scheme based on the SOCW model has been designed from the beginning to incorporate three basic features:

- 1) It is extendable, i.e. new substituent functional groups can be added to the scheme with the properties of the hydrocarbon backbone and other already determined groups unchanged by this addition.
- 2) The extension is always based on careful compilation and presentation of available data on all standard molar thermodynamic properties (including their

- 3) evaluation from experimental results on related quantities such as Henry's law constants, phase equilibrium data, dissociation constants etc.). The data base is open to be used in the future for parameterization of other models, if proved more suitable than the SOCW model.
- 4) Adding just a few functional groups at a time and collaboration with the prime experimental laboratories specialized in high temperature thermodynamics of aqueous systems allows supplementing the existing data bases with targeted experimental efforts, needed for reliable representation of the new functional groups in a wide range of conditions. This approach was already used in case of anilines, phenols, ketones, ethers and esters (on-purpose experimental studies were published preceding the extension of the group contribution scheme).

Project Objectives

The purpose of the project is to extend the high temperature group contribution scheme by addition of nitro- functional group directly bound to aromatic ring and of phenolate (charged) functional group. Aromatic nitro compounds are often applied technologically and their effluents belong among the most environmentally sensitive systems. Phenolates appear in large amounts namely as intermediates in the production of phenol and due to their solubility constitute an important part of waste waters from such processes.

The project has two main objectives:

- 1) To develop the extended group contribution scheme by simultaneous treatment of all available standard thermodynamic data for nitro- and phenolate aqueous systems. In both cases it is expected that, in addition to NO_2^- and $-\text{O}^-$ first order groups, the second order functional groups will be also needed, correcting for near neighbor interactions (namely two substituents in *ortho*- position). The model extension will be based on literature compilation and data evaluation that will have to include high temperatures as well as the reference conditions (298 K, 0.1 MPa) used as integration constants in the SOCW model.
- 2) To supplement the existing scarce experimental results available for these aqueous systems at high temperatures by measurements of the ionization constants of isomeric *ortho*-, *meta*-, and *para*-nitrophenols up to 250°C using hydrothermal indicators and UV-VIS spectroscopy. A unique apparatus of this type is available at the University of Guelph, where the experimental part of the project should be accomplished. The choice of nitrophenols as target solutes had two reasons: i) their solubility is larger than solubility of non-polar aromatic

- 3) solutes, e.g. nitrobenzene, allowing measurements of the standard derivative properties to be made also. (It is expected that Ms. Ehlerova will complete the experimental study by measuring the standard molar heat capacities of nitrophenols to high temperatures at Universite Blaise Pascal, Clermont-Ferrand: this stay will be financed by the European exchange program Socrates); ii) as weak acids, nitrophenols are suitable for measurements of the ionization constants and include both functional groups of interest.

The work at Guelph will be carried out under the co-supervision of Dr. Sedlbauer, Dr. Tremaine and Dr. Liliana Trevani. The project will make use of the high-temperature UV-visible flow system developed by Trevani *et al.* (*J. Solution Chem.* 2001, **30**, 585–621) and thermally stable colorimetric indicators developed by Keith Johnston's group at the University of Texas (Austin), as used in our laboratory at temperatures up to 350 °C (Clarke *et al.*, *Geochim. Cosmochim. Acta* 2005, **69**, 3029-3043; Bulemela *et al.*, *J. Solution Chem.* 2005, **34**, 769–788). The nitro-phenol UV-visible spectra overlap with the colorimetric indicator spectra, and it may be possible to measure the ionization constants at high temperature directly, by determining the ratio of the ionic and neutral forms in standard buffers with known pH. Both approaches will be tried.

Justification for IAPWS Support

The IAPWS funding will make it possible for the young scientist to spend at the University of Guelph for four months in a single stay starting in the fall of 2006. The purpose of this visit will be collaboration with Prof. Tremaine and Dr. Trevani on experimental determinations of the ionization constant of nitrophenols under a wide range of conditions using high temperature UV-visible spectroscopy. Subsequently the two teams from the University of Guelph and from the Technical University of Liberec will cooperate on development of the extended group contribution scheme for aqueous nitro-substituted aromates and aqueous phenolates. Involved in this part of the project will be also Prof. Mayer from the Blaise Pascal University in Clermont-Ferrand.

Budget (in \$US)

Subsistence for 4 months: IAPWS Young Scientist Grant.....	\$6000
Travel (round trip): to be paid by TU Liberec.....	\$1500
Chemicals, supplies, equipment: to be paid by U. Guelph.....	\$4500
Total	\$12000

**PRESS RELEASE FOR IAPWS ANNUAL MEETING AT WITNEY, OXFORDSHIRE, UK
September 3-8, 2006**

Sixty scientists and engineers from thirteen countries attended the annual meetings of the International Association for the Properties of Water and Steam (IAPWS), September 3-8, 2006 on in Witney, Oxfordshire, United Kingdom. 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.

The IAPWS delegates were joined by an additional 36 people from England and Ireland for a symposium on power cycle chemistry. New methods of power generation and current issues in power cycle chemistry, such as the use of amines for pH control were featured. In a separate session, issues in nuclear power plant chemistry, particularly those related to flow assisted corrosion, were featured.

A highlight of the 2006 meeting was the workshop on seawater properties and standard seawater. Representatives from the International Association for the Physical Sciences of the Ocean (IAPSO) explained the difficulties in the IAPSO standards. IAPSO and IAPWS will cooperate in developing new seawater standards. This cooperation will require extending the IAPWS-95 formulation to subcooled water, since seawater freezes below the current lower limit of the triple point of water.

A new IAPWS Release “Equation of State for H₂O Ice Ih” was approved and should appear on the IAPWS website shortly. Work continues on new documents which will describe the viscosity of water and the ionization of constant of water.

IAPWS produces Certified Research Needs (ICRN) as guidance for funding agencies and as an aid to people doing research in defining important research. This year several ICRN's were approved in principle at the meeting and will appear on the IAPWS website as they are made final. The ICRN's approved this year concerned thermophysical properties associated with ultra-supercritical coal-fired steam generators; mechanism of decomposition of ion-exchange resin; development and application of ambient and high temperature sensors; and improved analysis of low concentration of metals.

Equations for thermophysical properties of water and aqueous systems have long been and continue to be an interest of IAPWS. The IAPWS Helmholtz Award lecture this year, “Corresponding States: A General Theory Including Aqueous States,” by Hong Wei Xiang of the Chinese Academy of Sciences, provided additional insights in this field. 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.

A plan to understand the corrosion and catalysis at metal surfaces related to ultrasupercritical power plants continues. It includes a symposium on “Interfacial Electrochemistry and Chemistry in High Temperature Media” to be conducted at the Joint Electrochemical Society (ECS)-IAPWS Symposium (Washington, D.C., 2007). The aim of the

symposium is to provide deeper insight into chemical and electrochemical processes at all kinds of interfaces and to elucidate the significant effects of the interfacial processes on the properties and behavior of materials in high temperature aqueous environments. Of particular interest are the high temperature interfacial processes related to water cycles in current and next-generation fossil fuel and nuclear power plants, fuel cells and batteries, hydrogen production and storage, photovoltaics, hydrothermal/electrochemical synthesis of materials, corrosion and passivation of high-performance alloys, etc. (Links will appear on the IAPWS website when the symposium is organized.)

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. The book is expected to be completed by the end of 2006.

In response to advanced energy cycles identified by industrial members, a revision to IAPWS-IF7 (Industrial Formulation) will increase the upper pressure limit of Region 5, which covers the high temperature range of steam from 800 to 2000°C, from 10 MPa to 50 MPa. It is anticipated that this revised release will be adopted by IAPWS at next year's annual meeting.

An international collaboration project on "Predictive Scheme for Standard Thermodynamic Properties of Aqueous Substitutes Benzenes over a Wide Range of Temperatures and Pressures" will be carried out by Jana Ehlerova, a Czech Republic student, from the Technical University of Liberec at the University of Guelph (Canada). A second international collaboration on improvements in power plant sampling techniques will send Piti Srisukvatananan from the University of New Brunswick to Alstom in Switzerland and Elsam Power in Denmark.

The next IAPWS meeting will be in Switzerland, near the start of September, 2007. Details of the meeting will be available through links from the IAPWS website at www.iapws.org. Minutes of the 2006 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*, are available (see link on Website). The 15th International Conference on Properties of Water and Steam is planned for Berlin, Germany in September 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 (bdooley@epri.com).

**BRITISH AND IRISH ASSOCIATION FOR
THE PROPERTIES OF WATER AND STEAM
(BIAPWS)**

A Member of the International Association for the Properties of Water and Steam
www.biapws.org

BIAPWS Annual Report to IAPWS for 2005/06.

BIAPWS continues with a strong membership, with 13 Industrial Sponsors, all of whom are associated with the power generation industry. BIAPWS maintains links, through corresponding members, with academic institutions but has only one active academic member of the committee. Currently, BIAPWS has no active links with any research based institution.

BIAPWS has recently become a member of the British Standards Institute, representing the power generation industry on aspects of steam and water chemistry in the power cycle relative to recently issued European standards on boiler water chemistry.

The BIAPWS Award scheme has been modified to offer an undergraduate bursary for summer vacation work experience in a suitably relevant industry.

Membership.

There has been one additional industrial sponsor of BIAPWS in the past year. The sponsors of BIAPWS are currently: power generation companies (8); power plant manufacturers (2); chemical instrumentation suppliers (2); and technical support organisations (1).

The academic support remains as last year with 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 four 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. Two further ex power company associates are corresponding members

BIAPWS is a member of the British Standards Institute.

BIAPWS is sponsored by: Alstom Power Ltd; ABB Ltd; Amec NNC Ltd; British Energy Generation Ltd.; EDF Energy plc; ESB (Eire); E.ON UK plc; PX Ltd; Hach Ultra Analytics Ltd; Rolls-Royce plc; RWE-npower plc; Scottish Power plc; Thames Power Services Ltd.

Chairman: Dr R R Harries, Power Chemistry Consulting, 6, Montague Drive, Loughborough, Leics. LE11 3SB., UK.

Secretary: Mr M Ball, 48, Leconfield Road, Loughborough, Leics. LE11 3SQ., UK.

Treasurer: Mr E G Huff, Plush Hill, All Stretton, Shropshire, SY6 6JP., UK

Research.

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 in the BIAPWS agenda. The level of academic research into topics of interest to BIAPWS/IAPWS, appears to remain low in the UK. However, with IAPWS expanding its sphere of interest into environmental areas the scope for research may increase.

British Standards Institute.

BIAPWS has been invited to become a member of the British Standards Institute, the body responsible for issuing British Standards and European Standards in Britain. BIAPWS will represent the power industry views in the area of steam and water chemistry as applied to power generation cycles.

Education and Outreach.

BIAPWS continues to see 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.

A large number of alternative schemes have been raised and discussed by BIAPWS.

BIAPWS Symposia.

BIAPWS continues to organise regular symposia on topics of interest to power plant operators and suppliers. This theme is continued in 2006 with the BIAPWS Symposium incorporated into the IAPWS Annual Meeting on the topic "Advances in power plant chemistry; current trends and future developments". This has an environmental bias as well as addressing traditional water and steam cycle chemistry issues.

BIAPWS Award.

The BIAPWS Award was conceived 4 years ago, offering a cash prize to undergraduates for submission of final year project reports on topics relevant to the measurement or application of the properties of water and steam. For various reasons the award has only been made once. The quality of the (few) submissions was not high and there appeared to be a clear problem in accessing UK academic institutions, although chemistry, chemical engineering and mechanical engineering departments were all circularised.

There is an implication that BIAPWS (and IAPWS) does not have a high profile in UK universities and attempts to open dialogue with learned institutions on the possibility of joint awards have also foundered.

BIAPWS Student Bursary.

To overcome some of the above problems 2006 has seen BIAPWS institute a student bursary, initially for one undergraduate student, where BIAPWS jointly funds a summer vacation placement with one of its industrial sponsors. The first such placement, with the technical and engineering department of a power generation company, has been very successful. The candidate gained an appreciation of the wide application of chemistry of water and steam in power plants as well as gaining skills in research tools and report writing.

BIAPWS Future.

BIAPWS will continue to act as the central point for co-ordinating the properties of water and steam and their application to industry, particularly power generation in the UK and Ireland.

BIAPWS will continue to seek ways to widen the knowledge of the properties of water and steam and their industrial applications, particularly through financial support to undergraduate students and other appropriate initiatives.

Richard Harries
Chairman BIAPWS
September 2006.

IAPWS CANADIAN NATIONAL COMMITTEE

Annual Report 2006

Executive: *Peter Tremaine (Chair); David Guzonas (Secretary Treasurer); Igor Svishev (Past Chair); Derek Lister (Member at Large); Candu Owners Group Representative (TBD).*

1. Canadian National Committee: Dues for the Canadian National Committee are supported by the National Research Council, which requires an industrial partner. Three years ago, the Canadian Electrical Association withdrew as the industrial partner for IAPWS, and it has been replaced by the Candu Owner's Group ("COG") on a three year trial basis. The Canadian Committee must submit a proposal this fall for continued participation and funding. Interest from the thermal industry has fallen, but the creation of ("UNENE") has created a vibrant research climate in nuclear R&D and we are optimistic..

2. University Network of Excellence in Nuclear Engineering (UNENE). The Canadian government and nuclear industry are co-funding an initiative to create a number of NSERC University Research Chairs which will form a research network, and common postgraduate MSc program in nuclear engineering. Companies are: Atomic Energy of Canada Ltd. Ontario Power Generation, Bruce Power, CANDU Owners Group. Some of the Chairs relevant to IAPWS are listed below:

Roger Newman (University of Toronto): Corrosion, materials performance, electrochemistry.in primary secondary coolant

Dave Shoesmith (University of Western Ontario): Electrochemistry, materials performance and corrosion for high-level nuclear waste repositories.

Clara Wren (University of Western Ontario): Radiolysis and radiochemistry under nuclear reactor primary-coolant conditions, and reactor accident scenarios.

Three Canadian IAPWS National Committee Members are involved with UNENE, as sponsoring industrial participants or as members of universities who are associate members in UNENE are:

Derek Lister: (University of New Brunswick, Associate Member of UNENE) Primary and secondary coolant chemistry, activity transport, corrosion.

Peter Tremaine: (University of Guelph, Associate Member): Solution thermodynamics, phase relations, and solubility in sub-critical and super-critical water; also D₂O isotope effects under CANDU-PHW conditions.

Dave Guzonas (Atomic Energy of Canada Ltd.) Section Leader, Reactor Chemistry Group. Materials performance and chemistry control in primary and secondary coolant circuits.

3. Other Research Relevant to IAPWS

Other researchers with active programs in high-temperature water chemistry are:

Vladimiro Papangelakis (University of Toronto) Hydrometallurgy of pressure-leach processes involving nickel, cobalt, copper and zinc ores.

Paul Percival (Simon Fraser University): Muonium ion chemistry and radiolysis in sub-critical and super-critical water using the TRIUMF cyclotron national facility.

Alan Anderson (St. Francis Xavier University); Solubility and phase relations in supercritical water using diamond anvil cell methods.

Proposals to fund a 1.5 M\$ experimental laboratory for high-pressure, high-temperature water chemistry at the University of Guelph, and a \$300,000 supercritical autoclave loop at the University of New Brunswick are under review by the Canadian “CFI” program.

A new program to fund research on a Generation IV super-critical water reactor is expected to be announced in early 2007.

**THE CZECH NATIONAL COMMITTEE
INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM**

REPORT on IAPWS related activities – August 2005 / August 2006

Submitted to the EC Meeting of IAPWS, Witney – September 2006.

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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 and Department of, 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 Theory and Design of Power Plants, Univerzitní 8, CZ-306 14 Plzen

SKODA POWER, Plzen, Inc., 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, Sigmunda, Lutín

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

- Dr. Hruby (IT) investigated nucleation and measured properties of supercooled water and surface tension. He was the chairman of IAPWS team for evaluation of formulation of thermodynamic properties of ice. Refs [1, 2].
- Prof. Mares (UWB) was charged with chairmanship of the IAPWS task group on evaluation of a new formulation for viscosity of water. Ref. [3].
- Prof. Mares (UWB) with his collaborators measured surface tension of supercooled metastable water and extrapolated the Formulation IAPWS-95 to region of the supercooled metastable liquid down to -37°C. Refs [4 to 6].

- Prof. Mares (UWB) prepared extension of the region 5 of the formulation IAPWS-IF97. Ref. [7].
- Prof. Marsik (IT) coordinated research in the metastable states and nucleation and lectured on modeling of fuel cells. Refs. [8 to 11].
- Prof. Sedlbauer (TUL) and his team collaborated with Profs. Majer (France) and Wood (U.S.A.) and investigated thermodynamic properties of hydration for selected organic solutes. Refs [12 to 16].
- Dr. Patek (IT) prepared formulation of the thermodynamic properties of LiBr-H₂O solutions. Ref. [17].
- Research activities at the (CTU) have continued during the period 8/2005 – 6/2006 in further improvement of current knowledge on the following subjects:
 - Diagnostics of wet steam i.e. measurement of droplet size spectra and steam quality. The tests were carried out in the fossil (210 MW) and (360 MW) LP steam turbines with optical extinction probe.
 - 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 nozzle and in the new special sampling line supplied both with the laboratory steam.
- Research activities at the (TU) were oriented to:
 - Development of interactive graphical software "Moist Air" with IAPWS equations for application for heating, ventilation and air conditioning, Ref. [18].
 - Development of software for interferogram evaluation of refractive index and temperature fields in water with the IAPWS equations, Refs [19 to 22].
 - Measurements of bulk viscosity and speed of sound in water, Ref. [23]
- In SIGMA Research and Development Institute the activities included experimental and numerical modelling of bubble nucleation and cavitation in pumps as well as the investigation of the effect of water properties on these phenomena, Ref. [24].
- Dr. Jiricek (ICT-IE) with collaborators investigated corrosion processes and chemical effects in water and steam systems of power plants. Refs [25 to 27]. ICT-IE will organize the 6th International Power Cycle Conference (CHEO 6), held from 11th to 13th September, 2006.
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles and conference fulltexts are under Refs [28 to 38].
- Prof. Stastny (SKODA POWER) with co-workers studied effects of deposits on the blades of MP parts of steam turbine in fossil power station, measured degradation of steam turbine blade surfaces by deposits of chemicals, and compared numerical models of the water steam flow with hetero-homogeneous condensation in nozzles and in blade cascade, Refs [39 to 43].

- Dr. Kodl (SKODA POWER) prepared information on application of IAPWS data in calculation in SKODA, Ref. [44].
- Dr. Zmitko (NRI) studied effects of simultaneous influence of irradiation, water chemistry at high pressures and temperatures on behavior of nuclear power plants structural materials and components and collaborated with nuclear power plants mainly on water chemistry, corrosion problems and radiation control. Following activities were carried out:
 - monitoring and evaluation of primary water chemistry and radiation situation at units 1 and 2 of the Temelín Nuclear Power Station, Refs [45,46]
 - investigation of fuel rod cladding materials (eg. Zircaloy-4 alloy, Zr-1%Nb alloy) corrosion behavior at specific VVER water chemistry conditions.
 - 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).

Young Scientists IAPWS Fellowships

- T. Nemec, the fellowship holder of the 2003 Young Scientists IAPWS (CZ-US) Project "*Thermodynamics of Binary Homogeneous Nucleation in Superheated Steam*" under supervising Prof. Maršík, Dr. Hrubý, Dr. Palmer, and Dr. Simonson, submitted his PhD. thesis. Ref. [11]. His new publications are in Refs [8, 9, 11].
- O. Mican performs his Young Scientist IAPWS (CZ-US) 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.

His Final Report of the Project will be finished by the end of the year 2006. Preliminary results he will present at the 2006 IAPWS Meeting. Ref. [10].

- Prof. J. Sedlbauer (CZ) and Prof. P. R. Tremaine (Canada) (WG PCAS) prepared a Proposal for Young Scientist IAPWS Project for J. Ehlerova "*Predictive Scheme for Standard Thermodynamic Properties of Aqueous Substituted Benzenes over a Wide Range of Temperatures and Pressures*". The project has two main objectives:
 - to develop the extended group contribution scheme by simultaneous treatment of all available standard thermodynamic data for nitro- and phenolate aqueous systems,
 - to supplement the existing scarce experimental results available on these aqueous systems at high temperatures by measurements of the ionization

constants of isomeric nitrophenols to 250°C using hydrothermal indicators and UV-VIS spectroscopy.

The CZ NC PWS fully recommends this project to the EC IAPWS to support it.

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DANISH NATIONAL IAPWS COMMITTEE - DIAPWS

c/o IDA, Kalvebod Brygge 31 - 33, 1780 Copenhagen V

8 February 2005

IAPWS REPORT 2004 AND 2005

The research activities in 2004 and 2005 in Denmark in the field of properties of water and steam were mainly concentrated at the Technical University of Denmark, Copenhagen:

- Modelling of multicomponent aqueous electrolyte systems and application of models to the recycling process for fertilizer from straw ash residues.
- Measurements and modelling of density and viscosity of multicomponent aqueous electrolyte solutions are in progress. The aim is to predict the scaling in hydrogeological systems. Pressure parameters are added to the Extended UNIQUAC model presented by Thomsen and Rasmussen (1999). The improved model is used for correlation and prediction of solid-liquid equilibrium of scaling minerals (CaSO_4 , $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$, BaSO_4 and SrSO_4) at temperatures up to 300C and pressures up to 1000 bar. The results show, that the Extended UNIQUAC model with the proposed pressure parameters is able to represent binary, ternary and quaternary solubility data within the experimental accuracy in the temperature range from -20 to 300C, and the pressure range from 1 to 1000 bar.
- Modelling of ion exchange processes, particularly with focus on removal of vanadium from effluent waters.

The research at the utilities have concentrated on new methods for monitoring of carbon dioxide in water/steam cycle.

Publications:

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Svend-Erik Therkildsen, A 23 Years Old Reheater Acid Cleaned at Asnaes Power Plant, 14. ICPWS, Kyoto, Japan, Aug 29 – Sept. 3, 2004.

Karol Daucik, Solubility of Sodium Sulphate in Steam in the Vicinity of the Critical Point, 14. ICPWS, Kyoto, Japan, Aug 29 – Sept. 3, 2004.

Kaj Thomsen, Maria Iliuta, and Peter Rasmussen "Extended UNIQUAC model for correlation and prediction of vapor-liquid-liquid-solid equilibria in aqueous salt systems containing non-electrolytes. Part B. Alcohol (Ethanol, Propanols, Butanols) - water - salt systems". (Chemical Engineering Science 59(2004)3631-3647, issue 17)

Kaj Thomsen, Chapter on: "Thermodynamics of Electrolyte Systems of Industry", Published in Chemical Thermodynamics for Industry, (RSC books, 2004), Edited by T.M. Letcher

Ada Villafañila García, Kaj Thomsen, and Erling Stenby, "Prediction of Mineral Scale Formation in Geothermal and Oilfield Operations using the Extended UNIQUAC Model. Part I: Sulphate Scaling Minerals" (Accepted for publication in Geothermics).

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GERMAN NATIONAL COMMITTEE TO IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam

Report "Research in Progress 2006"

Baltic Sea Research Institute, Warnemünde, Germany, Dr. rer. nat. habil. R. Feistel

1. Final preparation of the „Release of an Equation of State of Ice Ih“, expected to be issued by IAPWS in 2006
2. Publication of “A New Equation of State of Ice Ih” by R. Feistel and W. Wagner, in J. Phys. Chem. Ref. Data, 35, 2 (2006) 1021-1047
3. New correlation equations of the sublimation pressure and the sublimation enthalpy of ice Ih between 20 K and 273.16 K, paper by R. Feistel and W. Wagner, accepted at Geochimica et Cosmochimica Acta, 2006.
4. New correlation equations of the melting pressure and the melting enthalpy of ice Ih between 0.1 MPa and 210 MPa, unpublished, to be presented at the IAPWS meeting in Witney.
5. A “Gibbs-Pitzer Function for High-Salinity Seawater Thermodynamics” by R. Feistel and G. M. Marion, valid for -7 to 25°C , 0.1 to 100 MPa, 0 to 110 g/kg salinity, submitted to Progress in Oceanography in Dec 2005

University of Applied Sciences Zittau/Görlitz, Faculty of Mechanical Engineering,
Department of Technical Thermodynamics, Prof. Dr.-Ing. habil. H.-J. Kretzschmar

1. Supplementary backward equations $p(h,s)$ for regions 1 and 2 of IAPWS-IF97
 - The comprehensive article on the backward equations $p(h,s)$ appeared in the "Journal of Engineering for Gas Turbines and Power" in 2006.
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 will appear in the "Journal of Engineering for Gas Turbines and Power" in September 2006.
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" was prepared.
4. Thermodynamic derivatives from IAPWS Formulations
 - The Advisory Note No. 3 was prepared.

5. Investigations on thermodynamic properties of humid air - part of the project "Advanced Adiabatic Compressed Air Energy Storage" (AA-CAES) of the European Union. –
 - Comparison calculations of different models for calculating thermodynamic properties of humid air were carried out.
6. Property libraries for water and steam, humid gases, and aqueous mixtures
 - The property library LibAmWa for Ammonia/Water mixtures was developed.
 - The Add-In FluidEXL for Excel® and the Add-On FluidMAT for Mathcad® were extended.
7. The download "Steam Tables on Pocket Calculators" were prepared for the IAPWS website.
8. The homepage www.iapws.de of the German National Committee of IAPWS was prepared.

Ruhr University Bochum, Germany, Faculty of Mechanical Engineering,
Department of Thermodynamics, Prof. Dr.-Ing. W. Wagner

1. Basic equation for region 5 of IAPWS-IF97
 - Development of a new basic equation for region 5 of IAPWS-IF97 that covers a pressure range up to 50 MPa.
 - A draft revised release on IAPWS-IF97 was prepared.
2. Investigations of the current IAPWS equations for the heat conductivity
 - The differences between the industrial equation and the scientific equation for the heat conductivity were investigated.

CURRENT STATUS OF RESEARCH ACTIVITIES IN JAPAN
Submitted to the Executive Committee Meeting, IAPWS, Witney, U.K.,
September 2006

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 continuing to play 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 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 conducted spectroscopic measurements of water and water-hydrocarbon mixtures at high temperatures and pressures. Infrared absorption of binary mixtures of water with hexane and decane were measured at temperatures and pressures in the 473-648 K and 70-350 bar ranges, respectively, and the anomalous volumetric behavior of the aqueous mixtures in the vicinity of the critical region was discussed [J. Chem. Phys., **122**, 204506 (2005)]. Near-infrared and ultraviolet spectra of water-NaCl-benzene mixtures were measured in the 473-573 K and 100-400 bar range, and it has been found that addition of NaCl in the aqueous phase suppresses transfer of water into the benzene-rich phase. The salting-out constant for the water-NaCl-benzene system increased significantly with increasing temperature. These facts seem to be explained by ion-induced electrostriction of the aqueous phase [J. Chem. Phys., **123**, 214504 (2005)]. Molecular dynamics study of anomalous volumetric behavior of water-benzene mixtures in the vicinity of the critical region was performed also [J. Chem. Phys., **123**, 244507 (2005)].

[contact: Prof. S. Ikawa; E-mail: sikawa@sci.hokudai.ac.jp].

At the Nuclear Science and Engineering Directorate, Japan Atomic Energy Agency, Tokai-mura, Dr. S. Uchida is promoting a second phase of the project on water chemistry of BWR, which has been supported by the Japan Society for the Promotion of Science (JSPS) [A Grant-in-Aid for Scientific Research: Subject No. 16360467 (2004-2006)]. In order to evaluate

the effects of H_2O_2 on corrosive conditions, static and dynamic responses of stainless steel exposed to H_2O_2 and O_2 in high temperature pure water were evaluated by analyzing ECP (electrochemical corrosion potential), FDCI (frequency dependent complex impedance), APP (anodic polarization properties) and CER (contact electric resistance) data. At the same time, multilateral surface analyses were carried out to determine characteristics of oxide film on the specimens. The following points were experimentally confirmed. 1) H_2O_2 resulted in a much higher ECP than O_2 with the same level oxidant concentration. ECP of the specimens exposed to 100 ppb H_2O_2 was as high as ECP of specimens exposed to 10 ppb H_2O_2 and it was not affected by co-existing O_2 . 2) The cathodic currents of the specimens exposed to H_2O_2 were determined by the H_2O_2 redox reaction, the anodic ones were determined mainly by H_2O_2 oxidation, and both were determined by $[\text{H}_2\text{O}_2]$. ECP was saturated against $[\text{H}_2\text{O}_2]$ and this resulted from the compensation of $[\text{H}_2\text{O}_2]$ dependences of anodic and cathodic currents. 3) Oxide layers were divided into inner and outer layers: Outer layers exposed to 100 ppb H_2O_2 consisted of larger corundum type hematite particles, while inner layers consisted of very fine Ni rich magnetite. Outer layers exposed to 200 ppb O_2 consisted of larger magnetite mixture particles, while inner layers consisted of fine Cr rich magnetite. 4) Particle density and size were changed by oxidant concentration. The average diameter of the particles decreased with $[\text{O}_2]$ and $[\text{H}_2\text{O}_2]$. A larger dissolution rate at higher $[\text{H}_2\text{O}_2]$ resulted in a thinner oxide film with smaller particles and larger hematite particles. 5) A sensor complex consisting of ECP and FDCI sensors was proposed as a $[\text{H}_2\text{O}_2]$ monitor in operating power plants. [Latest publication: (1) S. Uchida, "Latest Experience with Water Chemistry in Nuclear Power Plants in Japan", *Power Plant Chemistry*, 2006, 8 (5), (2) S. Uchida, T. Satoh, Y. Morishima, *et al.*, "Effects of Hydrogen Peroxide and Oxygen on Corrosion of Stainless Steel in High temperature water", *Proc. 12th Int. Conf. Environmental Degradation of Materials in Nuclear Power Systems – Water Reactors*, Snowbird, Aug. 15-18, 2001, TMS, (2005) (CD), (3) S. Uchida, T. Satoh, T. Miyazawa, *et al.*, "Dissolution of Oxide Film on Stainless Steel Surface in High Temperature H_2O_2 Water", *Proc. Symp. Water Chemistry and Corrosion of Nuclear Power Plants in Asia*, 2005, 145, Gyeongju, Korea, Oct. 11-13, Korean Atomic Energy Research Institute (2005) (CD)]

[contact: Prof. S. Uchida; E-mail: uchida.shunsuke@jaea.go.jp].

At the Graduate School of Environmental Studies, Tohoku University, Sendai, Profs. N. Yamasaki and H. Enomoto were retired in March 2006, but they are still active. Prof. N. Yamasaki was back to Kochi (his hometown) and he had established private company on science and technology on water. Prof. N. Yamasaki keeps excellent research on use of dry steam for material and environmental processing, and he is conducting research project on refinement of asbestos. Profs. H. Ishida and K. Ioku, they are covering development of new material by hydrothermal treatment. They published excellent papers: porous hydroxyapatite with tailored crystal surface was prepared by the hydrothermal method (K. Ioku *et al.*, *Key Eng. Mater.*, 284-286, (2005), 353-356). They also tried to prepare high performance bioceramics: novel

bioceramics of calcium phosphates composed of rod-shaped particles were prepared by the hydrothermal method (K. Ioku et al., *J. Hard Tissue Biology*, 14 (2005), 136-137). Geofluid science research group □ Prof. N. Tsuchiya □ is conducting water-rock interaction under sub- and supercritical condition, including multi-phase and multi-component solutions. They published experimental studies and field observation on hydrothermal reaction of geomaterials. (Hara and Tsuchita, *Geofluids*, 5 (2005), 251-26; Batkhisg et al., *Resource Geology*, 55(2005), 1-8). We organized 3rd workshop of WATER DYNAMICS in 16-17th November 2005 in Sendai International Center, which focused on the role of water in Earth processes, Life science and Material and Energy Process Design. The workshop was unique objectives covering very wide range of water and steam properties and utilization. We are planning 4th workshop of WATER DYNAMICS in 7-8th November 2006 in Matsushima (sightseeing place close to Sendai and University campus). The web site of WATER DYNAMICS is the follows:
<http://geo.kankyo.tohoku.ac.jp/events/WD4/index.html>. We can provide 1st and 2nd workshop proceedings, and proceedings of 3rd workshop was published as AIP (American Institute of Physics) conference series (vol. 833). [contact Prof. N. Tsuchiya; tsuchiya@mail.kankyo.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, NMI-Australia, 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. Kuetsgens, 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. In 2006, the uncertainty of the density measurement of 1 kg silicon spheres has been reduced down to 3.6×10^{-8} , being close to the final target of the uncertainty for replacing the kilogram 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. 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. Nanotechnologies 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," *Proc. 14th ICPWS*, Kyoto, 2004, 112-115]. Preliminary data on the falling velocity measurement are being obtained at the NMIJ. 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. [contact: Dr. K. Fujii, Chief, Fluid Properties Section, NMIJ; E-mail: fujii.kenichi@aist.go.jp].

Mr. K. MIYAGAWA assessed 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 the time. The aim of the assessment was to compare them on the common and state-of-the-art platforms. He tested the computing times of 43 IAPWS-IF97 equation programs and compared them with those of 66 reference programs on 7 modern PC environments. It was found that the IAPWS-IF97 equations are 8.3 times as fast as the previous international formulation. Modern computer systems are optimized for "simple" computational operations and therefore favor the simple structure of IAPWS-IF97. Provision of "backward equations", which are approximation of inverse equations, is one of the features of IAPWS-IF97. The backward equations showed much shorter computing times than iterative routines, which had been used to calculate with several independent variables. For users who still require iterative routines for inverse equations to achieve very high numerical consistency, the backward equations give good initial guess for iteration process. IAPWS-IF97 is faster than the equations of IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95) by factors of 70 to 200. The results will be presented at the IAPWS annual meeting in 2006. [contact: Mr. K. Miyagawa; E-mail: miyagawa.kiyoshi@nifty.com]

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 of solid sample, in order to understand corrosion of metals and steels in high temperature water up to 673 K. The Raman spectroscopy system enables continuous *in situ* observation for several hundred hours [*J. Nucl. Sci. Technol.*, **43**, 675-680 (2006).]. They are also conducting immersion tests under several redox conditions in high temperature water at 623 K and 723 K, to evaluate stability of chromium oxide. The samples are Pt plates coated with

chromium oxide, which is artificially formed by metal organic chemical vapor deposition. After the immersion tests, weight loss and [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 study the behavior of thermodynamic properties of aqueous mixtures by means of the PVT measurements, isobaric specific heat capacity measurements, and the critical parameter measurements. The UEMATSU group measures the PVT properties of aqueous ammonia mixtures in the temperature range from 350 K to 600 K at pressures up to 200 MPa by a metal-bellows variable volumometer. The preliminary results were presented at the ICCT-2006 held in Boulder, Colorado, USA by Dr. N. Sakoda. The Cp measurements of water + methanol mixtures were finished in the temperature range from 280 K to 360 K at pressures from 0.1 MPa to 15 MPa by the thermal relaxation method. The results were also presented at the ICCT-2006 by I. Fujita. The calorimeter, principle, and results to confirm the reliability of the apparatus were described in Review of Scientific Instruments, 77-3 (2006) 035110. The apparatus for the critical parameter measurements by a metal-bellows variable volumometer with an optical cell is reconstructed in order to measure the critical properties of aqueous ammonia mixtures. We proposed a new method to determine the critical point by image analysis which is available on line in the Journal of Chemical Thermodynamics. [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, *J. Chem. Phys.* **124**, 024510 (2006)] 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 and the cluster near the surface. [Y. Andoh and K. Yasuoka, *Langmuir*, **21**, 10885-10894 (2005); Y. Andoh and K. Yasuoka, *J. Phys. Chem. B.*, in press.] 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).; T. Koishi et al., *Phys. Rev. Lett.*, **123**, 204707 (2005).] [contact: Dr. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.jp].

At the Department of Mechanical Engineering, Kanagawa Institute of Technology, Atsugi, Dr. K. Oguchi and his group are measuring the pVT_x properties of ammonia + water mixtures. They have already measured new 49 points of the pVT_x properties of aqueous solutions of ammonia along four isochors in the range of temperatures from 295 K to 308 K, pressures

from 0.29 MPa to 17.17 MPa, densities from 818 kg/m³ to 825 kg/m³, and compositions from 0.5036 mol/mol to 0.5221 mol/mol. [contact: Dr. K. Oguchi; E-mail: oguchi@kait.jp]

At the Department of Mechanical Systems Engineering, National Defense Academy, Yokosuka, Prof. N. Kagawa and his group are developing a twin-cell type adiabatic calorimeter for water + alcohol and water + ammonia mixtures. This apparatus was designed based on results by another twin-cell type adiabatic calorimeter which had measured water + alcohol and hydrocarbon mixtures. The new one will measure liquid isochoric heat capacities of these mixtures for temperatures from 220 to 420 K and pressures to 30 MPa including super critical region. [contact: Prof. N. Kagawa; E-mail kagawa@nda.ac.jp]

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their co-workers study the structure, dynamics, and reactions in super- and subcritical water by means of multinuclear NMR (nuclear magnetic resonance) spectroscopy and computer simulation. Their current focus are (1) the thermodynamics, structure, and dynamics of hydration over a wide range of thermodynamic conditions [“A new high-temperature multinuclear-magnetic-resonance probe and the self-diffusion of light and heavy water in sub- and supercritical conditions”, K. Yoshida, C. Wakai, N. Matubayasi, and M. Nakahara, J. Chem. Phys. 123, 164506 (10 pages) (2005)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions. [“Hydrothermal Carbon-Carbon Bond Formation and Disproportionations of C1 Aldehydes: Formaldehyde and Formic Acid”, S. Morooka, C. Wakai, N. Matubayasi, and M. Nakahara, J. Phys. Chem. A 109, 6610-6619 (2005)]. [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 tetraalkylammonium bromides (R₄NBr) in liquid methanol along the liquid-vapor coexistence curve up to about 180 °C to examine the validity of the Hubbard-Onsager (HO) dielectric friction theory. The translational friction coefficients z of relatively small ions, Me₄N⁺ and Et₄N⁺, were remarkably smaller than the prediction of the HO theory at high densities and low temperatures. However, the negative deviation from the HO theory gradually disappears with decreasing density and increasing temperature. For relatively large ions, Pr₄N⁺ and Bu₄N⁺, the experimental friction coefficients lay in the validity range of the HO theory in all the conditions studied here [T. Hoshina, K. Tanaka, N. Tsuchihashi, K. Ibuki, and M. Ueno, J. Chem. Phys., 122, 104512 1-8 (2005)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

**U.S. NATIONAL COMMITTEE TO IAPWS
2006 REPORT ON ACTIVITIES OF POTENTIAL INTEREST TO IAPWS**

Communicated from Arizona State University, Tempe, AZ:

It is shown that the corresponding-states correlations exist for families of similar compounds between the reduced values of the infinite dilution solute – water direct correlation function integrals (DCFI) when plotted against water density over the density ranges 500-1000 kg·m⁻³. The value of DCFI for a solute is calculated from its partial molar volume and thermophysical properties of pure water. The reduced DCFI is defined as the ratio of the DCFI at some T and water density to its value at 298 K and atmospheric pressure. The following classes of aqueous solutes are separated: simple fluids (Ar, CH₄,...), nonpolar compounds (CO₂, C₂H₄, aliphatic hydrocarbons,...), polar organic and inorganic compounds, and compounds with chemically bonded water (water itself, H₃BO₃, aqueous silica, ...). It is expected that neutral hydroxides of metals and nonmetals belong to the last class, and the partial molar volumes of these solutes in water at elevated T and P can be estimated using the proposed correlations.

Reference: Plyasunov A.V., Shock E.L., O'Connell J.P. (2006) Corresponding-states correlations for estimating partial molar volumes of nonelectrolytes at infinite dilution in water over extended temperature and pressure ranges. *Fluid Phase Equil.*, **247**, 18-31.

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

The Energy Institutes' Electrochemical Laboratory at Penn State University strives to be at the front edge of fundamental and applied research in a variety of electrochemical and materials science technologies. The Laboratory aims to promote and facilitate the use of electrochemical methods in the areas of science and technology related to traditional and renewable energy generation systems. We lead interdisciplinary studies on electrochemistry of high temperature aqueous systems in a variety of scientific areas including corrosion and protective coatings, proton exchange membrane and solid oxide fuel cells, thermochemical hydrogen production, etc. The main research directions and key publications in 2005-2006 are as follows: **(1) High-Temperature Thermodynamics of Aqueous Solutions** (Bandura A. V., and Lvov S.N. The Ionization Constant of Water over Wide Ranges of Temperature and Density, *J. Phys. Chem. Ref. Data*, 2005, **35**, 15-35); **(2) High-Temperature Aqueous Electrochemistry** (Lvov S.N. Electrochemical Techniques for Studying High-Temperature Subcritical and Supercritical Aqueous Solutions, in "*Encyclopedia of Electrochemistry*", v. 5, A. Bard, M. Stratmann, and D. Macdonald, and Patrick Schmuki, Eds., 2006, Wiley-VCH); **(3) High-Temperature Surface Electrochemistry** (Lvov S.L., Chalkova E., Fedkin M. V., Komarneni S., and Wesolowski D. J., Surface Electrochemistry of Composite Materials for High-

Temperature PEM Fuel Cells, *ECS Transactions*, 2006, v. 1, p. 215-225); **(4) High-Temperature Proton Exchange Membrane Fuel Cells** (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.*, 2005, **152**, A1742-A1747, 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, **152**, A1035-A1040); **(5) High-Temperature Aqueous Corrosion** (Z.F. Zhou, E. Chalkova, S.N. Lvov, P. Chou, and R. Pathania, Development of a hydrothermal deposition process for applying zirconia coatings on BWR materials for IGSCC mitigation, *Corrosion Science*, 2006, in press).

Communicated from The University of Delaware, Newark, DE:

The research group of R. Wood produced the following work on high-temperature aqueous electrolyte systems:

“Conductance of Aqueous Na₂SO₄, H₂SO₄, and their mixtures: Limiting Equivalent Ion Conductances, Dissociation Constants, and Speciation to 673K and 28 MPa,” by Lubomir Hnedkovsky, Robert H. Wood, and Victor N. Balashov, *J. Phys. Chem. B*, 2005, **109**, 9034-9046; “Conductance study of association in aqueous CaCl₂, Ca(CH₃COO)₂, and Ca(CH₃COO)₂.nCH₃COOH from 348 to 523 K at 10 MPa,” by Lucila P. Méndez De Leo and R. H. Wood, *J. Phys. Chem. B*, 2005, **109**, 14243-14250; “Multiple ion association and sulfate ion mobility in aqueous Li₂SO₄ and K₂SO₄ from measurement of conductance at temperatures from 523 to 673K,” by Victor N. Balashov, Andrei V. Sharygin, Robert H. Wood, Brian K. Grafton, and Caibin Xiao. Accepted *Geochim. Cosmochim. Acta*; “Structure of an accurate *ab initio* model of the aqueous Cl⁻ ion at high temperatures” By Haitao Dong, Wenbin Liu, Douglas J. Doren, and Robert Wood. Accepted *J. Phys. Chem.*

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

A collaboration is continuing with Richard Wheatley at the University of Nottingham, developing intermolecular pair potentials for aqueous systems for the quantitative calculation of second virial coefficients. This approach produces second virial coefficients that for the most part have smaller uncertainties than those obtained by experiment. Water with nitrogen has been completed, and preliminary results have been obtained for water with oxygen. Calculations for water with “air” based on a combination of these results look promising. A similar collaboration with the University of Delaware has produced similar results for water with methane.

References: Akin-Ojo, O., Harvey, A.H., and Szalewicz, K., 2006. "Calculations of the cross second virial coefficient with quantum corrections for the methane—water system using an *ab initio* potential energy surface," *J. Chem. Phys.* **125**, 014314; Tulegenov, A.S., Wheatley, R.J., Hodges, M.P., and Harvey, A.H., 2006. "Intermolecular potential and second virial coefficient of the water—nitrogen complex," *J. Chem. Phys.*, submitted.; Wheatley, R.J., and Harvey, A.H., 2006. "Intermolecular potential and second virial coefficient of the water—oxygen complex," *J. Chem. Phys.*, in preparation; Harvey, A.H., and Huang, P.H., 2006. "First-Principles Calculations for Humidity Standards: The Air-Water Second Virial Coefficient," *Int. J. Thermophys.*, in preparation.

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 has been refitted and is ready for evaluation by IAPWS. Work has started on the low-density portion of the thermal conductivity.

Communicated from Oak Ridge National Laboratory, Oak Ridge, TN:

The solubilities of cupric and cuprous oxides were measured in water over the range 25 to 350 °C in the presence of various chemical agents (NaOH, NH₃, B(OH)₃, H₃PO₄, (OHCH₂)₃CNH₂, (OHCH₂)₃CN(OHCH₂CH₃)₂, HF₃CSO₃, HNO₃ and mixtures thereof) as a function of pH, and in steam to 400 °C as a function of pressure. Large discrepancies exist between the various experimental studies, especially at high temperatures for cuprous oxide, where the current solubilities are orders of magnitude lower. The solubilities of both oxides in water are highly pH dependent exhibiting unexpected changes in the speciation of dissolved copper with temperature, but are virtually pH independent in steam.

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