**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

**ASSOCIATE MEMBER**

Switzerland

**EXECUTIVE SECRETARY**

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# Minutes of the Meetings

# of the

# Executive Committee

# of the

# International Association for the Properties of

# Water and Steam

## Lucerne, Switzerland
## 26 August – 1 September 2007

## Prepared by: Barry Dooley

IAPWS

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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
Lucerne, Switzerland
26 August – 1 September 2007

Plenary Session. Monday, 27 August 2007. 8:40am

The President of IAPWS, Jeff Cooper, welcomed the Executive Committee (EC) and other IAPWS members to Lucerne for the EC and Working Group (WG) Meetings of IAPWS. The President officially opened the 2007 EC Meetings by introducing the National Delegates. Each of the member countries of IAPWS was in attendance with the exception of Argentina/Brazil, France, and Italy.

The President asked the head of the newly formed Swiss National Committee to provide some comments. Svoboda welcomed everybody to Switzerland and to the 2007 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 May 2007. There were no further agenda 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 to serve on this Committee. Another member will be added to the Committee. The Press Release is discussed in Minute 16.1 and Attachment 9.

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 Attachment 8.

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 2008 award would consist of a member from Germany, Greece, Japan, Russia and USA. The President asked the German delegate (Rukes) 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 new guidelines had been adopted for the selection of Helmholtz awardees at the Whitney meetings in 2006 and suggested that the amended age limit could possible eliminate candidates who would be eligible under the old guidelines. He suggested that the EC reflect on this and that Friend, Bellows and himself provide an amendment at the Friday EC meeting. (See Minute 15.1)

2.3.2 Honorary Fellow Award Committee

The President requested that Tremaine take over as the Chairman of this committee from Daucik for 2008. Watanabe was added as the other member. The IAPWS President would be ex. Officio.

2.3.3 Gibbs Award Committee

The President indicated that the Gibbs Award was the most prestigious international award at IAPWS, and because the Executive Secretary had only received one nomination that the time period to receive nominations would be extended until 5PM on Tuesday. The Gibbs Award Committee had already been formed in Whitney and they would report back to the EC on Friday. (Minute 15.3).

2.4 Host Country for 15$^{th}$ ICPWS

The President requested the German Delegate to provide an update. Rukes indicated that preparations are in very good shape to organize the 15$^{th}$ ICPWS in Berlin in 2008. Rukes indicated that the International Program Committee would meet during the week as well as the German Organizing Committee. Full information, including a budget, would be provided at the EC Meeting on Friday (Minute 16.2).

2.5 and 2.6 IAPWS Member Countries and IAPWS Statutes and By-Laws

The President indicated that these two items are closely related and would be dealt with together. He first indicated that a committee had been assembled in Witney under the Chairmanship of Watanabe to review the Statutes and By-Laws, and a second committee to look into reorganizing IAPWS to allow individual memberships in addition to National memberships. The President next requested Harvey to provide a short presentation on a number of items within the Statutes which might need to be addressed by the committee. He then requested that Watanabe as Chairman, meet with his committee during the week and report back to the EC on Friday. The committee will consist of Cooper, Harvey, Hruby, Svoboda, Daucik and Alexandrov. This report is provided in Minute 16.3.

2.7 IAPWS Education and Outreach

The President requested the Chairman of this committee to provide a short report. Kretzschmar indicated that the committee had suggested four proposals in Whitney and that his committee would research the activity during the week and provide a status report to the EC on Friday (Minute 16.4).

2.8 Acknowledging Contributions to IAPWS Documents

The President indicated that the Executive Secretary had received a note from the Head of the US National Committee on this topic. Friend had not yet arrived in Switzerland so Harvey indicated that IAPWS Documents do not have named authors and asked whether it would be possible to give credit to people who had contributed. Lvov then presented an example acknowledgement in a current release. Some discussion ensued from the EC reflecting that IAPWS needed to take a closer look at this. A committee was formed with Friend (Chairman), Lvov, Hiegemann, and Wagner with the President as ex-officio. The Chairman was requested to report to the EC on Friday (Minute 16.5).

2.9 Other Business Considered to Require Special/Extensive Discussions

No other business was raised by the EC.

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 and ICRNs that would need action by the WGs and the EC during the week. The Executive Secretary indicated that four final Draft Releases had been forwarded in April, May and July to the Heads of National Committees. No comments had been received prior to the meeting so the TPWS/IRS and PCAS WGs need to provide a final review prior to presenting them to the EC on Friday for approval.

The Executive Secretary then noted that six ICRNs (16-21) had been forwarded to the National Committees in October 2006. Three (18,19,20) had been approved and are available on the IAPWS Website. ICRNs 16, 17 and 21 had received comments and would need action by the WGs during the week.

3.2 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 Cooper 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, 5, 6, and 7).

The President closed the opening session of the EC at 10:03am.

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 "Interaction of Water and Steam with Materials in Power Plants" 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, 31 August 2007

President Cooper opened the continuation of the EC Meeting at 8:35am. All members of IAPWS were present except Argentina/Brazil, France, Greece, and Italy. Cooper 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 Cooper asked for comments and changes to the minutes of the EC meeting held in Witney, England in September 2006. No changes were noted, thus the 2006 Minutes were accepted.

6. President's Report

President Cooper indicated that IAPWS was in a very healthy condition both financially and in terms of a broad range of activities. He particularly wanted to highlight the expansion of IAWPS into Seawater and the activities associated with the Workshop and ICRNs. He hoped that other opportunities would arise in the future.

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 a draft of a Revised Release on the Melting and Sublimation Curves of Water and that a Task Group had been set up. The plan is to have the Revised Release ready for approval in Berlin in 2008.

7.2 The Task Group on the Properties of Liquid Water at Atmospheric Pressure had been authorized to develop a draft of a Supplementary Release for approval at the EC meetings in Berlin 2008. An Evaluation Task Group had also been formed.

7.3 A new release on Viscosity of Water and Steam will be proposed to the EC next year. Chairman Kretzschmar indicated that this will be forwarded

to the Executive Secretary for Postal Ballot following review by the Editorial Committee.

7.4 The Chairman indicated that the Release on the Transport Properties of Heavy Water had been reviewed by both TPWS and IRS. The WGs recommended that the EC approve this Release which had been circulated to all National Committees prior to the EC Meetings.

**The EC approved this Release unanimously.**

7.5 The Chairman reported that a workshop had been held on the Properties of Humid Air and Humid Combustion Gases jointly with IRS, PCAS and PCC. ICRN #14 on Thermophysical Properties of Humid Air and Combustion Gas Mixtures will be updated by the next EC meetings in 2008. Also a new ICRN on Dew Point Determination for Combustion Gases will be prepared by a Task Group before the next EC Meetings.

7.6 Kretzschmar reported that at the Workshop on the Properties of Seawater a draft Release on the Properties of Seawater had been presented by Feistel. Adoption of this Release is planned for the Berlin EC meetings in 2008. The Chairman also indicated that an updated version of ICRN 16 on Seawater had been approved by TPWS, IRS and PCAS, and he requested that this now be sent to National Committees for approval.

7.7 With regards to IAPWS-IF97 for the Calculation of the Density for Determining the Dielectic Constant, Refractive Index, Ionization Constant etc., the TPWS and IRS WGs request that the EC ask National Committees if they have any input on the question: "is there any need for instructions from IAPWS about using IAPWS-IF97 in conjunction with formulations for quantities that have been based on IAPWS-95 (dielectric constant, refractive index, ionization constant, etc)". The Chairman requested that each National Committee (NC) will report the results next year. Discussion by the EC suggested that the IRS Chairman should arrange to draft a brief statement to make it clear exactly what is required from each NC. Replies are expected by 1st March 2008.

7.8 Kretzschmar next informed the EC that in relation to the liaison with CCM, Harvey had been instructed to prepare a joint paper regarding using IAPWS-95 outside of the range of validity of the CCM standard for liquid water.

7.9 With regards to membership of TPWS, the Chairman requested that three new members be added to the WG: V. Ochkov (Moscow Power Institute), P. Spitzer (PTB Germany) and M. Wendland (University of Applied Life Sciences, Vienna, Austria).

**The EC approved these membership additions unanimously.**

The Chairman also indicated that the Czech Republic National Committee had requested that Kadrnozka be withdrawn from membership of TPWS.

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 5. 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 first informed the EC that IRS has decided to change its Approval of Minutes procedure. The Chairman will distribute an electronic version to all working group members. Any comments or additions will be reflected in an updated version. After a specified period of time when no further comments are received, the minutes will be considered approved.

In discussion by the EC, the Japanese Delegate (Watanabe) suggested that all WGs adopt the same procedure.

8.2 The Chairman then reported on the Release concerning Region 5 Extension of IAPWS IF-97 to 50 MPa. TPWS and IRS had reviewed the draft release and the results of the Evaluation Task Group. The Working Groups recommend to the EC that the revised release be accepted. This Release had been circulated to all National Committees prior to the EC Meetings.

**The EC approved this Release unanimously.**

8.3 With regards to future Industrial Requirements for Steam Properties the Chairman informed the EC that he had given the WGs a presentation on the future needs of industry with special emphasis on computational fluid dynamics. As a result two Task Groups had been formed. The first Task Group will define Industrial Requirements in connection with CFD Calculations and other industrial applications which would benefit having very fast property calculations. This Group will be chaired by Parry. The second Task Group will investigate homogeneous nucleation as steam is expanded from a dry to wet condition. This Group will be chaired by Hruby.

8.4 With regards to Advisory Note No. 3 on Thermodynamic Derivatives from IAPWS Formulations, the Chairman reported that the WGs had thoroughly reviewed the Release and the results of the Evaluation Task

Group. The Working Groups recommend to the EC that the Advisory Note be accepted. This Advisory note had been circulated to the National Committees prior to the EC meetings.

**The EC approved this Advisory Note unanimously.**

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

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

9.1 An international collaboration proposal on "Equilibrium Constants and Speciation of Aqueous Transition Metal Chlorocomplexes over a Wide Range of Temperatures and Pressures" was developed and submitted by Tremaine (Canada) and Sedlbauer (Czech Republic). The President thanked PCAS and indicated that this would be dealt with later (Minute 14.1)

9.2 The IAPWS Release on "Ionization Constant of Water over Wide Ranges of Temperature and Density" had been reviewed by PCAS. All comments had been addressed, editorial changes had been made, and the Release had been circulated to National Committees. This release had included as an example a proposed "Acknowledgements Section" as discussed in Minute 2.8. However at this stage in the EC Agenda, the committee to address acknowledgements had not presented its finding to the EC (Minute 16.5), so the President proposed that the Release be approved by the EC and that if the acknowledgement section is approved later it would be added to the Release. If the acknowledgements section is not approved then the Release would remain approved without an acknowledgements section.

**The EC approved the Release unanimously with this caveat.**

9.3 Final Report on IAPWS International Collaboration on "Irreversible Thermodynamics of PEM Fuel Cells" by Mican, Marsík, and Lvov has been completed and submitted to the Executive Secretary for the IAPWS files.

9.4 Final Report on IAPWS International Collaboration (in PowerPoint format) on "The ionization constant of o-, m, and p-nitrophenol under hydrothermal conditions" by Ehlerova, Tremaine and Sedlbauer has been completed and submitted to the Executive Secretary for the IAPWS files.

9.5 It will be necessary to rearrange the joint IUPAC/IAPWS Project on Standard Partial Molar Properties of Solutes following receipt of a letter from Majer explaining that he has left his position as Director of the

Thermodynamics Lab at Blaise Pascale and will not continue the work. Lvov indicated that he had sent an e-mail letter to Majer asking for a number of clarifications about the project. This lead to much discussion by the EC. Finally Tremaine indicated that PCAS was simply alerting the EC of the problem, and that PCAS would await a response from Majer until taking any action. The US Delegate (Friend) proposed postponing all expenditures by IAPWS and that a new Proposal should be prepared by PCAS for a postal ballot.

**The EC agreed unanimously with this proposal.**

9.6 Lvov proposed that the WG would be renamed from "Physical Chemistry of Aqueous Solutions" to "Physical Chemistry of Aqueous Systems" as this more closely agreed with the work within the PCAS WG.

**The EC approved this WG name-change unanimously**

Chairman Lvov finalized his report by indicating: a) that the joint symposium with ECS will take place on 7 October 2007, b) that the IAPWS Data Book (Valashko) had six of seven chapters in good shape, and c) that PCAS would review its leadership and direction to make the WG work more effectively within IAPWS. A recommendation will be provided at the 2008 Berlin meetings.

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

Chairman Svoboda highlighted those activities that needed action/approval by the EC. A full written report of the PCC WG activities forms Attachment 7.

10.1 PCC Workflow. Svoboda first reported to the EC that the WG had spent time during the week to define a Mission Statement and the major Relevant Documents which PCC produces. As well as ICRNs and Technical Publications by PCC members, the WG is developing a new guidance document which at this time is called an IAPWS Technical Application Guidance (ITAG). This will be brought to the EC for approval in Berlin.

10.2 ICRNs. Svoboda reported that three ICRNs are pending. The first (ICRN 21) on Ultra-Supercritical Plants and the second (ICRN 17) on Amines are in review following comments from National Committees. The third ICRN (22) is new and needs to be harmonized with the current ICRN 13 on Surface Tension. All three ICRNs will be forwarded to the Executive Secretary for postal ballot.

10.3 International Collaboration. The Chairman indicated that the 2006 International Collaboration Project on "Improved analysis of low concentrations of particulate oxides in water/steam cycles" had been completed and circulated for peer review within PCC. When completed it

will be forwarded to the Executive Secretary for the IAPWS files, and submitted for publication. The overall project was completed well below the budget estimate because of the raising of local funds. Here the Danish Delegate proposed that the remaining funds could be used to send the student to the Berlin ICPWS to present a paper on the topic.

**The EC approved this no-cost extension for the project unanimously.**

10.4 Guidance Document on Mechanical Carryover. The PCC Chairman reported that draft number 16 was still circulating within PCC but was expected to be finalized by the end of 2007. This will be the first of the new PCC Guidance documents.

The President initiated discussion on the process to be used for approval of this new document and the issue of the exact name for these documents The consensus of the EC was that it was not necessary to rigidly fix the name of the document until the National Committees have reviewed the first one. The process to be used for approval will be: a) review by WG, b) review by Editorial Committee, c) Postal Ballot for review by NCs, and d) approval by EC.

**The EC approved this suggested process unanimously.**

10.5 PCC Membership. The Chairman proposed one new members for PCC: Dr. Andreas Drexler (Areva, Germany). He also indicated that PCC had elected a second Vice-Chairman: Marc deWispelaere (Laborelec, Belgium)

**The EC approved these membership and officer changes unanimously.**

The Chairman informed the EC that two PCC members (McGrath and Mathur) had retired and wished to be removed from the membership list.

10.6 The Chairman next informed the EC that PCC had formed three Task Groups on: a) Carryover, b) Risk for Asset Damage, and c) Review of the European Standard EN 12952.12. With reference to the last, the Task Group will prepare a uniform technical statement that will be used by National EN committees to support an update of this standard.

With regards to this item, the President asked the EC for comment. After much discussion focused on IAPWS commenting on standards, a proposal was made that the technical statement will be circulated to the Members of the EC for review and approval with a two weeks time period for response.

**The EC approved this process unanimously.**

10.7 PCC Public Relations. The Chairman indicated that the commented and edited Minutes would be submitted to PPChem for publication, and that a presentation of IAPWS/PCC will be made at the VGB "Chemistry in Power Plants" conference in October 2007.

11. Editorial Committee Report

Chairman Harvey reported that the Editorial Committee (Harvey and Cooper) had reviewed and approved four items during the year: a) Revised Release on the IAPWS Industrial Formulation 1997, b) Advisory Note #3 (thermodynamic derivatives), c) Release on the Ionization Constant of $H_2O$, and d) Revised Release on Viscosity and Thermal Conductivity of Heavy Water Substance. The Committee had also provided preliminary input on the proposed viscosity release.

Harvey then raised the following issues:

1. Reminder to the WGs to allow sufficient time for Editorial Review.
2. The names and contact of the President and Executive Secretary need to be updated on all future documents.
3. There is a need to agree on a procedure for updating references in Releases without going through a long approval process. A motion was developed to "allow the Editorial Committee to make small changes to IAPWS Documents without needing EC approval".

   **The EC approved this simplification unanimously.**

4. Should the IAPWS document come before or after the journal publication? After much discussion, the consensus of the EC was that there is no need to have a release first, and the procedures should allow for both approaches.
5. Should the Editorial Committee review ICRNs? After some discussion which reviewed the initial simple and quick concept for ICRNs, the consensus of the EC reflected that if a National Committee, during review, indicated that Editorial Review was necessary then the ICRN would be sent to the Editorial Committee. This process should be included in the revised Statutes and By-Laws.
6. The final item was a request by Harvey to the President and EC that a third person should be added to the Editorial Committee.

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 June 2007), the following countries had not paid the 2007 IAPWS dues: Argentina/Brazil, Canada, Denmark, France, and Russia. The Executive Secretary further reported that in 2006 France

Russia and the Argentinean/Brazil National Committee had not paid the dues. In 2005 France and Russia had not paid the dues. The Canadian Delegate (Tremaine) told the EC that the Canadian NC had been undergoing changes in personnel and in support. He considered the Canadian committee was now stable and would be able to pay the 2007 dues relatively soon. The Russian NC had paid the 2007 dues to the Executive Committee earlier this week.

12.2 New Associate Member

The Executive Secretary reported that earlier in August he had received an application for IAPWS Associate Membership from the newly formed Swiss National Committee. The President requested the Head of the newly formed committee to say a few words. Svoboda reported that the Swiss National Committee will probably have about 12 individual members, and were going to test the feasibility of developing a joint membership with Austria, and that they hoped to be able to soon apply for full IAPWS membership.

13. Executive Secretary's Report

13.1 Financial, Auditors and Dues

The Executive Secretary reported that IAPWS remained on a sound financial footing with currently over SFrs 81,017 in the Swiss bank account and about $27,935 in the US account for a total of $94,569 combined. The status as at 30 June 2007 in the bank accounts had been provided to each National Delegate present at the EC meeting.

The Executive Secretary next reported that the 2006 financial statements had been forwarded to the Auditors in January 2007. Both VDI in Germany and Mr. Miyagawa in Japan had reviewed the financial statements. The Auditors' reports had also been provided to all the National Delegates present.

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

**The EC approved this unanimously.**

The Executive Secretary proposed to the EC that the dues structure for member countries remain unchanged for 2008.

**The EC unanimously agreed to this proposal.**

The Executive Secretary also provided a rough estimate of the income and known planned expenditures for 2007.

13.2 Time and Place of the 2008 and 2009 Meetings

The Executive Secretary reminded the EC that the 15th ICPWS would be held in Berlin in September 2008 and that a status report would be presented later (Minute 16.2). He then explained that the next logical host countries to hold IAPWS annual EC and WG meetings were Canada, Czech Republic and the USA. He had spoken to the Canadian Delegate, who had suggested that 2010 would be a much more convenient time. During the week, the IAPWS Executive Secretary had asked Zeijseink to explore the possibility of hosting the 2009 meetings in The Netherlands and to present an invitation at the 2008 EC Meetings in Berlin. If it will not be possible, then Zeijseink will inform the Executive Secretary. The 2009 meetings would then revert to Canada if possible.

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 (Parry) to report on the discussions during the week. The Chairman indicated that the Committee had only reviewed one proposal for international collaboration. The details of this proposal are provided in Attachment 8. The Chairman then summarized the proposal for the EC.

"Equilibrium Constants and Speciation of Aqueous Transition Metal Chlorocomplexes over a Wide Range of Temperatures and Pressures". The IAPWS sponsors are Tremaine (Canada) and Sedlbauer (Czech Republic). The young scientist will be Jitka Felcmanova at the Technical University of Liberec, Czech Republic. The requested contribution from IAPWS is $14,000 for subsistence for 10 months.

The Chairman recommended to the EC that IAPWS support this proposal. Members of the EC indicated that the contribution was a little higher than in the past and questioned whether this fell within the spending guidelines of IAPWS in relation to the large expenditures needed over the next year to support the 15th ICPWS. After some discussion and analysis

**The EC approved the Collaborative Project unanimously.**

15. IAPWS Awards

15.1 IAPWS Helmholtz Award

The President reported that Dr. Karsten Meier had been selected as the 2007 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 German Delegate for the names of the 2008 Helmholtz Award Committee. The 2008 Helmholtz Committee would consist of: Chairman Wagner (Germany), Assael (Greece), Nakahara (Japan), Petrova (Russia) and Anderko (USA). Nominations will be due to the Executive Secretary by January 31, 2008.

The President next asked the Chairman of the Helmholtz Procedures Committee to review the results of this committee's further discussions during the week (Minute 2.3). Friend indicated that the committee (Cooper and Bellows) had discussed only the issue of the age requirement for the Helmholtz Award. Initially it had been set at age 40. Then last year this had been changed to 10 years after the highest degree. The President had raised this as a limiting requirement so the Committee now proposes 12-15 years after the highest degree as being the upper limit. After some discussion the Canadian Delegate (Tremaine) modified the "12-15 year" proposal to 15 years

**The EC approved this modification to the Helmholtz requirements unanimously.**

15.2 IAPWS Honorary Fellowships

The President reported that Palmer (USA) had been elected Honorary IAPWS Fellow, following the established procedures and after unanimous approval through the postal ballot conducted by the Executive Secretary. In Palmer's absence, the Fellowship Award had been presented at the IAPWS Dinner on Thursday evening to the Head of the US National Committee.

The President reminded the EC of the Awards Committee for 2008 with Tremaine as Chairman and Watanabe as member with the IAPWS President as ex.-officio member. Nominations are due to the Executive Secretary by January 31, 2008.

15.3 IAPWS Gibbs Award

The President requested that the Chairman of the Gibbs Award Committee, Nakahara, present the results of his committee's discussions

during the week. Nakahara reported that the committee agreed with the Presidents extension of the nomination time to Tuesday at 5pm. The committee had reviewed the nomination of Professor Wolfgang Wagner and recommended him as the 2008 IAPWS Gibbs Award.

**The EC approved this nomination unanimously.**

16. New Business

16.1 Press Release

The President requested that Bellows project the Press Release for review by the EC. Suggestions were provided by the EC and the final version is contained in Attachment 9.

16.2 15th ICPWS

The President requested the Head of the German National Committee to provide a status report on the 15th ICPWS. Rukes delegated this to Weber, who reported on the following items:

- The German Organizing Committee had met 2 times since Witney and several times during the current IAWPS week
- The International Program Committee met twice during the current IAPWS week. 17 Symposia subjects with Chairmen have been developed.
- First Announcement has been distributed through IAPWS and VDI. The second announcement and call for papers will be issued in October 2007. Submission and review of Abstracts will take place before the meeting of the International Program Committee on 21/22 February 2008 in Berlin.
- Web site is online (www.icpws15.de)
- Title, Dates, Location and Hotel have been decided upon
- Preliminary Schedule for the conference week exists, with option for 4 parallel sessions
- An initial Program and Timeline has been developed
- Conference fees and projected participants have been developed so that a preliminary budget could be presented to the EC.

Weber then requested that the EC support the Conference with the remainder of the donation approved at the Witney meeting in 2006.

**The EC unanimously approved the remaining $20,000 of the IAPWS donation to the 15th ICPWS.**

16.3 IAPWS Member Countries, and Statutes and By-Laws

The President requested that Chairman Watanabe report on the activities of the Task Group, which had been formed on Monday (Minutes 2.5 and 2.6). Watanabe indicated that the six person committee had met twice during the week. The Committee was asked to: a) assess ways to improve participation in IAPWS of countries and individuals, and b) consider other needed changes to the IAPWS Statutes and By-Laws for adoption at the 2008 15th ICPWS. The Chairman then asked Harvey to present the suggestions from the Committee on only those items where the EC needs to provide decision or guidance. Harvey then provided discussion on the following five items:

1. General Meeting. The recommendations here were: a) to continue with the General Meeting, make it only informational and give the responsibility for the Statutes to the EC, and b) changing the Statutes should not become too easy. These recommendations resulted in much discussion by the EC. The Canadian Delegate (Tremaine) proposed the first motion to the EC which was that "Non-members should not have voting rights at the General Meeting". This was seconded and

   **The EC approved this motion unanimously**

   The German Delegate (Rukes) next proposed a motion "That the authority to vote on the Statutes and General Policy should be changed from the General Meeting to the EC". This was seconded and

   **The EC approved this motion by 6 votes to 2 of Members present.**

   The US Delegate (Friend) then proposed the motion that "The Statutes Committee should include that the EC should vote only on the Statutes at a General Meeting". This was seconded and

   **The EC approved this motion by 4 votes to 3 with one Member abstaining.**

2. Members Defaulting on Dues. Here Harvey reminded the EC that the Statutes already include that after three years of a member defaulting on payment of dues "its status will be changed to that of Associate Member". The Committee recommends that the EC should be allowed to make exceptions each year.

   **The EC approved this recommendation unanimously.**

The Committee also suggested, as a one-time experiment, that each member in default on dues payment should send a written report to the President and Executive Secretary by 31st December on the health of its National Committee.

3. Role of Individuals in IAPWS. Harvey indicated that this was already covered in the Statutes, but it would be made clearer in the Statutes and on the IAPWS Web Site that individuals can be members of a WG even if their country is not an IAPWS Member. Observers from non-member countries (and affiliated countries) are welcome to attend EC meetings.

4. Document Procedures. First Harvey provided the recommendation that for Releases and Guidelines, the procedures should be revised and clarified for faster processing now that electronic communication was used. Adequate time would still be incorporated for review by National Committees.

   **The EC unanimously approved that these Statutes changes should be implemented**

   With regards to ICRNs the Committee recommends that the Statutes be changed so that minor comments do not delay the approval process.

   **The EC unanimously approved this recommendation**

5. Speakers Invited to Meetings. Harvey indicated that the Committee wanted to remind annual meeting organizers to arrange for one-day registrations, and to consider ways to provide partial support to invited people who can help in advancing the interest of IAPWS. The Statutes already include this but currently there are no mechanisms to activate the process. The EC suggested that a Task Group consisting of Friend and Harries develop a set of procedures to support invited speakers and present this to the EC at the 2008 meeting. The EC accepted the principle and suggested leaving it up to the President and Executive Secretary to make a local decision for the 2008 meetings.

As a final item, the President wished to develop a series of next steps to address the revision of the IAPWS Statutes and By-Laws. After some discussion with EC, the following steps were formulated:

1. A Task Group to draft the revision was formed and consisted of Harvey (Chair), Cooper, Watanabe, Hruby and Alexandrov
2. Once drafted the Executive Secretary will circulate copies to the Heads of National Committees at least six months prior to the Berlin EC meeting.

3. Comments will be reviewed by the Task Group and changes will be made. The final version will be circulated to the Heads of NCs about one month before the Berlin EC meeting. A vote for approval will be taken at the Sunday EC meeting.
4. The final vote will be taken at the General Meeting.

**The EC approved these steps unanimously.**

16.4 IAPWS Restructuring: Education and Outreach

At Monday's EC Meeting (Minute 2.7), the President had asked the Chairman of the Education and Outreach Committee (Kretzschmar) to meet with his committee members during the week and report to the EC on Friday. The Chairman presented his Committee's report which is Attachment 10. Only item 3 of this report needed discussion by the EC as this was new in the suite of items. The Committee suggested to the EC that there should be 10 Awards for Students at the ICPWS at an amount high enough to offset a significant portion of the travel costs (500 Euros). Much discussion resulted in the US Delegate (Friend) proposing to the EC that "the EC allocate 2500 Euros from IAPWS for 5 students to attend the 15$^{th}$ ICPWS with the local committee making the selection".

**The EC approved this proposal unanimously.**

16.5 Acknowledging Contributions to IAPWS Documents

At Monday's EC Meeting (Minute 2.8), the President had formed a Committee to investigate whether acknowledgements should be added to IAPWS documents: Friend (Chair), Lvov, Hiegemann and Wagner. Friend presented the findings and first indicated that his Committee recommends that the EC exercise maximum flexibility in approving or removing an Acknowledgements section in any future IAPWS document.

The Committee further recommended that the primary authors of an IAPWS document provide a draft with the content and format of any Acknowledgement appropriate to that document. The Evaluation Committee, the Working Group(s), the Editorial Committee, and the Executive Committee should review and revise any Acknowledgement section and explicitly give its recommendation for inclusion in the final document.

These two recommendations lead to much EC discussion. The President asked the WG Chairmen for their WG's specific response. TPWS/IRS did not recommend any acknowledgements in any IAPWS documents. PCC and PCAS recommended that acknowledgements should be included. This

lead to further discussion as to whether different documents could/should have different approaches. The President then asked if the EC agreed with the Committee's recommendations. This lead to two motions to the EC. The first was proposed by the Canadian Delegate (Tremaine) and seconded by the US Delegate (Friend): "All IAPWS documents have acknowledgements, which include the names of those who prepared the document and the Evaluation Committee".

**The EC rejected this proposal by a vote of 5 to 1 with 2 abstentions**

The second was proposed by the US Delegate (Friend) and seconded by the Canadian Delegate (Tremaine): "All IAPWS documents may have acknowledgements, which include the names of those who prepared the document and the Evaluation Committee and the names of WG members who had prepared the document".

**The EC rejected this proposal by a vote of 5 to 2 with 1 abstention.**

As a result of these votes by the EC, the President announced that the inclusion of acknowledgements in IAPWS documents had been rejected by the EC. He also indicated that a letter should be sent to the author of the Ionization Constant Release.

**Action: The President will send a thank-you letter to the author of the Ionization Constant Release which will clearly provide attribution of his contribution.**

16.6 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 11 |
| Czech Republic | Attachment 12 |
| Germany | Attachment 13 |
| Japan | Attachment 14 |
| Russia | Attachment 15 |
| USA | Attachment 16 |

16.7 Participants

Attachment 17 provides a list of participants at the IAPWS EC and WG Meetings in Lucerne, Switzerland in August 2007.

16.8 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 Lucerne 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 the new Swiss National Committee for organizing the 2007 Annual IAPWS Meetings, and then he formally closed the 2007 EC meeting at 4:20 pm.

**AGENDA for the EXECUTIVE COMMITTEE of IAPWS**

## LUCERNE, SWITZERLAND. 26 AUGUST – 1 SEPTEMBER 2007

**Monday, 27 August 2007. Opening Session (8:30 – 10:00am)**

Opening Remarks and Welcome by IAPWS President and Head of Swiss Committee
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). (Discussion on Helmholtz follows from Witney Minute 15.1)
   - 2.4 Host Country for 15th ICPWS (German NC) (Witney Minute 17.2)
   - 2.5 IAPWS Member Countries (Witney Minute 12.2.4)
   - 2.6 IAWPS Statutes and By-Laws (Witney Minutes 11 and 12.2)
   - 2.7 IAWPS Education and Outreach (Witney Minute 17.3)
   - 2.8 Acknowledging contributions to IAPWS Documents (US NC)
   - 2.9 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 WG Directions
4. Preview by WG Chairpersons of Week's Activities

**Friday, 31 August 2007. 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)
13. Executive Secretary's Report
    - 13.1 Financial, Auditors and Dues
    - 13.2 Time and Place of 2008/2009 Meetings
14. Guidelines, Releases, Certified Research Needs, and International Collaborations
    - 14.1 International Collaborations
15. IAPWS Awards
    - Helmholtz Award and Procedures Committee
    - Honorary Fellowship
    - Gibbs Award
16. New Business
    - 16.1 Press Release
    - 16.2 15th ICPWS (German NC Report)
    - 16.3 IAPWS Member Countries, Statutes and By-Laws
    - 16.4 Education and Outreach
    - 16.5 Acknowledging IAPWS Contributions
17. Adjournment

THE 2007 ANNUAL IAPWS MEETING
**GRAND HOTEL EUROPE, LUZERN, SWITZERLAND**

Wednesday 29 August 2007

**THE IAPWS 2007 SYMPOSIUM**

**08:00 Begin registration**

**09:00 - 10:00 Helmholtz Award**

Presentation of the Helmholtz award to Karsten Meier (Institut für Thermodynamik, Helmut-Schmidt-Universität, Universität der Bundeswehr Hamburg)

Helmholtz Award Lecture: Dr.K.Meier
"Development of an instrument for highly accurate measurements of the speed of sound in fluids at high pressures"

**10:15 - 16:30 IAPWS Symposium**
**"Interaction of water and steam with materials in power plants"**
Chairman: Dr.H.Venz (NOK Kernkraftwerk Beznau, Switzerland)

Dr.R.Svoboda (Alstom Power, Chairman SCPWS)
Welcome and Introduction

Prof.D.H. Lister and Dr.D.R. Morris (University of New Brunswick, Canada):
"The Dissolution of Hydrogen in Reactor Coolants"

Dr.Shunsuke Uchida (Japan Atomic Energy Agency, Japan):
"Latest Experience with Water Chemistry in Nuclear Power Systems in Japan "

Prof.Horst Michael Prasser (ETH Zürich, Switzerland):
"Water hammer experiments in the frame of the WAHALoads project"

Dr.Barry Dooley (Structural Integrity, USA):
"State of knowledge and future aspects of fossil and combined cycle chemistry"

12:30 - 14:00 Lunch

Dr.Geoff Bignold (GJB Chemistry for Power Ltd, UK):
“The consequences of dissolution of protective metal oxides in water.”

Dr.Andreas Drexler, Dr.Bernhard Stellwag (AREVA NPG Erlangen, Germany):
"Dissolution Behaviour of Ni and NiO Particles in Simulated PWR Reactor Coolant at Temperatures below 100 °C"

Dr.Irene Mailand / Dr.Hartmut Venz (NOK Kernkraftwerk Beznau, Switzerland):
"Influence of the stability of nickel iron oxides on the procedure of the shutdown chemistry at Beznau NPP"

Prof.Serguei Lvov (Pennsylvania State University):

" A New Wave of Basic Research on Materials Under Extreme Environments in the United States"

Final Discussion and Closing Remarks

**16:30 Coffee**

# Schedule of IAPWS Meetings
# Lucerne, Switzerland. 26 August – 1 September 2007

(All meetings will be at the Grand Hotel Europe, Lucerne)

| | | |
|---|---|---|
| Sunday 26 Aug. | 6:30pm | Informal Get-together, Cocktails and Registration<br>(Hosted by SCPWS Committee. Grand Hotel Europe) |
| Monday 27 Aug. | 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<br>**Research on Physical Chemistry for Power Generation** |
| Tuesday 28 Aug. | 8:30am. | PCAS Workshop (other WG Members will be welcome)<br>**Physical Chemistry of High Temperature Aqueous Systems** |
| | 8:30am. | TPWS/IRS/PCC Joint Working Group Meeting<br>**Properties of Humid Air and Humid Combustion Gases** |
| | 10:30am. | All WG Separate or Joint Meetings |
| | 1:30pm | Separate or Joint WG Meetings |
| | 2:30pm | All WGs Joint Meeting<br>"**Workshop on Properties of Seawater"** |
| Wednes. 29 Aug. | 9:00 – 5:00 | **IAPWS Symposium**<br>**" Interaction of Water and Steam with Materials in Power Plants "**<br>**(Registration commences at 8:00am. Helmholtz Lecture at 9am. Symposium at 10:15am)** |
| Thursday 30 Aug. | 8:30am. | IRS and PCC Separate WG Meetings |
| | 8:30am. | TPWS/PCAS Joint WG Meeting<br>"**Ionization Constant of Water"**<br>"**Symposium on Molecular Simulation"** |
| | 1:30pm. | Separate meetings of Working Groups<br>(If needed to prepare for Executive meeting) |
| | 6:30 pm. | **IAPWS Dinner/Banquet**.<br>(Location to be announced) |
| Friday 31 Aug. | 8:30am. | Executive Meeting **(8:30am - 1: 00pm)**<br>(Will include at least one member from each National Delegation) |
| Saturday 1 Sept. | 8:15am. | Technical Visit to NAGRA **(8:30am - 6:00pm)**<br>(Includes Lunch) |

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

Barry Dooley
25 August 2007

## *Minutes*

## IAPWS Thermophysical Properties of Water and Steam WG

**LUCERNE, SWITZERLAND AUGUST 27-30, 2007**

NOTE: Items are listed according to their order on the agenda, which is attached as Attachment A. **Bold print** denotes significant actions. These minutes include some items (4, 8-12, 16, 18) that were done jointly with the WG IRS and also the jointly held workshops on humid air (13) and on seawater (14).

1-3. The meeting was opened on Monday, August 27 by the Chair, Hans-Joachim Kretzschmar. The agenda (Attachment A) was adopted after a few revisions. Allan Harvey was appointed Clerk of Minutes. The minutes of the 2006 TPWS WG meeting in Witney were approved. It was decided that, starting with 2007, circulation and approval of WG minutes would be by email as soon as possible after the meeting.

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

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

8. W. Wagner presented the background of the proposed Revised Release for the melting and sublimation curves, consistent with the IAPWS formulations for fluid water and for ice. **An Evaluation Task Group was appointed consisting of Cooper (Chair), Mares, and Miyagawa. The planned schedule for possible adoption of this document at the 2008 IAPWS meeting will be as follows:**

**Dec. 31, 2007 Completion of evaluation by Evaluation Task Group**
**Jan. 15, 2008 Evaluation report and revised release distributed to Working Group**
**Feb. 15, 2008 Deadline for input from WG members**
**Mar. 1, 2008 Finalized draft of Release to Editorial Committee**
**April 1, 2008 Approval by Editorial Committee**
**Apr. 15, 2008 Distribution by Executive Secretary to National Delegates**

9. A. Harvey and J. Hruby presented a report on their efforts to produce convenient formulations for properties of liquid water at 1 bar pressure. This involves a single self-consistent formulation for the thermodynamic properties, and separate equations for the viscosity, thermal conductivity, and static dielectric constant. It was pointed out that these equations should not extend beyond the range of the underlying full IAPWS formulation; this is particularly an issue for the thermal conductivity. **Harvey and Hruby were authorized to prepare a draft of a Supplementary Release. An Evaluation Task Group was appointed consisting of Sengers, Mares, and Miyagawa. The group will discuss among themselves to select a Chair. The proposers will send supplementary information to the Evaluation Task Group when they send them the draft document. The planned schedule for possible adoption of this document at the 2008 IAPWS meeting will be as follows:**

**Jan. 31, 2008 Completion of evaluation by Evaluation Task Group**
**Feb. 15, 2008 Evaluation report and revised release distributed to Working Group**
**Mar. 15, 2008 Deadline for input from WG members**

**Apr. 1, 2008 Finalized draft of Release to Editorial Committee**
**May 1, 2008 Approval by Editorial Committee**
**May 15, 2008 Distribution by Executive Secretary to National Delegates**

10. R. Feistel presented an update on the project to achieve an improved description of the ideal-gas heat capacity of water, especially at very low and high temperatures. The work is being done in collaboration with the group of Prof. Tennyson at University College London. It is hoped that the technical work will be complete before next year's IAPWS meeting.

11.1 J. Sengers reported on the development of the new viscosity Release, and the work done on the document since last year, with many improvements due to the helpful input of the Evaluation Task Group. R. Mares presented the report of the Evaluation Task Group, which has endorsed the work but had some suggestions about the way some material should be presented, particularly about the simplification obtained by omitting the critical enhancement and what should be said about industrial use. After much discussion, the WG concluded that the simplification should be presented as something for all (not just industrial) users, and that it was very important that our recommendation for industrial use clearly tell people only one way to do things (without extra options that would cause confusion). A temporary Task Group (Harvey, Friend, Sengers, Weber, Mares, Okita) was appointed to draft changes to the document consistent with the discussion. The new draft language was brought back to the WG later in the week.

The item was taken up again on Thursday, and the new language was endorsed with minor revisions. In addition, it was decided to add a footnote to reflect work done by Mr. Miyagawa about the region where the critical enhancement becomes insignificant. **The Working Groups endorsed the document, subject to these revisions and minor editorial changes. We ask the Executive Secretary to distribute it for Postal Ballot following review by the Editorial Committee.**

11.2 J. Sengers described the work toward a new thermal conductivity formulation. The database has been completed and the functional form has been chosen. The data to be used near the critical point have been identified. It is desired to include the Evaluation Task Group at earlier stages compared to the viscosity release, so they can agree on issues such as the database. An Evaluation Task Group will be appointed in 2008.

12. J. Cooper presented the work on modification of the formulations of the transport properties of heavy water. A. Harvey presented a brief evaluation report on behalf of K. Miyagawa; the recommendation was to endorse the revisions and the new document. **The Working Groups TPWS and IRS approved the draft Revised Release and recommended its approval by the EC (subject to some very minor editorial changes for formatting).**

13.1. M. Wendland presented his results on "Measurements of the Water Vapor Concentration Enhancement in Compressed Air, Nitrogen, and Argon with FTIR Spectroscopy."

13.2. A. Harvey presented his results on "First-Principles Calculation of Interaction Second Virial Coefficients Between Water and Common Gases Including Air." Discussion ensued on discrepancies between the model calculations and various experimental results. It is clear that more research and discussion is needed to resolve these discrepancies.

13.3 N. Okita presented his report, and a proposed ICRN, from the Task Group on the dew point of combustion gas. J. Hruby presented some calculations of the dew point of mixtures of water and sulfuric acid.

The IRS WG chairman pointed out that the problem statement of the draft was not yet clear enough. Some discussion evolved around this topic. It was the common understanding that there are two steps involved in this matter:

1. The first step is the conversion of the sulfur in the fuel to $SO_2$ / $SO_3$ in the flue gas including the conversion rate between $SO_2$ and $SO_3$.
2. The second step is the determination of the dew point based on a known $SO_2$ / $SO_3$ content in the flue gas.

It was the feeling that step 1 is somewhat outside the scope of IAPWS. For step 2 apparently quite a few investigations were published recently. There wouldn't be any progress to be expected through an involvement of IAPWS. N. Okita presented an updated draft of an ICRN, however it was the feeling of the WGs that the draft still needs some clarification. **A task group was formed to establish an ICRN on this topic requiring only formal acceptance at the 2008 IAPWS meeting. Members of the task group are N. Okita (chair), J. Hruby, B. Rukes, R. Span. Timeline for the task group is:**
**2008-01-31: Circulate updated draft of ICRN to members of WGs**
**2008-03-31: Deadline for comments, transfer of the finalized draft to the editorial committee**

13.4 R. Span discussed the existing ICRN #14 on properties of humid air and combustion gases, which is expiring in 2008. There was consensus that this was still an area in need of work, with some shift in focus to humid combustion gases. **Prof. Span was authorized to proceed forward to produce a revised ICRN for 2008. The requested timeline is that a revised ICRN should be circulated to the Working Groups by March 31, 2008.**

14. The Workshop on Seawater was done as a joint session on Tuesday afternoon. The presentations were as described on the agenda (Attachment A).

The new standard for the definition of salinity was discussed, and IAPWS had no objection to this proposal.

R. Feistel presented a Draft Release on thermodynamic properties of seawater. It was agreed to proceed forward for possible adoption in 2008, with the Release being from PCAS and TPWS. An Evaluation Task Group was appointed consisting of Hruby (Chair), Kretzschmar, Cooper, Miyagawa, and Tremaine. The evaluators were instructed to think about the relevance of the Release for desalination conditions. The timetable will be as follows:
**Jan. 31, 2008 Completion of evaluation by Evaluation Task Group**
**Feb. 15, 2008 Evaluation report and revised release distributed to Working Group**
**Mar. 15, 2008 Deadline for input from WG members**
**Apr. 1, 2008 Finalized draft of Release to Editorial Committee**
**May 1, 2008 Approval by Editorial Committee**
**May 15, 2008 Distribution by Executive Secretary to National Delegates**

R. Feistel presented a draft ICRN for seawater properties. **The Working Groups endorsed this ICRN and request that it be sent out for approval.**

15. [The joint PCAS/TPWS workshop is reported in the PCAS minutes.]

16. A. Harvey reported that there would be no update this year on the IAPWS Fundamental Constants document, but that an update would be prepared for 2008.

The contents of Advisory Note #2 are affected by some of the documents to be adopted at this meeting. **Cooper and Harvey were authorized to update this Advisory Note by the usual procedure.**

H.-J. Kretzschmar reported on the Steam Tables for pocket calculators now available at a site linked from the IAPWS website. There have been 452 downloads of this software so far.

V. Ochkov reported on the software he has developed for convenient calculation of water and steam properties in many formats and languages. It is available through a site linked from the IAPWS website. He also reported on some useful implementations that allow online checking and calculation of IAPWS formulations.

J. Cooper reported that there was nothing to report regarding liaison with the IEC.

A. Harvey reported on the efforts toward making 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. Progress along the original plans (where a comprehensive paper would be produced) has been stopped due to concerns on the CCM side. The WG was not in favor of a joint publication which only had a few comparisons but was not comprehensive. The consensus was in favor of an alternative where only a brief paper would be written as a joint statement, without any technical information. **Harvey was instructed to proceed forward on these lines.**

17. We were informed by the Czech delegation that **Prof. Kadrnozka is withdrawn from TPWS membership. It was voted to accept V. Ochkov, P. Spitzer, and M. Wendland for membership in TPWS.**

18.1 Prof. Wagner informed the Working Groups about the fact that calculations of the IAPWS dielectric constant and refractive index are still good if IAPWS-IF97 is used to calculate density. He pointed out that the current releases specify calculation with IAPWS-95, which could be a problem for any people using the Industrial Formulation who wish to calculate these properties. Some discussion ensued about whether there was a need to amend the releases or otherwise provide guidance. It was decided that this question should be on the TPWS/IRS agenda in 2008. In addition, **we request the EC to ask National Committees if they have any input on the following question: "Is there a need for instruction from IAPWS about using IAPWS-IF97 in conjunction with formulations for more scientific quantities that have been based on IAPWS-95 (dielectric constant, refractive index, ionization constant, etc.)."**

18.2 There was nothing further on this item.

18.3 There were no collaborative projects proposed from TPWS or IRS.

18.4 The issue of Acknowledgments in IAPWS documents was discussed. **The combined WGs TPWS and IRS considered a motion that such Acknowledgments should not be allowed in IAPWS documents. The motion passed with 13 in favor, 4 opposed, and 4 abstaining.**

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

20. The meeting was adjourned at 5:20 PM on Thursday, August 30.

# *Agenda*

## IAPWS Thermophysical Properties of Water and Steam WG

### LUCERNE, SWITZERLAND, 26 – 31 AUGUST 2007

1. Opening Remarks; Adoption of Agenda
2. Appointment of Clerk of Minutes
3. Approval of Minutes of TPWS WG in Witney, UK (September 2006)
4. Potential International Collaborative Projects
5. Revised Release on IAPWS-IF97 Including the Extension of Region 5, joint with WG IRS
   - Report of the Task Group (W. Wagner)
   - Report of the Evaluation Committee (R. Mareš, K. Miyagawa)
   - Formal Consideration of the Revised Release by the WGs TPWS and IRS
6. Industrial Requirements for Steam Property Calculations (W.T. Parry), joint with IRS
   - 6.1 CFD – The Need for Speed
   - 6.2 Tradeoffs between Speed, Consistency, and Accuracy
   - 6.3 Metastable Considerations
7. Advisory Note No. 3 on Thermodynamic Derivatives from IAPWS Formulations, joint with WG IRS
   - Report of the Evaluation Committee (N. Okita in place of K. Miyagawa)
   - Formal Consideration of the Advisory Note by the WGs TPWS and IRS
8. Revised Release on the Pressure along the Melting and Sublimation Curves of Water, joint with WG IRS
   - Report of the Task Group (W. Wagner)
   - Appointment of an Evaluation Task Group
9. Properties of Liquid Water at Atmospheric Pressure, joint with WG IRS
   - Report of the Task Group (A.H. Harvey, J. Hruby)
10. Ideal-Gas Properties, joint with WG IRS
    - Report of the Task Group (R. Feistel)

11. Transport Properties of Water and Steam, joint with WG IRS

11.1 Release on the IAPWS Formulation 2007 for the Viscosity of Water

- Report of the Task Group (J.V. Sengers)
- Report of the Evaluation Task Group (R. Mares, K. Miyagawa)
- Formal Consideration of the Release by the WGs TPWS and IRS

11.2 Thermal Conductivity

- Report of the Task Group (J.V. Sengers)
- Appointment of an Evaluation Task Group

12. Transport Properties of Heavy Water, joint with WG IRS

- Report of the Task Group (J.R. Cooper)
- Report about the Evaluation Work (A. Harvey, K. Miyagawa)
- Formal Consideration of the Revised Release by the WGs TPWS and IRS

13. Workshop on Properties of Humid Air and Humid Combustion Gases, joint with WGs IRS, PCC, and PCAS (Tuesday morning, 8:30)

13.1 Measurements of the Water Vapor Concentration Enhancement in Compressed Air, Nitrogen, and Argon with FTIR Spectroscopy (M. Wendland, Univ. of Agriculture Wien)

13.2 First-Principles Calculation of Interaction Second Virial Coefficients Between Water and Common Gases, Including Air (A.H. Harvey)

13.3 Dew Point of Combustion Gas

- Report of the Task Group (N. Okita, R. Span, J. Hruby)

13.4 Update for ICRN-14: Thermophysical Properties of Humid Air and Combustion-Gas Mixtures (R. Span)

14. Workshop on Properties of Seawater (P. Tremaine), joint with WGs IRS, PCAS, PCC (Tuesday afternoon, 1:30)

14.1 Activities of the Task Group on Seawater, Liaison with IAPSO, Letters Between the IAPWS President and the President of IAPSO
- Report of the Task Group (R. Feistel, A.H. Harvey, M. Hiegemann, P. Tremaine)

14.2 Investigation of IAPWS-95 Properties Between the Freezing Points of Pure Water and Seawater
- Report of the Task Group (R. Feistel, M: Anisimov, J. Hruby, W. Wagner)

14.3 Composition of Standard Seawater, Reference Salinity Scale (R. Feistel, F.J. Millero, RSMAS, Miami, FL)

14.4 Uncertainty of Conductivity Measurements (P. Spitzer, PTB Braunschweig, Germany)

14.5 Release on the IAPWS Formulation for the Thermodynamic Properties of Seawater
- Report of the Task Group (R. Feistel)
- Appointment of an Evaluation Task Group

14.6 New Measurements for Density of Seawater (R. Feistel in place of F.J. Millero)

14.7 Formulation of an ICRN on the Properties of Seawater (R. Feistel)

14.8 Formula Symbols, e. g. for the Salinity of Seawater (R. Feistel)

15. Joint Meeting with PCAS (Thursday Morning, 8:30)

15.1 Release on the Ionization Constant of Water
- Report of the Evaluation Committee (A.H. Harvey, M. Nakahara, P. Tremaine)
- Formal Consideration of the Release by the WGs TPWS and PCAS

15.2 Workshop on Molecular Simulation (K. Yasuoka)
- Molecular Dynamics Study of Water and Amphiphile/Water: Sub- and Supercritical Water and Micellar Solution (N. Yoshii, Himeji Dokkyo University)
- Report of the Molecular Simulation Task Group (K. Yasuoka)

15.3 The Nucleation, Bubble Dynamics and Effects of the Physical Properties of Water on the Cavitation Erosion (M. Sedlar)

15.4 The Mechanism of Nucleation in Pure Water and the Surface Tension of Ice (T. Nemec).

15.5 Thermochemical Split of Water for Hydrogen Production (S.N. Lvov, P. Tremaine)

16. Reports on Other TPWS & IRS Activities

16.1 Fundamental Constants (A.H. Harvey), joint with WG IRS

16.2 Update of Advisory Note No. 2: Roles of Various IAPWS Documents. (A.H. Harvey, J.R. Cooper), joint with WG IRS

16.3 Download of Steam Tables for Pocket Calculators from the IAPWS Website

16.4 Steam Tables and Diagrams on Mathcad Calculation Server for Personal Computers, Pocket Computers, and SmartPhones (V.F. Ochkov, Moscow Power Institute), joint with WG IRS

16.5 New Internet Technology of IAPWS Formulations Checking, Publication, and On-line Calculation (V.F. Ochkov, Moscow Power Institute), joint with WG IRS

16.6 Liaison with IEC (J.R. Cooper), joint with WG IRS

16.7 Liaison with CCM (A.H. Harvey, R. Span), joint with WG IRS

17. Membership
18. Other Business
    - 18.1 Use of IAPWS-IF97 for the Calculation of the Density for Determining the Dielectric Constant and Refractive Index (W. Wagner), joint with WG IRS
    - 18.2 Topics for the 15th ICPWS 2008 in Berlin (B. Rukes, I. Weber), joint with WG IRS
    - 18.3 Report on International Collaborative Projects
    - 18.4 Acknowledgements in IAPWS Documents
19. Preparation of the Formal Motion to the EC
20. Adjournment

*August 30, 2007*

*H.-J. Kretzschmar (Chair) and A.H. Harvey (Vice-Chair)*

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

## Lucerne, Switzerland, 27. – 31. August 2007

Remark: Most of the IRS meetings were held as joint meetings with TPWS (marked by *). Of these joint meetings the IRS minutes cover the topics chaired by the IRS chairman.

1. **Opening remarks, Adoption of Agenda**
   Chairman B. Parry welcomed the WG members to Lucerne. The agenda was adopted with slight adjustments.

2. **Appointment of Clerk of Minutes**
   I. Weber was appointed clerk of minutes.

3. **Approval of Witney Meeting Minutes**
   The minutes of the 2006 IRS WG meeting were approved unchanged.

   A different procedure for a more effective approval of the minutes was suggested by members of the WG. The proposal is that the minutes are sent out to all WG members directly after the meeting requesting any comments / corrections within a defined time frame. Any comments will be incorporated and the updated minutes are distributed again. If no comments are received anymore the minutes are approved. The "approval of the minutes" topic of the WG agenda could be eliminated.
   The EC will be informed that WG IRS will proceed accordingly.

4. **Revised Release on IAPWS-IF97 including extension of Region 5***
   a. **Report of the Task Group**
      W. Wagner had presented a full report on the topic last year in Witney, no additional technical information was given this time. The proposed changes to the release were presented last year, the evaluation task group evaluated the equations and the revised release document.
   b. **Report of the Evaluation Committee**
      R. Mares presented the results of the evaluation on behalf of the task group chair K. Miyagawa. The evaluation task group found that the accuracy meets the requirements, that the computing speed is acceptable and that the wording of the draft is acceptable. The evaluation task group recommends to the WGs to adopt the revised release.
   c. **Formal Consideration of the Revised Release by the WGs TPWS and IRS**
      The WGs unanimously voted to recommend to the EC that the revised release is adopted.

5. **Industrial Requirements for Steam Property Calculations***
   Bill Parry presented an overview about the speed requirements for water / steam properties throughout the years - starting from the early times when speed was not a factor all the way to the requirements of Computational Fluid Dynamics (CFD). CFD modeling requires vast numbers of property calls, as an example simplified modeling of a low pressure section of a steam turbine requires property calls in the order of magnitude of $10^{13}$. Considering this huge number of calculations using the fastest existing method (TTSE) the calculation still would require roughly a day. However, the goal is a detailed CFD model with all nozzles, leakages, etc. This kind of calculation would again multiply the required property calls by a factor of 10000. I.e. the current speed capabilities are by no means acceptable for this type of calculation. Accuracy is an important factor, however consistency plays an even more important role. With the current quality of consistency CFD calculations will not be successful, additional iterations within the property function routines are required – causing additional time requirements. It was the opinion of the

WGs that table-lookup methods would be the method of choice for this type of application. Another aspect of CFD calculations is the question of modeling metastable states. Here the question arises how the expansion through the saturation line is to be modeled correctly. Some discussion evolved about the "metastable issue", it was mentioned that this topic has been discussed a few times already without any concrete result. Problem is that the behavior depends on many factors which partly are outside the pure thermodynamic field.
As a conclusion of the discussion the following tasks where identified:

- **a.** A task group was founded to establish requirements and current possibilities for high-speed property functions. Members of the task group are: W. Parry (chair), B. Rukes / I. Weber, M. Hiegemann, R. Mares, N. Okita, H.-J. Kretzschmar and K. Miyagawa. It was suggested to utilize the forthcoming 15th ICPWS to present future requirements for water/steam property routines for industrial use.
- **b.** J. Hruby agreed to found a task group for homogeneous nucleation. P. Blangetti agreed to contact Mr. Yamamati, an expert in this field. Additionally R. Feistel offered to contact people during the forthcoming meeting of the Organization on Nucleation Theory and Applications in Dubna / Moscow, Russia. Possibly some kind of workshop within the framework of the 15th ICPWS could be organized.

**6. Advisory Note No. 3 on Thermodynamic Derivatives from IAPWS Formulations***

- **a. Report of the Evaluation Committee**
  N. Okita presented the report of the evaluation task group consisting of K. Miyagawa and N. Okita. No major issues were found, only minor corrections were communicated. After amendment the advisory note was checked by the editorial committee. The evaluation task group recommends to the WGs to adopt the advisory note.
- **b. Formal Consideration of the Advisory Note by the WGs TPWS and IRS**
  The WGs unanimously voted to recommend to the EC that the advisory note is adopted.

**7. Development of New Equations for Melting Pressure and Sublimation Pressure***
See TPWS minutes.

**8. Properties of Liquid Water at Atmospheric Pressure***
See TPWS minutes.

**9. Ideal-Gas Properties***
See TPWS minutes.

**10. Transport Properties of Water and Steam***
See TPWS minutes.

**11. Transport Properties of Heavy Water***
See TPWS minutes.

**12. Properties of Humid Air and Humid Combustion Gases***
See TPWS minutes.

**13. Workshop on Properties of Seawater***
See TPWS minutes.

**14. Reports on Other TPWS & IRS Activities***
See TPWS minutes.

**15. Membership**
There were no membership items to be discussed this year.

**16. Other Business***

See TPWS minutes.

**17. Preparation of Report to Executive Committee**
The Chairman and Clerk of Minutes will prepare the report to the EC.

**18. Adjournment**
The Chairman adjourned the IRS working group meeting at 30. August 2007, 5:30pm.

# Agenda
# of
# Industrial Requirement and Solutions Working Group

## LUCERNE, SWITZERLAND, 26 TO 31 AUGUST 2007

1. Opening Remarks, Adoption of Agenda
2. Appointment of Clerk of Minutes
3. Approval of Minutes IRS WG in Whitney, UK (September 2006)
4. Revised Release on IAPWS-IF97 including extension of Region 5, joint with WG TPWS
   - Report of the Task Group (W. Wagner)
   - Report of the Evaluation Committee (R. Mares)
   - Formal Consideration of the Revised Release by the WGs TPWS and IRS
5. Industrial Requirements for Steam Property Calculations (W. Parry)
   - 5.1 CFD – The Need for Speed
   - 5.2 Tradeoffs between Speed, Consistency, and Accuracy
   - 5.3 Metastable Considerations
6. Advisory Note No. 3 on Thermodynamic Derivatives from IAPWS Formulations, joint with WG TPWS
   - Report of the Evaluation Committee (N. Okita)
   - Formal Consideration of the Advisory Note by the WGs TPWS and IRS
7. Development of New Equations for Melting Pressure and Sublimation Pressure, joint with WG TPWS
   - Report of the Task Group (W. Wagner)
8. Properties of Liquid Water at Atmospheric Pressure, joint with WG TPWS
   - Report of the Task Group (A.H. Harvey, J. Hruby)
9. Ideal-Gas Properties, joint with WG TPWS
   - Report of the Task Group (R. Feistel)
10. Transport Properties of Water and Steam, joint with WG TPWS
    - 10.1 Viscosity
      - Report of the Task Group (J.V. Sengers)
      - Report of the Evaluation Task Group (R. Mares)
      - Formal Consideration of the Release by the WGs TPWS and IRS
    - 10.2 Thermal Conductivity
      - Report of the Task Group (J.V. Sengers)
      - Appointment of an Evaluation Task Group
11. Transport Properties of Heavy Water, joint with WG TPWS
    - Report of the Task Group (J.R. Cooper)
    - Formal Consideration of the Revised Release by the WGs TPWS and IRS
12. Properties of Humid Air and Humid Combustion Gases (A.H. Harvey), joint with WGs IRS and PCC (Tuesday morning)
    - 12.1 Measurements of the Water Vapor Concentration Enhancement in Compressed Air, Nitrogen, and Argon with FTIR Spectroscopy (M. Wendland)
    - 12.2 First-Principles Calculation of Interaction Second Virial Coefficients Between Water and Common Gases, Including Air (A.H. Harvey)
    - Dew Point of Combustion Gas
      - Report of the Task Group (N. Okita, R. Span, J. Hruby)

Update for ICRN-14: Thermophysical Properties of Humid Air and Combustion-Gas Mixtures (R. Span)

13. Workshop on Properties of Seawater (P. Tremaine), joint with WGs IRS, PCAS, PCC (Tuesday afternoon)

14. Reports on Other TPWS & IRS Activities
    - 14.1 Fundamental Constants (A.H. Harvey)
    - 14.2 Update of Advisory Note No. 2: Roles of Various IAPWS Documents. (A.H. Harvey, J.R. Cooper)
    - 14.3 Download of Steam Tables for Pocket Calculators from the IAPWS Website
    - 14.4 Liaison with IEC (J.R. Cooper), joint with WG IRS
    - 14.5 Liaison with CCM (A.H. Harvey, R. Span)
15. Membership
16. Other Business (Joint with TPWS)
    - 16.1 Use of IAPWS-IF97 for the Calculation of the Density for Determining the Dielectric Constant and Refractive Index (W. Wagner)
    - 16.2 Topics for the 15th ICPWS 2008 in Berlin (B. Rukes, I. Weber)
    - 16.3 Report on International Collaborative Projects
    - 16.4 Gibbs Award Committee
    - 16.5 Acknowledgements on IAPWS Documents
17. Preparation of the Formal Motion to the EC
18. Adjournment

# IAPWS Annual Meeting 2007, Lucerne
# PCAS Minutes

## Monday Morning

***Present:*** *Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Uneo; Notiyuki Yoshi; Frantisek Marsik; Milan Sedlar; Pavel Safarik; Tomas Nemec; Jana Ehlerova.*

**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.

**2. Minutes from 2006 meeting (Witney)** were unanimously approved as written.

**Actions Arising:** One outstanding action from 2006. Horacio Corti has expressed concern about the difficulties he is having in attending meetings as co-chair. He was not able to come to Lucerne. The question will be discussed on Thursday.

**3. IAPWS International Collaboration:** Peter Tremaine presented the proposal by Canada (Tremaine) and the Czech Republic (Sedlbauer). Both national committees support the proposal. Questions related to two aspects of the proposal were discussed by Tremaine. (i) Budget: the budget of $16,000 is based on the stipend of a Canadian graduate student after tuition is deducted. (ii) The draft proposal was incorrectly sent to the Executive Director rather than to the Chair of PCAS for distribution. The project is for measurements on copper (II) complexation vs T as part of research to support the hydrogen co-generation as part of the Gen IV Initiative. Two students have been identified as candidates. The request for $16,000 is higher than past proposals. It will be reduced to $14,000 for a 10 month stay. The proposal identifies Ms. Jitka Felcmanova for the exchange, with Ms. Jana Eherlova as 2nd choice. Both are Dr. Sedlbauer's PhD students. Dr. Tremaine and Dr. Trevani will supervise the experimental portion of the project; Dr. Sedbauer will supervise fitting the SOW group additivity model to the new data. The project is not related to the recently completed collaborative project by Jana Eherlova, Tremaine and Sedlbauer, which was to develop group additivity models for aromatic organic solutes in high temperature water.

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

**4. ICRNs and Releases:** Lvov invited the committee to discuss reasons for so few ICRNs to arise from PCAS. It was agreed to identify possible new ICRNs and further discuss the issue on Thursday.

**ICRN Number 10 (pH Measurements) and ICRN Number 13 (Surface tension of Aqueous Solution)**: Members agreed in 2006 to transfer ICRN 13 to PCAS. Both were extended by 3 years at that time last year.

**New Release: Ionization Constant of Water.** The draft release prepared by Lvov was approved by the Evaluation Committee (A. Harvey, P. Tremaine, M. Nakahara). The question of whether releases should have an acknowledgement to indicate the members of the evaluation committee and other contributors. It was agreed that acknowledgements can be included where appropriate.

**5. New Members:** No new members were suggested.

**6. Task Groups and Committees**:

**6.1. Joint Electrochemical Society/IAPWS Symposium (Washington, 2007**): Dr. Lvov presented a status report on the Symposium. The call for papers attracted 25 submissions and will result in a 2-day symposium. The WG compliments Lvov on this very successful initiative.

**6.2. Data Book Project**: Dr. Lvov presented a status report on the Data Book Initiative, Prof. Valashkov (editor). The chapter 2 by Dr. Majer has been withdrawn and will be omitted. Three chapters

are complete, three are completed as drafts. The project is on schedule. The draft manuscript is expected to be submitted to the publisher by Prof. Valashkov by December 2007.

**6.3: Joint IUPAC/IAPWS Project on Standard Partial Molar Properties of Solutes** Dr. Lvov presented a letter from Dr. Fernandez Prini expressing concern about the status of the project, and a letter from Professor Majer to IUPAC explaining that he has left his position as Director of the Thermodynamics Lab at Blaise Pascale, and that the project cannot be continued. The committee expressed deep concern that IAPWS was not contacted by Dr. Majer to explore solutions.

***ACTION (Lvov):*** To write Dr. Majer requesting a wrap-up status report, and recommendations by which the project might be saved.

# Tuesday Morning

**Present:** *Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Uneo; Notiyuki Yoshi; Frantisek Marsik; Milan Sedlar; Pavel Safarik; Tomas Nemec; Jana Ehlerova.*

**7. Actions from Witney:**
**(7.1) Membership:** Horacio Corti has expressed concern about the difficulties he is having in attending meetings as co-chair. The question of attendance from several counties was 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.

**8. IAPWS International Collaboration:** Jana Ehlerova presented results from her recently completed collaborative project with Dr. Tremaine (University of Guelph) and Dr. Sedlbauer (University of Libercec), which was to measure values for the ionization constant of o-, m-, and p-nitrophenol under hydrothermal conditions as part of her PhD thesis project which is to develop group additivity models for aromatic organic solutes in high temperature water. A manuscript entitled "Spectrophotmetric Determination of the Ionization Constants of Aqueous Nitrophenols at Temperatures up to 225 EC" by Ehlerova, Trevani, Sedlbauer and Tremaine has been written and will be submitted to J. Phys. Chem.

The Working Group congratulated Ms. Ehlerova on her very successful project and report presentation.

***MOVED (Lvov):*** To accept the PowerPoint report, as successful completion of the project. ***APPROVED (Unanimous)***

***ACTION (Tremaine, Sedlbauer):*** To provide the manuscript by Christmas 2007, for information.

# Tuesday Afternoon (Joint with TPWS)

***Present (PCAS):*** *Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Uneo; Notiyuki Yoshi; Frantisek Marsik; Milan Sedlar; Pavel Safarik; Tomas Nemec; Jana Ehlerova..*
***Present (TPWS):*** *Hans Joachim Kretzschmar(Chair); Alan Harvet; Jan Sengers; Rainer Feistal; Dan Friend; Koichi Watanabe; Jeff Cooper; Alexandrov; Ines Stoecker, Petra Spitzer.*

**9. Seawater Symposium and Decisions**

Rainer Feisal and Petra Spitzer presented the talks on seawater as listed in the agenda. Rainer noted that the release is based on the new seawater formulation outlined in his presentation, and submitted for publication.

***IT WAS AGREED:*** that TPWS and PCAS should proceed on the understanding that approval will be contingent of acceptance of the new formulation by IAPSO.

***MOVED (R. Feisal)*** that the working groups accept the draft release, subject to review by the editorial committee. **APPROVED (Unanimous)**

# Thursday Morning (Joint with TPWS)

***Present (PCAS):*** *Serguei Lvov (Chair), Masaru Nakahara; Peter Tremaine (Clerk of Minutes); Masakatsu Uneo; Notiyuki Yoshi; Frantisek Marsik; Milan Sedlar; Pavel Safarik; Tomas Nemec; Jana Ehlerova..*
***Present (TPWS):*** *Hans Joachim Kretzschmar(Chair); Alan Harvet; Jan Sengers; Rainer Feistal; Dan Friend; Koichi Watanabe; Jeff Cooper; Alexandrov; Ines Stoecker.*

### 10. Release on the Ionization Constant of Water

A. Harvey presented the Editorial Committee report on the proposed release by S. Lvov. The Committee consisted of Alan Harvey (Chair); M. Nakahara, P. Tremaine, and D. Palmer (withdrew),
S. Lvov presented two additional changes:
(i) Q is now defined to be dimensionless
(ii) The limit at zero density of $K_w$ (hyp 1-m std state) is not equal to $K_w^G$ (ideal gas std state)
because the standard-state transfer term is non-zero.
The Working Groups discussed minor changes to the list of symbols to improve clarity.

***MOVED: (A. Harvey; second S. Lvov):*** that the working groups accept the formulation subject to minor correction by the Editorial Committee: ***APPROVED*** **(Unanimous).**

***ACTION (Hans-Joachim Kretzschmar):*** To raise the issue of whether the release must be based on a published paper and whether the release can deviate from the material in the paper on which it is based.

***ACTION (Working Party Members):*** Minor corrections must be submitted to A. Harvey by lunch time today.

### 11. Symposium on Molecular Simulation:

After the presentations, the working groups discussed two questions at PCAS request: (i) whether the IAPWS mandate should include Hydrogen Co-generation; (ii) whether TPWS would be prepared to initiate work on developing releases on the density and dielectric constant of $D_2O$ and NaCl(aq).

***IT WAS AGREED:*** that a strong effort should be made to support the symposium on cogeneration at the ICPWS.

***IT WAS AGREED*** that, if the need is clarified, TPWS would consider a request to produce an ICRN could be written to highlight the need for measurements and/or formulations for the density and dielectric constant of $D_2O$ and NaCl(aq).

***ACTION:*** **(Peter Tremaine, Jeff Cooper**) to draft a short statement of each problem with key references.

### 12. PCAS Meeting: Final Actions

**Collaborative Project:** Frantisek Marsik presented the report for the project of Andre Mican's project (S. Lvov and F. Marsik, supervisors).

***MOVED (Lvov):*** that the report be accepted. **APPROVED (Unanimous)**

**New name of the WG:** Serguei Lvov proposed to rename the WG to Physical Chemistry of Aqueous Systems. **APPROVED (Unanimous).**

**Future of PCAS:** Possible candidates for PCAS WG chair in the future were discussed. It was decided to continue the discussion at IAPWS 2008 meeting in Berlin.

**13. The meeting adjourned at 4:00 pm.**

# IAPWS Working Group Power Cycle Chemistry (PCC)

**Minutes of IAPWS PCC WG Meetings**

Lucerne Switzerland 27-30 August, 2007

Chairman: Robert Svoboda
Members present See Addendum A

Members attended 4 technical presentation sessions covering topics set out under the agenda, see Addendum B.

## 1. AGENDA

### 1.1 Amendments / Adoption of Agenda

The content of the agenda was agreed. The order of consideration of topics was adjusted to enable actions to be placed after full coverage of relevant topics.

### 1.2 Week program: PCC participation in joint workshops and task groups

It was agreed that the session on sea water properties would provide an opportunity for a further parallel PCC meeting session to be attended by those not wishing to attend the joint meeting.

## 2. APPOINTMENT OF CLERK OF MINUTES

Geoff Bignold agreed to record the minutes.

## 3. APPROVAL OF MINUTES OF PCC WG IN WITNEY, ENGLAND, 2006

The minutes were agreed without any corrections or additions.

## 4. PROGRESS REPORTS ON PCC ACTIVITIES 2006 / 2007

### 4.1 International Collaboration "Assessment of the State of the Art of sampling Corrosion Products from Water / Steam cycles"

Derek Lister reported that successful progress had been made. Piti Srisukvatananan, a student at New Brunswick University had spent time at Alstom under supervision of Robert Svoboda, and at a Danish plant under supervision of Karol Daucik. He had now produced a draft final report "Assessment of the state of the art of sampling of corrosion products from water/steam cycles":

The draft report will be circulated to PCC members for review with a deadline of 30 September. It will then be submitted for publication.

**Action RS**.

Derek Lister confirmed that the collaboration had been completed with cost below budget, due to unforeseeable additional resources in Switzerland and Denmark.

Barry Dooley stated that the final report will be retained within IAPWS records and that the Executive Committee need take no action other than to note the successful outcome.

### 4.2 ICRN

- ICRN 18 "Decomposition of Ion Exchange Resins",

- ICRN 19 "Improved Coolant Sampling and Analysis of Low Concentration Metals (Fe, Cu, Co, etc.),

- ICRN 20 "Sensors for Use at Elevated Temperature in the Plant Cycle of the Power Industry".

Have all been approved and issued.

Work on two other draft ICRNs continues. These are:

"Research of Amines for the Power Industry". Further drafting of this will be coordinated by Jim Bellows.

**Action JB**.

"Thermophysical Properties Associated with Ultra-supercritical Coal-Fired Steam Generators". Barry Dooley will contact Don Palmer with regard to further drafting of this.

**Action BD**.

### 4.3 PCC Guidance Document "Mechanical Carry-Over"

After 16 iterations within the task group, a draft guidance document on this topic has been circulated in PCC. To be discussed under item 10.1

### 4.4 European Standard EN 12952:12

Severe concerns have been expressed about the technical content of this European Standard. Consideration will be given to setting up a PCC Task Group to lobby for appropriate revisions. See item 10.3.

### 4.5 PCC Public Relations

Robert Svoboda urged PCC members to give consideration to the need to attract more young members into the working group and to ensure that the efforts of the group are demonstrably valuable to the supporting industry. See item 10.4

### 4.6 Other Action List Items

There were no reports on other actions at this stage.

## 5. PROPOSALS FOR INTERNATIONAL COLLABORATION

No new proposals for international collaborations were raised.

## 6. PRIORITY LIST REVIEW

A full review of the priority list was undertaken. The outcome is covered in Addendum C.

## 7. ICRN

There is intention for an ICRN on Priority List item #6. ("The relationships between the chemistry of the contaminants and their concentration at point of measurement"). Subject of possible paper for the 15th ICPWS.

**Action JB**

There is intention for an ICRN 7 on Priority List item #6 ("Quantification of Risk"). Subject of current task group activity, item 10.2

ICRN 13 – Surface Tension. It was agreed that a full formal closure statement is required. Frank Gabrielli has indicated that the interest in the topic has declined and that the closure statement will therefore be quite brief. Robert Svoboda will request that it be prepared.

**Action RS**.

ICRN 22 - Steam Chemistry in Turbine Phase-Transition Zone. A draft, prepared by Miroslav Štastnŷ has been circulated and some comments provided. Further suggestions for modifications, formulation into ICRN format, etc. will be incorporated and the ICRN will be circulated for approval by national committees

**Action BD, JB, RH**

## 8. SETTING UP PCC TASK GROUPS

New Task Groups established:

> Task Group on "Assessment of plant lifetime consumption resulting from operation outside of chemistry guideline targets". Karol Daucik (chairman). See item 10.2)
>
> Task Group of European members to lobby for "Review of Standard EN12952:12". Eric Maughan (chairman). See item 10.3

New ad hoc Task Groups established:

> Task Group on defining the role of PCC with regard to future activities and growth of wider support. – All PCC members invited to attend and contribute. See item 10.4.
>
> Task Group on liaison with other IAPWS working groups on chemistry and corrosion issues arising out of the ongoing work on the properties of humid air and humid combustion gases. – Jim Bellows to co-opt members and convene as appropriate.

## 9. OTHER BUSINESS

None.

## 10. TASK GROUP PROGRESS REPORTS

### 10.1 Task Group on PCC Guidance Document "Mechanical Carry-Over"

There was extensive debate about the final draft that had been circulated to members in advance of the meeting. Barry Dooley criticised the concentration on vaporous and mechanical carry over when the plant requirement is to monitor and control total carry-over. Plant operators and manufacturers have different requirements. Manufacturers need to demonstrate that the plant meets specification targets, whereas operators need to be alert to the development of faults. More emphasis on appropriate and sufficiently comprehensive sampling was required.

Despite the issues raised there was general agreement that the document should become a valuable IAPWS PCC product. However, there was not yet sufficient agreement to present it as a final draft for consideration by the Executive Committee at this time. Robert Svoboda agreed to make modifications based on the issues raised and then to invite comments from an editing task group comprising Malcolm Ball, Barry Dooley, Albert Bursik, Jim Bellows, Marc de Wispelaere, Andre Zeitjseink, Geoff Bignold. He would introduce the concept to the Executive Committee and indicate the PCC wish to

issue it under a new suggested category of document called an IAPWS Technical Application Guideline.

**Action RS**.

### 10.2 Task Group "Assessment of plant lifetime consumption"

PCC has set up a task group on "Assessment of plant lifetime consumption resulting from operation outside of chemistry guideline targets" (Priority List item # 7: "Quantification of risk of asset damage").

The task group consists of the following members of PCC:
K.Daucik (chairman), M. Rziha, B.Hughes, E.Maughan, A.Zeijseink, A.Rudge, S.-E. Therkildsen, J.Bellows

The goal of the task group is to investigate and to elaborate, as far as possible, the effect of corrosive contaminants, corrosion processes and deposition processes on the life time of the plant, respectively its components in order to provide a decision tool for plant managers and operators to evaluate commercial impacts on plant operation.

The following primary tasks were decided and distributed to the individuals as follows:

| | |
|---|---|
| Jim Bellows | - Information on deposition rates in steam turbines |
| Barry Hughes | - Experiences on the application of action levels |
| Eric Maughan | - Collection and comparison of literature on chemical indices |
| Andy Rudge | - Information about chem. indices in nuclear industry;<br>- Information about risk assessment programs |
| Andre Zeijseink | - Collection of literature on this topic (starting mid 1990's) |

The result of the primary tasks is due to be sent by 1st December 2007 to Karol Daucik who will then define further action.

**Action KD**

### 10.3 Task Group on "Review of Standard EN 12952:12"

EN 12952:12 and EN 12953:10 are due for review in 2008. Several PCC WG members from Europe have expressed their concern regarding these Standards that have been adopted by the European Community. The content of the Standards with respect to chemistry is not applicable to all steam generating plants. Considering that work may have begun at least a decade ago, it is feasible to present the CEN with additional views with respect to international plant cycle chemistry guidelines currently in use.

Recognizing the above-mentioned concerns, PCC has set up a task group on review of these guidelines to follow up this issue. The Task Group comprises WG members from European countries. Members of the WG from other countries are welcome to participate in the Task Group activities and to offer opinions.

Scope of the task group is to formulate a document detailing related issues into a common statement that can be used by the individual national committees to approach CEN via the official channels. If appropriate, the Task Group chairman may also contact CEN directly.

To be successful, the CEN and National Standards' Committees to be approached in each country should be assured that this Task Group is not confronting them but offering international expertise through the IAPWS PCC WG to the Technical Committee who will review and propose changes to the Standard.

Although the PCC WG agree in principle that this could be task for the IAPWS to provide input for the review of this Standard, it is strictly not an official activity but may in future prove to be a product coming from the PCC WG.

It was agreed that Eric Maughan should chair this task group and that he should co-opt all interested members.

Robert Svoboda will inform the Executive Committee of this initiative.

**Action RS**.

### 10.4 Ad hoc Task Group "Role, Identity and Public Profile of PCC"

Robert Svoboda opened the discussion by asking for views on what PCC should be undertaking in the future. The options ranged from proactive development of guidelines to merely advising IAPWS on industrial research needs.

Eric Maughan raised the concern that a number of the larger industrial entities (e.g. ESKOM and EdF) no longer attend the working group and that the key staff at VGB were now aware of the work.

Barry Dooley listed many of the achievements of PCC and recommended that they be used to justify the refreshment of the group in future. Discussion of future products of PCC followed, including guidance documents on sampling, on monitoring of concentrations of metals and on practical use of the volatility data.

Pat Coleman suggested a draft mission statement for PCC that was then debated and developed by the group. After significant debate an agreed statement (Addendum D) was prepared.

Robert Svoboda will report this to the Executive Committee.

**Action RS**.

## 11. CHANGES IN MEMBERSHIP, ELECTION OF OFFICERS

The group welcomed first time attendance of the following:

| | |
|---|---|
| Frank Udo Leidich | Germany |
| K. Balasubranianian | India |
| K.R. Sanjeev | India |
| Dimitris Sotiropoulos | Greece |
| Pangiotis Tsiampas | Greece |
| Denis Smetanin | Russia |

Robert Svoboda explained the route to full membership of PCC and encouraged the expansion of the group.

Andreas Drexler was nominated for membership. Nomination by Robert Svoboda, seconded by Michael Rziha and Jim Bellows and approved unanimously.

Ken McGrath has written retiring from his membership. His past contributions were noted with thanks and best wishes.

Ken Mathur has now retired and will not continue his membership.

Marc de Wispelaere was nominated for recommendation to the Executive Committee as a deputy chairman of PCC. The nomination was approved unanimously.

It was agreed that contact should be sought with a number of members who have not been able to attend in recent years:

| | |
|---|---|
| W.Allmon | Jim Bellows to contact. |
| A. Banweg | Robert Svoboda to contact. |
| J-P.Jensen | Karol Daucik to contact. |
| L Guinard | Robert Svoboda to contact. |
| V.Kritski | Tamara Petrova to contact. |
| P.Saidl | Robert Svoboda to contact. |
| J.Vosta | Miroslav Štastnŷ to contact. |

## 12. PREPARATION OF ACTION LIST 2007 / 2008, TASK DISTRIBUTION, NEXT YEAR'S AGENDA, ICPWS PROGRAM

Robert Svoboda will circulate the action list to members by e-mail.

## 13. PREPARATION OF PCC WG REPORT FOR EXECUTIVE MEETING

## 14. MISCELLANEOUS AND ADJOURNMENT

There was no other business.

**ADDENDUM A – Attendees**

| | |
|---|---|
| K. Balasubranianian | India |
| Malcolm Ball | U.K. |
| James Bellows | USA |
| Geoff Bignold | U.K. |
| Albert Bursik | Germany |
| Patrick Colman | Ireland |
| Karol Daucik | Denmark |
| Marc de Wispelaere | Belgium |
| Barry Dooley | USA |
| Andreas Drexler | Germany |
| Richard Harries | U.K. |
| J. Barry Hughes | U.K. |
| Frank Udo Leidich | Germany |
| Derek Lister | Canada |
| Kazuo Marugame | Japan |
| Eric Maughan | Germany |
| Masamichi Miyajima | Japan |
| Tamara Petrova | Russia |
| Michael Rziha | Germany |
| Andy Rudge | U.K. |
| K.R. Sanjeev | India |
| Dimitris Sotiropoulos | Greece |
| Denis Smetanin | Russia |
| Miroslav Štastnŷ | Czech Republic |
| Robert Svoboda | Switzerland |
| Pangiotis Tsiampas | Greece |
| Hiroshi Takaku | Japan |
| Svend-Erik Therkildsen | Denmark |
| Shunseke Uchida | Japan |
| Sonia Vidoikovich | Serbia |
| Masaki Yoshida | Japan |
| Andre Zeijseink | Netherlands |

**ADDENDUM B- PCC related Workshops**

All WG workshop (Tuesday morning)

**"Properties of Humid Air and Humid Combustion Gases" (A.H. Harvey)**

- Measurements of the Water Vapor Concentration Enhancement in Compressed Air, Nitrogen, and Argon with FTIR Spectroscopy (M. Wendland)
- First-Principles Calculation of Interaction Second Virial Coefficients Between Water and Common Gases, Including Air (A.H. Harvey)
- Dew Point of Combustion Gas.
  - Report of the Task Group (N. Okita, R. Span, J. Hruby)
- Update for ICRN-14: Thermophysical Properties of Humid Air and Combustion-Gas Mixtures (R. Span)

All WG workshop (Tuesday afternoon)

**"Properties of Seawater" (P. Tremaine)**

- Activities of the Task Group on Seawater, Liaison with IAPSO, Letters Between the IAPWS President and the President of IAPSO
  - Report of the Task Group (R. Feistel, A.H. Harvey, M. Hiegemann, P.Tremaine)
- Investigation of IAPWS-95 Properties Between the Freezing Points of Pure Water and Seawater- - Report of the Task Group (R. Feistel, M: Anisimov, J. Hruby, W. Wagner)
- Composition of Standard Seawater, Reference Salinity Scale (R. Feistel, F.J. Millero, RSMAS, Miami, FL)
- Development of an Extended Formulation for the Thermodynamic Properties of Seawater (R. Feistel)
- Uncertainty of Conductivity Measurements (P. Spitzer, PTB Braunschweig, Germany)
- Density of Seawater (F.J. Millero, R. Feistel)
- Formulation of an ICRN on the Properties of Seawater (R. Feistel)
- Formula Symbols, e. g. for the Salinity of Seawater (R. Feistel)

PCAS / PCC workshop (Monday afternoon)

**Research Presentations on Physical Chemistry for Power Generation (S. Lvov)**

PCC contributions:

- S. Uchida: "Radiation Chemistry for Determining Corrosive Conditions in Primary Coolant of Light Water Cooled Nuclear Reactors"
- E. Maughan. "The fate of a water/steam sample from extraction until point of measurement"
- D. Smetanin "Mathematical modelling in cycle chemistry monitoring systems"
- G. Bignold: "Amine dissociation at temperature"
- P. Tremaine: "The Generation IV Supercritical Water Reactor concept and its research challenges"
- S. Lvov: "New experimental system for electrochemical corrosion studies in high temperature water"

PCC workshop (Tuesday morning and Thursday morning)

**Presentations on Power Cycle Chemistry Research and Experience (R.Svoboda)**

- H. Takaku, M. Miyajima, M. Yoshida: "Essentials of revised guideline for water conditioning for boiler feedwater and boiler water in Japan; JIS-B-8223 published in Oct. of 2006"
- S.Vidojkovic: "Corrosion damages analyses in fossil plant"
- M.Stastny: " Condensation of Flowing Steam with Nucleation in Salt Solution Zone"
- T. Petrova, V. Kashinskiy, P. Nikolaev "Influence filming amines on corrosion rate of carbon steel in water at higher temperatures"
- A.Rudge: "Substantiating an amine for use in our once-through boilers".
- A.Rudge: The second is in a sense a prequel to the one above - how we have used our "Steaming boiler rig to investigate the corrosion risk posed by species that concentrate in the boiler".
- A.Rudge: "Plant trial with amine dimethylamine treatment". (optional)
- S.Uchida: ""Evaluation of Flow Accelerated Corrosion of PWR Secondary Components by Corrosion Analysis Coupled with Flow Dynamics Analysis".

**ADDENDUM C**

## PCC Priority List

**1. Interfacial situation in advanced ultra supercritical plants**

Formation and exfoliation mechanism of scale (oxide films) in steam lines
effects of chemistry (oxygen, ammonia ?)
Corrosion interactions materials / steam, influence / effect of
supercritical parameters, protective layers, radiation
Faster decomposition of chemicals (TOC, ammonia etc)?

*Joint PPC/PCAS ICRN (Palmer, Dooley) to cover some of these topics has been drafted; pending approval*

**2*. Mechanism of Decomposition of Ion-exchange Resin**

Operating conditions, quality control of resin; leak rates are slow, but sulphate is one of the products, organic leachables, oxidation
Additional information has to be researched

*ICRN Daucik -> ICRN # 18 has been issued*

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

ECP (nuclear, fossil application), ORP,
problem: abstract parameters, acceptance by plant operators

*Joint PPC/PCAS ICRN #20 has been issued*

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

Techniques for analysis are known, but problems with implementation
Additional problems with adequate sampling

*Key work on sampling has been done (PCC International Collaboration 2006/7), remaining questions see #6*

**5*. Corrosion mechanisms that are related to the presence of contaminants in steam/water circuits, particularly in boiler-water**

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

*ICRN to be considered for 2008 (Svoboda contact PCC by E-mail)*

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

Detailed definition of the problem

*ICRN: Lister + Daucik; ICRN #19 on sampling of corrosion products has been issued. International collaboration 2006/7 has been performed: Piti S.(Lister, Daucik, Svoboda)*

*Topic to be considered for a paper at ICPWS 2008,(Bellows, et al)*

**7*. The quantification of risk of asset damage**

problems of getting background data, important long-term issue
need: tool for operators, design engineers & commercial persons
PCC: to provide basic background data, e.g. corrosion / deposition rates
*PCC task group has been set up (chair: Karol Daucik), implement results from #10*

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

Outline established in PPC minutes 2004
Guidance document is needed;
*Draft document issued, to be processed by PCC 2007 / 08*

**9*. Improved understanding of condensation mechanisms**

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

*ICRN draft to be processed 2007 / 2008 (Stastny with support by RS, BD, RH)*

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

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

*To be considered in 2008 for ICRN (Bellows)*

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

Long term interest in power industry,

*Treated in TPWS*

**12*. Radiation chemistry of water**

Radiolysis

*2007 PCAS/PCC presentations have been made*

**13. Behaviour of Alumnium in the steam / water cycle**

- volatile carry-over and deposition in the turbine
- depsoition on boiler tubes
- behaviour in conensate purification

*To be considered for ICRN 2007 / 2008 (Rziha, Svoboda)*

**14. Water cooling of copper in electrical machines**

- generator stators
- accelerators

*Consider a paper for the 2008 ICPWS (Svoboda)*

**** includes input from the nuclear group***

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

**In addition, PCC should maintain awareness of the following items**

- Chemistry and corrosion related items to future nuclear generation systems (6-best-design-reactor concepts, fusion reactor)

**ADDENDUM D**

## Mission and Working Process of PCC

30 Aug 2007

## PCC MISSION

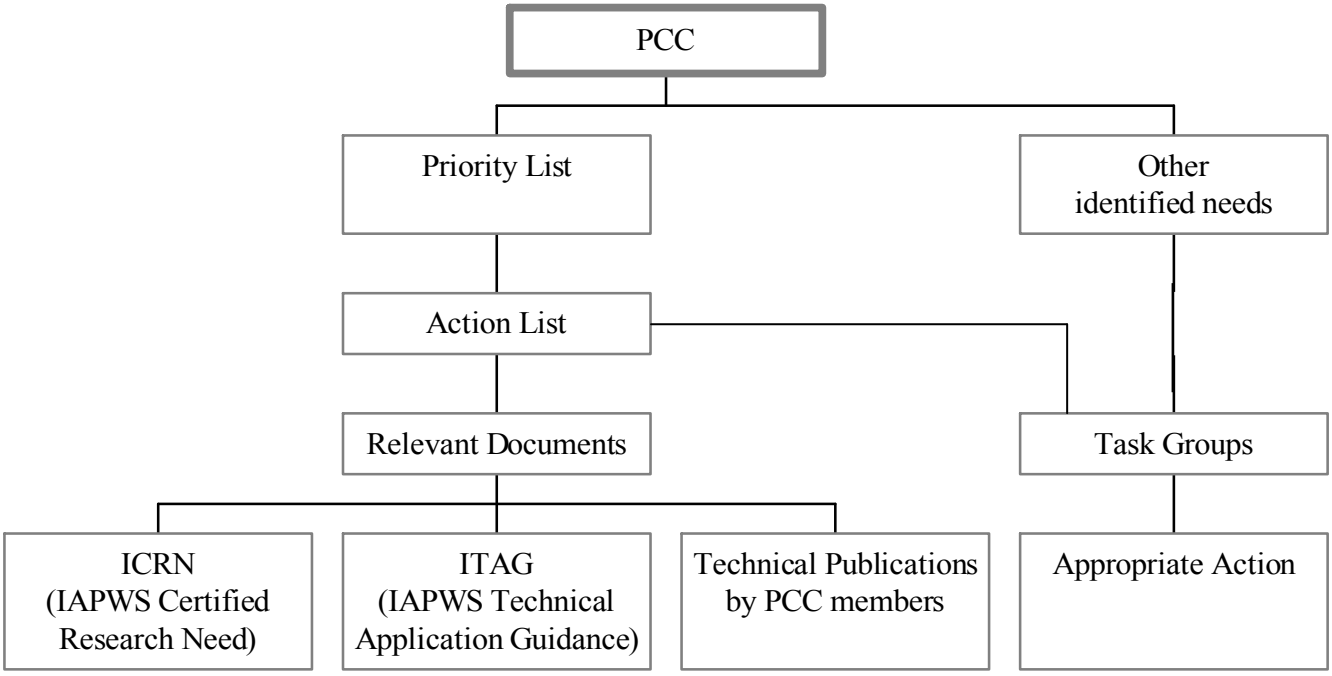
The Power Cycle Chemistry Working Group (PCC) brings together scientists and engineers from academia, research organizations, fossil and nuclear plant operators, equipment manufacturers and other relevant interested parties from around the world with an interest in power cycle chemistry to:

- Share results of scientific and engineering research and experience
- Identify gaps in technical information relating to power cycle chemistry
- Seek resolution of these gaps through international cooperative projects and the release of appropriate documents

for the benefit of industry.

**PCC WORKING PROCESS**

**Workflow**




(* ITAG: proposal for new type of IAPWS document, to be discussed within PCC)

**Working Tools**

- Discussions at annual IAPWS meeting (mainly for steering)
- Individual or group work on PCC assigned tasks throughout the year
- IAPWS International Collaboration

*Attachment 8*

# Young Scientist IAPWS Fellowship Project

# Equilibrium Constants and Speciation of Aqueous Transition Metal Chlorocomplexes over a Wide Range of Temperatures and Pressures

## *IAPWS Sponsors*

**Peter R. Tremaine**
Professor
Department of Chemistry
University of Guelph
Guelph, Ontario, Canada N1G 2W1

**Josef Sedlbauer**
Professor
Department of Chemistry
Technical University of Liberec
461 19 Liberec, Czech Republic

## *Young Scientist*

**Jitka Felcmanova**
PhD Student
Department of Chemistry
Technical University of Liberec
46119 Liberec, Czech Republic

August 22, 2007

## 1. BACKGROUND AND SCOPE

***The Supercritiscal Water Cooled Reactor:*** The "Generation IV" Super-Critical-WaterCooled Reactor ("SCWR") is a concept for a novel, extremely energy-efficient advanced reactor that has been chosen by eleven countries as one of six "best" options to replace the current generation of reactors, after 2025. Design work has not yet begun. This reactor concept would produce supercritical water at temperatures as high as 625°C to generate electricity, hydrogen and district heating. The six competing concepts are listed in:(i) US DOE web-site: http://nuclear.energy.gov/ genIV/documents/gen_iv_roadmap.pdf; (i) Natural Resources Canada Press Release, Feb. 28, 2005. The Canadian conceptual design for a Super-Critical-Water-Cooled reactor is based on a CANDUtype pressure tube reactor one light water loop that carries heat directly from the reactor core to the turbine at super-critical temperatures and pressures (450-625°C, 25 MPa). The other five Gen IV design concepts would produce much higher steam temperatures (800-1000°C, 25 MPa).

The integration of the primary and secondary coolant circuits and higher operating temperatures in the SCWR create a need for thermochemical and kinetic data to model transition metal complexation with chloride, sulfate and organic ligands up to and above the critical point of water.

***Hydrogen Co-generation by Thermal Processes:*** A requirement of all the SCWR concept designs is an ability to co-generate hydrogen from high temperature steam. The proposed project will contribute to research aimed at applying nuclear heat from Canada's Generation IV reactor Super-Critical Water Reactor to the thermochemical production of hydrogen. The nuclear reactor would be separated from the hydrogen production plant, but coupled through an intermediate heat exchanger that supplies heat to the thermochemical cycle. Over 200 processes for thermal hydrogen production have been evaluated by the US Department of Energy and, of these, three "best" processes have been selected for use at at temperatures below 550 °C (Petri *et al.*, 2006). As yet, only one of these, the copper-chloride cycle, has been shown to have promise as a practical process. This part of the "Gen IV" research program aims to optimize heat transfer between the SCWR and the various process loops of the Cu-Cl process. It will identify cycle modifications to maximize heat recovery, minimize heat losses and match the demands of the different thermochemical steps. The Canadian research is led by the University of Ontario Institute of Technology in a collaboration with Atomic Energy of Canada Ltd., Argonne National Laboratory and other Ontario universities.

The copper-chloride cycle, as currently developed by Argonne (Petri *et al.*, 2006), consists of five steps:.

***Step 1:*** $2\ Cu(s) + 2\ HCl(g) \rightarrow CuCl(l) + H_2(g)$, [430 - 470 °C]

***Step 2:*** (a) $4\ CuCl(s) + 4\ Cl^-(aq) \rightarrow 4\ CuCl_2^-(aq)$; [Dissolution + complexation, t < 100 °C]

(b) $4\ CuCl_2^-(aq) \leftrightarrow 2\ Cu(s) + 2\ CuCl_2(aq) + 4Cl^-(aq)$, [Electrolysis; t < 100 °C]

***Step 3:*** $4\ CuCl_2(aq) \rightarrow 2\ CuCl_2(s)$; [Evaporation, t > 100 °C]

***Step 4:*** $2\ CuCl_2(s) + H_2O(g) \rightarrow Cu_2OCl_2(s) + 2\ HCl(g)$, [300-375 °C]

***Step 5:*** $Cu_2OCl_2(s) \rightarrow 2\ CuCl(l) + 1/2\ O_2(g)$ [450 - 530 °C]

The existing Argonne process involves temperatures and pressures of less than 70°C and 2 MPa for the aqueous liquid phase, with HCl concentrations below ~ 6 m, for which the literature is quite complete. The Canadian research program may investigate the use of HCl concentrations up to 13 mol/kg, temperatures up to 130 °C and pressures of 30 MPa, for which copper(I) and copper(II) chloride solubility and complexation constant data are required. For example, a key need for step 3 is for better solubility data for the $CuCl/CuCl_2/HCl/H_2O$ system, up to the maximum saturation temperature, and an ability to model the formation of $Cu_2OCl_2(s)$ in step 4 at temperatures above 300°C, both at steam pressures as high as 0.5 MPa

## 2. THERMOCHEMICAL DATA FOR COPPER COMPLEXATION.

***Existing Data:*** The steps of the Cu-Cl cycle have been individually demonstrated, but more information is needed on their kinetics and yields as a function of temperature, pressure and reactor feed compositions. The thermochemical properties of the aqueous copper (I) chloride system have been studied at elevated temperatures by several authors, because of its importance to the geochemistry of ore-body formation (Liu *et al.*, 2002; Var'yash, 1992; Xiao *et al.*, 1998). The recent UV-visible study by Brigger *et al.* (2001) provides the only reliable data for the stepwise formation of copper (II) species above room temperature and these extend only to 90 °C. The themodynamic properties of $Cu_2OCl_2(s)$ are also not well known, although recent measurements at Brigham Young University have provided accurate data up to 25 °C (M. Lewis, Pers. Commun.).

***"Equations of State" for Standard Partial Molar Properties:*** Two major methods have been developed to model and extrapolate standard partial molar properties of ions to hydrothermal conditions. These are reviewed by Majer *et al.* (2004) in the recent IAPWS "Atlas" publication. The first approach, which is now widely used, was developed by Helgeson and his co-workers who developed an equation of state based on the Born equation for ionic hydration. (Shock *et al.*, 1992). Briefly, the Helgeson-Kirkham-Flowers (HKF) model consists of expressions for standard partial heat capacity and volume functions, and assumes that the standard molar Gibbs energy and enthalpy of formation of each species at 298.15 K and 0.1 MPa are known properties. Sverjensky *et al.* (1997) have applied this to develop predictive equations for the properties of chloro-complexes, based on the limited high temperature data available. The second approach, which was developed by Sedlbauer, O'Connell and Wood (2000) is based on solution fluctuation theory. The "SOCW"model has had much success in modelling and predicting high temperature data for ions and neutral species, but has not as of yet been applied to transition metal complexes.

## 3. PROPOSED RESEARCH AND JUSTIFICATION FOR IAPWS SUPPORT

***Project Objective:*** The purpose of the collaborative project with IAPWS is to measure and model stepwise formation constants for the copper(II) chloride complexes at temperatures from 75 to 250°C. The low end of this range will provide thermochemical data needed for process design and optimization of the reactor and heat exchanger. The higher temperature data are of fundamental value for steam generator design, both for the SCWR and more conventional power stations.

***Work Plan:*** This proposal seeks funding from IAPWS to support a visiting young scientist who will supplement the existing scarce experimental results available for these aqueous complexes at high temperature by measuring the stepwise formation constants $Cu^{2+}$(aq) with $Cl^{-}$(aq) up to 250°C using UV-VIS spectroscopy. The measurements will be made in solutions of LiCl(aq), to be consistent with the high quality measurements by Liu *et al.* (2002) on copper (I) complexation. A small excess of HCl(aq) will be used to prevent the precipitation of hydroxides. The experimenta work will be carried out in Guelph under the co-supervision of Dr. Tremaine and Dr. Liliana Trevani. The project will make use of the high-temperature UV-visible flow system developed by Trevani *et al.* (2001) which uses titanium or platinum flow cells to measure spectra under oxidizing or reducing conditions, respectively, up to 350 °C and 30 MPa. The upper temperature limit in this work will likely be determined by the precipitation of CuCl2 (s). Because spectra of the complexes overlap one another the interpretation of the UV-visible results require sophisticated statistical techniques (Trevani *et al.*, 2001; Brugger *et al.*, 2001). This part of the work will be done initially at Guelph and, carried on in Liberec if necessary. Subsequently the two teams from the University of Guelph and from the Technical University of Liberec will cooperate on development of models to describe the equilibrium constants and partial molar properties the aqueous complexes of copper(I) and copper(II) using both the Sedlbauer-O'Connell-Wood (SOCW) and the Helgeson-Kirkham-Flowers "equations of state".

Considering the wide range of concentrations, a suitable treatment for the activity coefficients must be included in the model. It might be interesting to test the Mean Spherical Approximation ("MSA") model for this purpose, as the Sedlbauer group has a good deal of experience with its extrapolation abilities, and has found it to require many fewer parameters than Pitzer's virial expansion for ions at high temperatures (Sedlebauer and Wood, 2004). The MSA treatment is computationally more difficult and requires a knowledge of solution densities. The Tremaine group has a high temperature densimeter suitable for such measurements if needed.

***Justification for IAPWS Funding:*** The IAPWS funding will make it possible for a young scientist to spend at the University of Guelph for ten months in a single stay starting in May or September of 2008. Two PhD students have been identified. Ms. Jitka Felcmanova is a PhD student in Dr. Sedlbauer's group and is in the early stages of her program. Ms. Jana Ehlerova would use the project as the final stage in her PhD work. She has experience with the equipment from her previous IAPWS fellowship, and is an expert in statistical methods. Timing of this collaboration is important. In the event that Jitka's participation is not possible or delayed, Jana Ehlerova would come in her place. The funding will allow one of these students to collaborate with Prof. Tremaine and Dr. Trevani on the experimental determinations of the stepwise complexation constants of copper(II) with chloride using UV-visible spectroscopy, and will contribute to the Gen IV

International Forum by providing basic research, student training and collaborative links between the Czech Republic and Canada.

## 4. BUDGET (in $US)

Subsistence for 10 months: IAPWS Young Scientist Grant.....$14000
Travel (round trip): to be paid by TU Liberec.....$ 1500
Chemicals, supplies, equipment: to be paid by U. Guelph .....$ 4500
Research Assosiate support, to be paid by U. Guelph .....$ 10000

**Total Cost.....$30,000**
**Request from IAPWS: .....$14,000**

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## 6. Curriculum Vitae

**Jitka Felcmanova**

**Born**

1982

**Education**

2001-2006 Technical University of Liberec, Faculty of Textile Industry, 2006 MSc.

2006- Technical University of Liberec, Faculty of Mechatronics and Interdisciplinary Engineering Studies, programme Science Engineering, Ph.D. study

**Employment**

2006- TUL, Department of New Technologies and Applied Informatics

**Research interests**

-thermodynamic properties of aqueous solutions at high temperature conditions
-experimental calorimetry

# Press Release for IAPWS Annual Meeting at Lucerne, Switzerland, August 26-31, 2007

Seventy-one scientists and engineers from fifteen countries attended the annual meeting of the International Association for the Properties of Water and Steam (IAPWS), August 26-31, 2007 in Lucerne, Switzerland. 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.

This year IAPWS welcomed a Swiss national committee as a new member.

The IAPWS delegates were joined by an additional five people from Switzerland for a symposium on power cycle chemistry. The chemistry of nuclear power plants and new research in materials for advanced power plants were features of this symposium. Nuclear power plant chemistry and flow-assisted corrosion were prominent topics in the discussions of the Power Cycle Chemistry Working Group.

Dr. Karsten Meier presenting the Helmholtz Award Lecture on speed of sound measurements at high temperatures and pressures.

A highlight of the 2007 symposium was the Helmholtz Award Lecture (see picture). The Helmholtz Award is given annually to a young scientist for work of interest to IAPWS. It includes a trip to the IAPWS meeting to present a paper.

IAPWS adopted a modification of the IAPWS Industrial Formulation 1997 that extended the high temperature region to higher pressures and a new "Release on the Ionization Constants of $H_2O$." IAPWS also approved "Revised Releases on the Viscosity and Thermal Conductivity of Heavy Water." New documents should appear on the IAPWS website shortly. Work continues on new documents which will describe the viscosity of water and the melting and sublimation curves of ice.

IAWPS produces Certified Research Needs (ICRN) as guidance for funding agencies and as an aid to people doing research in defining important research. Several new ICRN's have been approved in the last year and appear on the IAPWS website. The ICRN's approved this year concerned mechanism of decomposition of ion-exchange resin; development and application of ambient and high temperature sensors; and improved analysis of low concentration of metals.

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). Details of the symposium may be found at the IAPWS website under IAPWS News.

IAPWS is preparing a Databook, with six chapters: Phase equilibria, pVTX, 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 2007.

An international collaboration project on "Equilibrium Constants and Speciation of Aqueous Transition Metal Complexes over a Wide Range of Temperatures and Pressures" will be carried out by Jitka Felcmanova, a Czech Republic student, from the Technical University of Liberec at the University of Guelph (Canada). A task group was set up to support European members in a European Standards matter. This task group illustrates the organization's support of its members with expertise in their national concerns.

The next IAPWS meeting will be at the 15th International Conference on Properties of Water and Steam, to be held in Berlin, September 8-11, 2008. Details of the meeting will be available through links from the IAPWS

website at www.iapws.org, and at the Conference website www.icpws15.de. Minutes of the 2007 meeting will appear on the IAPWS 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).

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, Structural Integrity Associates, Inc., 2904 South Sheridan Way, Suite 303, Oakville, Ontario L6J 7L7, Canada, email: bdooley@structint.com. People do not need to be citizens or residents of member countries to participate.

**IAPWS Annual Meeting, Lucerne 2007**

**Educational Task Group:**
H.-J. Kretzschmar (chair), M. Assael, H. Corti, P. Safarik, S. Lvov, P. Tremaine

# Educational Issues

1. 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.
   4 PhD students attend the IAPWS meeting in Lucerne.
   In particular, the German and the Czech National Committees should make an effort to encourage students to participate at the 15th ICPWS in Berlin.

2. The committee recommends that the annual-meeting and conference fees for students are reduced drastically (to the amount for food).
   The 15th ICPWS conference fee for students was reduced from 500 EUR to 200 EUR.
   The Conference Organisation Committee should identify less expensive accommodations for students.

3. Either the Conference Organizers and/or IAPWS should create a number of awards for students who are presenting papers to attend the conference. We suggest that the amount be enough to offset a significant portion of travel costs (500EUR) per award, and that there be at least 10 awards.

4. The IAPWS Website is to be used for educational purpose.
   The item "Education" was added on the left menu bar in the IAPWS website.
   More than 450 Downloads of the Steam Tables on Pocket Calculators were registered in period from August 2006 to August 2007.
   Further software for students and appropriate papers from the IAPWS meetings should be placed in the related page.

5. It has been suggested that, for the future, IAPWS Summer Schools (2 or 3 days) could be offered in the week before the IAPWS meeting.
   In the opinion of the committee it is not feasible to do so at this time.

*H.-J. Kretzschmar, S. Lvov, P. Safarik, P. Tremaine*

**BIAPWS Annual Report to IAPWS for 2006/07.**

**Summary.**

BIAPWS has increased it industrial sponsorship membership to 16 and is a power industry representative body for boiler steam and water chemistry in the British Standards organisation.
BIAPWS continues its role in technical education and outreach within the power generation industry. This past year has seen each BIAPWS committee meeting preceded by a technical seminar which is open to a wider audience from our industrial sponsors.
The BIAPWS Award scheme, modified to offer an undergraduate bursary for summer vacation work experience, was very successful in 2006 and has been repeated in 2007.

**Membership.**
BIAPWS membership of industrial sponsors has increased by three in the past year to now stand at 16 industrial members. This includes 11 power generation companies, 2 power plant manufacturers, 2 chemical instrument manufacturers and one technical support company. BIAPWS membership now includes almost all of the major electricity generating companies in the UK and Ireland (see footer for list).

BIAPWS links with the academic field 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

**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. Research is ongoing in the UK power industry but little is reported in the open scientific, engineering or technical press. The level of academic research into topics of interest to BIAPWS / IAPWS, appears to remain low in the UK. A list of recent publications that have been brought to the notice of BIAPWS is appended.

**British Standards Institute.**
BIAPWS acts as the UK generating industry representative body on the British Standards committee that is concerned with the design and operation of steam raising boilers, with particular reference to the steam and water chemistry requirements. BIAPWS has initiated discussion of the latest European standard in that area EN 12952 part 12 (water tube boilers) and EN 12953 part 10 (shell boilers) with the aim of instituting a major review of these standards. To this end, the European members of IAPWS will discuss EN 12952:12 in Luzern with the aim of producing a common position that will ensure effective revision of these standards.

**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.

**BIAPWS Symposia.** The most recent BIAPWS Symposia was at the 2006 IAPWS International meeting, Witney. The next symposium is planned for spring 2008, when they will revert to an annual frequency at a fixed calendar period.

**BIAPWS Technical Seminars.** To enhance the value of BIAPWS membership regular technical seminars have been organised for the morning preceding each BIAPWS committee meeting. These have been opened to a wider audience from our industrial sponsors where active participation and discussion is encouraged, particularly by newer entrants to the power industry.

**BIAPWS Award.** In 2006 the BIAPWS Award was redefined as a co-sponsored undergraduate student bursary to enable a student to gain experience for at least 10 weeks working in an industry with relevance to the interests of IAPWS and BIAPWS. The co-sponsorship has been with one of BIAPWS industrial sponsors. In 2006 the Award went to a chemistry undergraduate from Nottingham University, co-sponsored by E.ON (UK). In 2007 the Award has been co-sponsored by Thames Power Services (Barking Power) with a chemical engineering undergraduate from Imperial College (London). The selected candidates have both been of high calibre and have benefited from their industrial experience.

**BIAPWS Future.**
BIAPWS remains committed to its role as a power industry representative body as well as developing further its role as the central point for co-ordinating and disseminating information on the properties of water and steam and their application to industry.

Richard Harries, Chairman BIAPWS
August 2007.

Published Papers and Associated Work.

J Cooper and J Sengers have examined the effect on the values of properties calculated from the IAPS Release on the Viscosity and Thermal Conductivity of heavy water Substance 1982 using ITS-90 temperatures. A draft revised release has been produced for presentation to the IAPWS 2007 meeting.

The behaviour of ammonia, amines, carbon dioxide and organic anions during condensation in an air cooled condenser. Bignold GJ., 2006. *Power Plant Chemistry. 8(2), 68-73.*

Supercritical Carbon Dioxide in Water Emulsion Templated Synthesis of Porous Calcium Alginate Hydrogels. Darr J. A.; Partap, S. and Rehman, I.U., *Advanced Materials. 18, 2006, 501 - 504.*

Instant Nano-Hydroxyapatite; A Continuous and Rapid Hydrothermal Synthesis. Boldrin P.; Chaudhry, A.A.; Khalid, F.; Darr J. A. and Rehman, I.U., *J. Chem. Soc., Chem. Commun. 2006, 2286 - 2288*

Recent Developments in Processing and Surface Modification of Hydroxyapatite. Norton, J.; Malik, K.R.; Rehman, I.U. and Darr, J. A., *J. Adv. Appl. Ceram., 105, 2006, 113-139*

# The Czech National Committee

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

## REPORT on IAPWS related activities – August 2006 / August 2007

Submitted to the EC Meeting of IAPWS, Luzern – August 2007.

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Head: Dr. Jan Hruby, E-mail: hruby@it.cas.cz

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

**Institute of Thermomechanics** (IT) AS CR, v.v.i., 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, Energy Institute, Department of Power Engineering and Department of Thermodynamics and Environmental Engineering, Technicka 2, CZ-616 69 Brno

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

**University of West Bohemia** (UWB), Faculty of Mechanical Engineering, Department of Power System Engineering, Univerzitni 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**, Jana Sigmunda 79, CZ-783 50 Lutin

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 surface tension of supercooled water. Refs. [1 to 4]. His research team investigated thermo-dynamic properties of water at pressure 0.1 MPa and dew point of combustion products (namely $H_2O$-$H_2SO_4$).
- Prof. Mares (UWB) with his collaborators measured surface tension of super-cooled water and tested formulation IAPWS-IF97 in this region at ambient pressure. Ref. [5]. As the chairman of the Task Group he tested the new formulation for viscosity of water. Refs. [6 to 9].
- Prof. Marsik (IT) coordinated research in the metastable states. nucleation and lectured on thermodynamic modeling of fuel cells. Refs. [10 to 19].

- Prof. Sedlbauer (TUL) and his team collaborated with Prof. Majer (France) and investigated thermodynamic properties of selected aqueous solutes. Refs [20 to 26].
- Research activities at the (CTU) continued in further improvement of the knowledge on following subjects: Determination of the particles in the super-heated steam using a new sampling technique. The probe is designed for sampling superheated steam in the range of 170 to 400°C and 0.13 to 4 MPa. Ref. [1]. Thermodynamic analysis of hydrogen direct-fired Rankine steam cycle and hybrid $H_2/O_2$ Solid Oxide Fuel Cell – Steam Turbine. Refs. [27 to 30].
- The activities of the SIGMA Research and Development Institute included solution of erosion effects of cavitation bubbles on the blades of water pumps and changes of the hydraulic machinery performance due to a cavitation. Refs. [10, 31]
- Dr. Jiricek (ICT-IE) with collaborators investigated corrosion processes and chemical effects in water and steam systems of power plants. Refs. [32 to 39].
- ICT-IE organized the 6$^{th}$ International Power Cycle Chemistry Conference (CHEO 6), held from 11$^{th}$ to 13$^{th}$ September 2006. Selected contributions are given in [40 to 55].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles and conference contribution are under Refs. [56 to 64].
- Prof. Stastny (SKODA POWER) with co-workers studied effects of deposits on the blades of HP steam turbine in fossil power plant by chemical analysis, measured degradation of steam turbine blade surfaces by deposits of chemicals and compared numerical models of the water steam flow in nozzles with NaCl binary nucleation and condensation. Refs. [32, 42, 65 to 67].
- Ing. Kodl (SKODA POWER) applied his own procedure for the evaluation of region 5 of IAPWS-IF97 enlarged up to 50MP; results were sent to Mr. Miyagawa the chairman of evaluation task group. He also tested the programming of the new formulation of viscosity.
- 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. New research activities are turned to the role of the coolant chemistry and decontamination on formation of corrosion product deposits on the fuel cladding and on the out-of-core surfaces. Refs. [68 to 71]

**Young Scientists IAPWS Fellowships**

- O. Mican finished the 2006 Young Scientist IAPWS (CZ-US) Project "*Irreversible Thermodynamics of Fuel Cells Membrane Transport*" under supervising Prof. F. Marsik, and Prof. S. Lvov. The project was 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 is in Appendix 1. The publications of the fellowship holder are in Refs.[13,18].

- J. Ehlerova performed her Young Scientist IAPWS (CZ-Canada) Project "*Predictive Scheme for Standard Thermodynamic Properties of Aqueous Substituted Benzenes over a Wide Range of Temperatures and Pressures*" under supervising of Prof. J. Sedlbauer, and Prof. P. R. Tremaine. The project had 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.

  Her Final Report of the Project will be finished by the end of the year 2007.
  Preliminary results she will present at the 2007 IAPWS Meeting. Ref. [26].

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# German National Committee to IAPWS

**Research Activities on the Thermodynamic Properties of Water and Steam**

**Report "Research in Progress 2007"**

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

1. „Release of an Equation of State of Ice Ih“ was issued by IAPWS in Witney 2006

2. IAPWS Certified Research Need „Thermophysical Properties of Seawater”, draft presented in Witney 2006, further edited for issue by IAPWS in Lucerne, 2007

3. Publication of R. Feistel, G.M. Marion: “A Gibbs-Pitzer Function for High-Salinity Seawater Thermodynamics”. Progress in Oceanography, 74 (2007) 515–539

4. Publication of R. Feistel, W. Wagner: “Sublimation pressure and sublimation enthalpy of H2O ice Ih between 0 and 273.16 K”. Geochimica et Cosmochimica Acta 71 (2007) 36–45

5. Publication of R. Feistel, F.J. Millero, T. J. McDougall: “Eine neue Zustandsgleichung für Meerwasser“. DGM-Mitteilungen, 2/2006, 19-21

6. Publication of F.J.Millero, R. Feistel, D.G. Wright, T.J. McDougall: “The Composition of Standard Seawater and the Definition of the Reference-Composition Salinity Scale”. Deep-Sea Research, submitted. To be presented in Lucerne 2007.

7. Certified Research and Development Need “Refractive Index of Seawater”. SCOR/IAPSO Working Group 127, Reggio di Calabria, May 2007

8. Publication of R. Feistel “A Gibbs Function for Seawater Thermodynamics for -2 °C to 80 °C and Salinity up to 120 g $kg^{-1}$”. Draft presented at the WG127 meeting, Reggio di Calabria, May 2007. In preparation for submission.

9. Chairing the TPWS Taskgroups “Seawater”, “Metastable Liquid”, “Ideal Gas” and “Correlation Equations”

10. W. Wagner, R. Feistel: Draft “Revised Release on the Pressure along the Melting and Sublimation Curves of Ordinary Water Substance” for presentation in Lucerne 2007

11. R. Feistel: Draft “Release on the IAPWS Formulation for the Thermodynamic Properties of Seawater” for presentation in Lucerne 2007

12. Liaison with SCOR/IAPSO WG127 on Thermodynamics and Equation of State of seawater

## 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 $v(p,T)$ for region 3 of IAPWS-IF97
   - The comprehensive article on the backward equations for the "Journal of Engineering for Gas Turbines and Power" was prepared.

2. Thermodynamic derivatives from IAPWS Formulations
   - The evaluation of the "Advisory Note No. 3 Thermodynamic Derivatives from IAPWS Formulations" was supported.
3. Development of fast property algorithms based on spline interpolation for non-stationary calculations of heat cycles and steam turbines
   - Different spline-interpolation methods and their implementation in Assembler programs were investigated.
4. Investigations on thermodynamic properties of humid air - part of the project "Advanced Adiabatic Compressed Air Energy Storage" (AA-CAES) of the European Union
   - The PTB Report "Determination of Thermodynamic and Transport Properties of Humid Air for Power-Cycle Calculations" was prepared.
5. Property libraries for water and steam, humid gases, and aqueous mixtures
   - The Add-On FluidMAT for MATLAB® was developed.
6. The homepage www.iapws.de of the German National Committee of IAPWS was hosted.

**Recent Publications**


- Kretzschmar, H.-J., Cooper, J. R., Dittmann, A., Friend, D. G., Gallagher, J. S., Harvey, A. H., Knobloch, K., Mareš, R., Miyagawa, K., Okita, N., Stöcker, I., Wagner, W., and Weber, I., Supplementary Backward Equations $T(p,h)$, $v(p,h)$, and $T(p,s)$, $v(p,s)$ for the Critical and Supercritical Regions (Region 3) of the Industrial Formulation IAPWS-IF97 for Water and Steam, *Journal of Engineering for Gas Turbines and Power*, Vol. 129 (2007) No. 1, p. 294-303
- Kretzschmar, H.-J., Cooper, J. R., Dittmann, A., Friend, D. G., Gallagher, J. S., Harvey, A. H., Knobloch, K., Mareš, R., Miyagawa, K., Okita, N., Span, R., Stöcker, I., Wagner, W., and Weber, I., Supplementary Backward Equations $p(h,s)$ for the Critical and Supercritical Regions (Region 3), Equations for the Region Boundaries, and an Equation for the Two-Phase Region of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam, *Journal of Engineering for Gas Turbines and Power*, Vol. 129 (2007) No. 7
- Kretzschmar, H.-J.; Stöcker, I.; Jähne, I.; Seibt, D.; Kunick, M.: Berechnung der thermodynamischen Zustandsgrößen und Transporteigenschaften von feuchten Verbrennungsgasen, feuchter Luft und Absorptionskältemittelgemischen in fortschrittlichen Energieumwandlungsprozessen (Calculation of the thermodynamic properties of humid air, humid combustion gases and absorption refrigerants in advanced power cycles). VDI-Berichte 1924 (2006) p. 417-423
- Knobloch, K.: Gleichungen für thermodynamische Umkehrfunktionen von Wasser und Wasserdampf im kritischen und überkritischen Zustandsgebiet für energietechnische Prozessberechnungen (Equations for thermodynamic backward functions of water and steam in the critical and supercritical regions for modelling power cycles. Fortschritt-Berichte VDI, Reihe 6, No. 542 (2006)


## 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
   - A draft revised release on IAPWS-IF97 was prepared.
2. Equations for the melting pressure and the sublimation pressure of ice Ih
   - Development of new equations for the melting pressure and the sublimation pressure of ice Ih. The equations were not developed based on experimental data, but the input *T*-*p* values were

calculated from IAPWS-95 and the equation of state for ice Ih by the application of the phase equilibrium condition.

– A draft revised release on the pressure along the melting and sublimation curves of ordinary water substance was prepared.

Current Status of Research Activities in Japan

# Submitted to the Executive Committee Meeting, IAPWS, Luzern, Switzerland, August 2007

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 countinuing 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.

Dr. S. IKAWA, emeritus Prof. of Hokkaido University, Sapporo, conducted study on volumetric behavior of water-methanol mixtures in the vicinity of the critical region, in collaboration with Prof. P. Tremaine and his coworkers of University of Guelph, Canada. Densities of water-methanol mixtures at 573 and 588 K and at pressures in the 100-200 bar range have been measured with a vibrating-tube densimeter. A large negative-to-positive sigmoidal change of the excess molar volumes as a function of methanol mole fraction was interpreted on the basis of an estimated locus of the mixtures. The behavior of the water-methanol mixtures at the lower methanol mole fractions was discussed in terms of the local solute-solvent structure by estimating radial distribution functions and self-diffusion coefficients from molecular dynamics calculations. [Fluid Phase Equilib., **245**, 125 (2006)].
[contact: Dr. 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 has finished the 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)] and then made his effort to promote development of evaluation method on flow-induced vibration and corrosion of components in two-phase flow by combined analyses of flow dynamics and corrosion [Innovative and Viable Nuclear Energy Technology Development Project of the Ministry of Economy, Trade and Industry]. 1) The six year research project on hydrogen peroxide was rewarded as the 2006 Award for Distinguished Technology of the Atomic Energy Society of

Japan, "Establishment of Experimental Technology for the High Temperature High Pressure Hydrogen Peroxide Water Loop - Concentration Control of Hydrogen Peroxide in the High Temperature Water Loop and *In-situ* Measurements of Its Concentration and Effects on Corrosion Behavior". 2) A model based on combined analyses of flow dynamics and corrosion has been developed to predict corrosive conditions in PWR secondary cooling system and pipe wall thinning due to flow accelerated corrosion. 3) Standard procedures were proposed to determine corrosive conditions in BWR primary cooling system based on combined analyses of water radiolysis and mixed potential models. [Latest publication: (1) T. Miyazawa, T, Terachi, S. Uchida, et al., "Effects of Hydrogen Peroxide on Corrosion of Stainless Steel (V) - Characterization of Oxide Film with Multilateral Surface Analyses", *J. Nucl. Sci. Technol*., 43, 884 (2006), (2) S. Uchida, T. Satoh, N. Kakinuma, et al., "An electrochemical sensor complex for in-situ measurements of oxide film electric resistance in high temperature water", *ECS Transactions,* Volume 2, Issue 25, 37, 209th ECS Meeting, May 7-May 12, 2006, Denver, Colorado, Electrochemical Society (2006)., (3) S. Uchida. K. Otoha, and K. Ishigure, "Water Chemistry – One of the Key Technologies for Safe and Reliable Nuclear Power Plant Operation", *Proc. the 15th Pacific Basin Nuclear Conference* (in CD), (2006), (4) S. Uchida, T. Satoh, T. Tsukada, et al., " Properties of Oxide Films on Stainless Steel Exposed to Hydrogen Peroxide and Oxygen in High Temperature Water", *Proc. Int. Conf. Water Chemistry of Nuclear reactor Systems 2006*, Oct. 23-26, 2006, Jeju, Korea, Korean Atomic Energy Research Institute (2006). (in CD)., (5) T. Satoh, S. Uchida, T. Tsukada, et al., "Effects of Hydrogen Peroxide and Oxygen on Polarization Curves of Stainless Steel in High Temperature Pure Water", *Proc. Int. Conf. Water Chemistry of Nuclear reactor Systems 2006*, Oct. 23-26, 2006, Jeju, Korea, Korean Atomic Energy Research Institute (2006). (in CD)., (6) E. Kadoi, H. Takiguchi, K. Otoha, et al., "Mitigation of Flow Accelerated Corrosion in Pure Neutral Water - Japan-Canada Collaboration Studies on FAC", Proc. Int. Conf. Water Chemistry of Nuclear reactor Systems 2006, Oct. 23-26, 2006, Jeju, Korea, Korean Atomic Energy Research Institute (2006) (in CD), (7) S. Uchida, M. Naitoh, Y. Uehara, et al., "Evaluation Method of Corrosive Conditions in Cooling Systems of Nuclear Power Plants by Combined Analyses of Flow Dynamics and Corrosion", Power Plant Chemistry, 9, 3, 143-156 (2007), (8) S. Uchida, Y. Morishima, T. Hirose, et al., "Effects of Hydrogen Peroxide on Corrosion of Stainless Steel (VI) - Effects of Hydrogen Peroxide and Oxygen on Anodic Polarization Properties", *J. Nucl. Sci. Technol.*, 44, 758 (2007). (9) T. Satoh, Y. Shao, W. G. Cook,, et al., "Flow-Assisted Corrosion of Carbon Steel under PWR Secondary Water Conditions", *Corrosion*, in press.
[contact: Dr. S. Uchida; E-mail: uchida.shunsuke@jaea.go.jp].

The research center of Suerpcritical Fluid Technology, Graduate School of Engineering, Tohoku University has been performed the density measurement of aqueous solutions at supercritical state of water. In these years, the densities of water-methanol and water-ethanol mixtures were measured with the laser-doppler type vibrating densimeter at 400 C in the pressure range of 25-40 MPa. The composition dependences of the excess molar volumes for both water-alcohol mixtures were estimated from the experimental values and fitted with the Redlich-Kister equation. The excess molar volumes of all mixtures were positive in the whole composition range at 400 C. The composition dependences of the excess molar

volumes showed maxima around 30-40 mol% of alcohol in water and the pressure dependences around 30 MPa at 400 C. [The Joint Meeting of ISHR-8 and ICSTR-7 (August 2006); T. Ono, T. Hoshina, T. Aida, M. Watanabe, Y. Sato, and H. Inomata□AIChE 2006 Annual Meeting (November 2006)□T. Hoshina, T. Ono, T. Aida, T. Matsushita, M. Watanabe, Y. Sato, R. L. Smith, Jr., and H. Inomata]

At the Institute of Multidisciplinary Research for Advanced Materials at Tohoku University, Prof. M. KAKIHANA and coworkers have discovered a series of new water-soluble, stable and non-toxic titanium complexes, which were proved to be very promising reagents from an environmental point of view for the preparation of titanium-containing functional materials using water-based synthesis methods. The hydrothermal treatment of these newly designed water soluble titanium complexes is one of the key synthesis techniques which allows the perfectly selective synthesis of nanocrystalline $TiO_2$ polymorphs including single phase brookite, anatase, rutile and $TiO_2$ (B). It was established that both brookite and $TiO_2$ (B) exhibited higher photocatalytic activities in NO decomposition reaction than commercially available anatase/rutile based TiO2 photocatalysts.[K. Tomita, V. Petrykin, M. Kobayashi, M. Shiro, M. Yoshimura and M. Kakihana, Angew. Chem. Int. Ed. 45 (2006) 2378-2381.]. Prof. T. SATO and co-workers studied on the panoscopic assembling of ceramic materials applicable for environmental clean-up, energy saving, preventing the healthy damage, etc. by solvothermal reactions. Visible light responsive photocatalysts such as nitrogen-doped titania and strontium titanate nanoparticles, ceria based new inorganic UV-shielding materials showing low photocatalytic activity, high performance de$NO_x$ catalyst of $\gamma$-$Al_2O_3$/Ag nanocomposite, high performance rare earth oxide nanoparticle phosphors, zinc oxide film possessing superhydrophilicity and superhydrophobicity, etc. were synthesized by the solvothermal reactions using various alcoholic aqueous solutions as reaction media [J. Photochem. Photobiol. A: Chem., 179, 105 (2006); J. Mater. Sci., 41, 1433 (2006); Chinese J. Process Eng., 6, 472 (2006); J. Europ. Ceram. Soc., 26, 2735 (2006); J. Photochem. Photobiol. A: Chem., 187, 72 (2007), J. Oleo. Sci., 55, 249 (2006); Appl. Surface Sci., 252, 5063 (2006). Adv. Sci. Technol., 45, 668 (2006); Adv. Sci. Technol., 45, 673 (2006); Adv. Sci. Technol., 45, 679 (2006); Adv. Sci. Technol., 45, 685 (2006); Chinese J. Process Eng., 6, 633 (2006); J. Photochem. Photobiol. A: Chem., 187, 72 (2007); J. Luminescence, 126, 427 (2007); Key Engineering Materials, 352, 293 (2007)]. Prof. A. MURAMATSU and co-workers have been studied the synthesis of monodispersed particles and their formation mechanism in liquid and/or solution phase. The Gel-sol method is originated and novel procedure to prepare the particles precisely controlled in size, shape, structure and composition with rather higher productivity, based on the well controlled nucleation and growth via selective chemical reaction such as a forced hydrolysis, selective reduction, and selective sulfurization. Now, it has been applied to the formation of ITO particles as a transparent conductive film component, $BaTiO_3$ as dielectrics and/or piezoelectric material, ferric oxides as a magnetic material and so on. Also, they have been making their maximum efforts on the hybridization of monodispersed particles with organic material such as liquid crystals, in order to obtain multi-functional materials. In addition to these original methods, the Liquid-Phase Selective Deposition has also been developed as a novel preparation method of heterogeneous catalysts for industrial use in dilute solution of metal precursory complexes. [Chemistry Letters, 35(6), 570-571(2006), Journal of Surface Science and Nanotechnology,

4(1), 352-358 (2006), The Journal of Physical Chemistry B,110 (12), 6224-6228 (2006), Catalysis, 48(4), 271-276 (2006)]. Prof. T. ADSCHIRI and co-workers studied on nano-bio reactions and organic–ingorganic reactions at hydrothermal conditions. Recently Prof. Adschiri proposed a new method to synthesize organic-inorganic hybrid nanoparticles at supercritical hydrothermal conditions. By introducing organic species (aminoacids, carboxylic acids, amines, alcohols, aldehydes etc.) during supercritical hydrothermal synthesis, nanoparticles whose surface was modified with organic molecules were synthesized. This is due to the homogeneous phase formation for organic substance and aqueous solution at supercritical conditions. Particle size was in the range from 2 nm to 10 nm, and particle size dispersion is extremely narrow. Crystal shape can be controlled to be sphere, nano-cube, nano-ribbon etc. By selecting a proper modifier, particles could be dispersed perfectly in organic solvents or in aqueous solutions. By drying the colloid, we obtained self-assembly structure of nanocrystals. [Analytical Sciences, 22(11),1417-1423(2006.11), Chemistry Letters, 35, 636-637 (2006), Chemistry Letters, 35, 732-733 (2006), Combustion Science and Technology, 178, 509-536 (2006), Journal of Materials Science, 41, 1445-1448 (2006), Funtai Kogaku Kaishi, 43, 440-444 (2006)] [contact: Prof. T. Adshiri; ajiri@tagen.tohoku.ac.jp]

At the Graduate School of Environmental Studies, Tohoku University, Sendai, we have several laboratories which studies hydrothermal experiments in material and Earth sciences. Prof. K. IOKU published excellent papers: hydrothermal preparation of tailored hydroxyapatite (K. Ioku et al., J. Mater. Sci., **41** [5], (2006), 1341-1344). He also tried to analyze bio-phenomena of materials prepared by hydrothermal methods: the effect of the microstructure of β-tricalcium phosphate on the metabolism of subsequently formed bone tissue (Ioku et al., Bimaterials, **28**, (2007), 2612-2621). Prof. H. Ishida's group studied about mesoporous materials which were prepared by the hydrothermal process using metakaolinite, quartz and slaked lime (Maeda et al. J. Ceram. Soc. Jp., 114 (2006) 743-747). The mesoporous materials had a broad pore size distribution more than 3 nm, which contributes to humidity control in the middle humid range. The humidity change in the vessel with the mesoporous materials was suppressed by water vapor adsorption-desorption of the materials. 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 new conceptual model of supercritical fluid in terms of chemical reactions (Tsuchiya and Hirano, Island Arc, 6 (2007), 6-15). Prof. N. Tsuchiya had an award on research of hydrogen production from $H_2S$ by hydrothermal reaction in International Symposium of Renewable Energy 2006. Petroleum Engineering research group studies hydrothermal cracking for unconventional heavy crude oil such as tar sands to develop new on-site partial upgrading process with high temperature and high pressure water in supercritical region was performed. (Kishita et al., J. of Japan Petroleum Institute, 49 (4), (2006), 177-185). We are planning 5$^{th}$ International Workshop of WATER DYNAMICS in 25-27$^{th}$ September 2007 in Sendai International Center. WATER DYNAMICS is unique objectives covering very wide range of water and steam properties and utilization, which focused on the role of water in Earth processes, Life science and Material and Energy Process Design. The web site of WATER DYNAMICS is the follows: http://geo.kankyo.tohoku.ac.jp/wd/wd5/index.html. We

published workshop proceedings as AIP (American Institute of Physics) conference series (vol. 833 and 898)
[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, viscosity, and refractive index standards. A determination of the Avogadro constant is being conducted in this section as an international project organized by the Comité International des Poids et Mesures (CIPM). This project continues 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 fundamental physical constants. Most recent situation of this project is given in a paper [K. Fujii, A. Waseda, N. Kuramoto, S. Mizushima, P. Becker, H. Bettin, A. Nicolaus, U. Kuetgens, S. Valkiers, P. Taylor, P. De Bièvre, G. Mana, E. Massa, R. Matyi, E. G. Kessler, Jr., and M. Hanke, "Present state of the Avogadro constant determination from silicon crystals with natural isotopic compositions," IEEE Trans. Instrum. Meas., 2005, 54, 854-859]. In 2007, the uncertainty of the density measurement of 1 kg silicon spheres has been reduced down to $3.6 \times 10^{-8}$ [Kuramoto N., Fujii K., Azuma Y., Mizushima S., and Toyoshima Y., "Density Determination of Silicon Spheres using an Interferometer with Optical Frequency Tuning," IEEE Trans. Instrum. Meas. 2007, 56, 476-480]. Using the silicon crystals as a solid density standard, densitt standard liquids are calibrated by a magnetic suspension densimeter 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 $4 \times 10^{-6}$ has been achieved in the density measurement of organic liquids. A revised densimeter is being developed in this section as a joint research with the Keio University [Y. Kano, Y. Kayukawa, K. Fujii, and H. Sato, "A new method for correcting a force transmission error due to magnetic effects in a magnetic levitation densimeter," Meas. Sci. TEchnol., 2007, 18, 659-666]. Review articles are given for the density standard [K. Fujii, "Present state of the solid and liquid density standards," Metrologia, 2004, 41, S1-S15] and for the hydrostatic weighing [K. Fujii, "Precision density measurements of solid materials by hydrostatic weighing," Meas. Sci. Technol., 2006, 17, 2551-2559]. 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]. 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. 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. The results were published as a technical brief entitled "Assessment of the Computing Time for the IAPWS-IF97 Equations", ASME Journal of Engineering for Gas Turbines, Volume 129, Issue 3, pp. 885-887, July 2007. [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 stability of chromium oxide in high temperature water up to supercritical region by *in situ* Raman spectroscopy and analyses after immersion tests. Experimental results of immersion tests of $Cr_2O_3$ film formed by metal organic chemical vapor deposition on Pt were published [CORROSION2007, Paper 07411 (2007).]. At 623 K, stability of $Cr_2O_3$ depends on redox conditions, and can be explained by oxidation of Cr(III). At 723 K, weight of $Cr_2O_3$ film was reduced to some extent irrespectively of redox conditions, but cristalinity of $Cr_2O_3$ increased. Stability of $Cr_2O_3$ film formed on stainless steel substrate in high temperature water was measured by *in situ* Raman spectroscopy. Under all conditions of temperature and redox environment examined, $Cr_2O_3$ was stable. The difference of $Cr_2O_3$ stability between Pt and stainless steel substrates can be attirbuted to interaction of $Cr_2O_3$ with oxide film formed on surface of stainless steel substrate.
[contact: Dr. M. Domae; E-mail: domae@criepi.denken.or.jp]

At Energy Engineering Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Kanagawa, Dr. NAKANO and his coworkers are studying on the efficiency improvement of geothermal power plant. They developed the software based on the heat and mass balance analysis, "General purpose program for analysis of thermal efficiency of power generation systems". Using this software, they estimate the relationship between vacuum and power outputs, the influence that non-condensible gas extractor systems are replaced, and, the actual effects generated by repair of cooling tower. [contact: Dr. Nakao; E-mail: y-nakao@criepi.denken.or.jp]

At the Department of Mechanical Engineering, Keio University, Yokohama, Prof. M. UEMATSU and his group study the behavior of thermodynamic properties of water + ammonia mixtures by means of the PVTx measurements, and the critical parameter measurements. The PVTx properties of water +

ammonia mixtures is measuring in the temperature range from 450 K to 550 K at pressures up to 200 MPa by a metal-bellows variable volumometer. The critical parameter of water + ammonia mixtures is measuring by a metal-bellows variable volumometer with an optical cell. The Cp measurements of water + ammonia 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. [I. Fujita, T. Suzuki, and M. Uematsu, Accepted for publication 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, Prof. K. YASUOKA and his group are studying the molecular dynamics (MD) simulation to clarify the thermodynamic stability of structure-I, II, and H clathrate hydrate by estimating the free energy difference. [E. Sato, T. Miyoshi, R. Ohmura, K. Yasuoka, *Jap. J. Appl. Phys.*, in press.; T. Miyoshi, M. Imai, R. Ohmura, K. Yasuoka, *J. Chem. Phys.*, **126**, 234506 (2007).; .; T. Miyoshi, R. Ohmura, K. Yasuoka, *J. Phys. Chem. C*, **111**, 3799-3802 (2007).; T. Miyoshi, R. Ohmura, K. Yasuoka, *Mole. Simul.* **33**, 65-69 (2007).] They reported the supercritical phenomena on the 2D of liquid-vapor water surface and the cluster near the surface. [Y. Andoh and K. Yasuoka, *J. Phys. Chem. B.*, **110**, 23264-23273 (2006).; Andoh and K. Yasuoka, *Mole. Simul.* **33**, 139-145 (2007).] They reported the Spontaneous self-assembly process for threadlike micelles. [N. Arai, K. Yasuoka, Y. Masubuchi, *J. Chem. Phys.*, **126**, 244905 (2007).] [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 finished the measurements of the pVTx properties of ammonia + water mixtures. They are preparing to design the set-up for the iso-choric specific heat capacity of ammonia + water mixtures, and to correlate the equation of state for ammonia + water mixtures. [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 a diabatic calorimeter for water + alcohol and water + ammonia mixtures. By the apparatus, liquid isochoric heat capacities will be measured for temperatures from 220 to 520 K and pressures to 30 MPa including super critical region. One isochore of propane was measured from 310 K to 350 K preliminary. The data showed behavior similar to the previous measurements by another twin-cell type adiabatic calorimeter apparatus which had measured water + alcohol and hydrocarbon mixtures. But, the preliminary data were quieter than the pre vious. [contact: Prof. N. Kagawa; E-mail kagawa@nda.ac.jp]

Prof. H. TAKAKU was retired from Faculty of Engineering of Shinshu University at the end of March of 2006, but at present he is entrusted by Shinshu University as the Professor in charge of education. He and his coworkers, including also some researchers of Japanese utility and makers, are conducting the corrosion researches of steam turbine materials for geothermal power plants, the corrosion of boiler tube materials for fossil power plants, and other subjects related to the corrosion and water chemistry for both of the fossil and nuclear power plants. As the chairman of the committee, he contributed to the revision of JIS-B-8223 entitled on “Water conditioning for boiler feed-water and boiler water”, and this revised JIS

(Japanese Industrial Standard) was published on October 20 of 2006. Their main publications are "Behavior of Organic Sulfate Ions of PWR plants; and also The Anticorrosive Magnetite Layer Formed by Amine-Carboxylate Aqueous Solution Treatment on Boiler Tubes; both papers presented at the International Conference on Interaction of Organics and Organic Cycle Treatment Chemicals with Water, Steam and Materials, organized by EPRI-Power Plant Chemistry, Oct.2-4 (2005)", Stuttgart, Germany, "Water conditioning for boiler feed-water and boiler water; JIS B 8223-2006, published by Japanese Standards Association, Oct. 20 (2006), "Influence of Chloride and Carbon Dioxide on General and Crevice Corrosions of Steam Turbine Materials for Geothermal Power Plants, *Power Plant Chemistry*, **8** (2006), 558-565", and so on. [contact: Prof. H. Takaku; E-mail: takaku06@ybb.ne.jp]

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their coworkers study the structure, dynamics, and reactions in super- and subcritical water by means of multinuclear NMR (nuclear magnetic resonance) spectroscopy and computer simulation. Their current focus are (1) the thermodynamics, structure, and dynamics of supercritical aqueous solution over a wide range of thermodynamic conditions, especially the diffusion dynamics in very dilute region ["Self-diffusion of supercritical water in extremely low-density region", K. Yoshida, N. Matubayasi, and M. Nakahara, J. Chem. Phys. 125, 074307 (7 pages) (2006); 126, 089901 (2 pages) (2007) (erratum)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions in connection to next-generation hydrogen fuel technology. ["Kinetic and Equilibrium Study on Formic Acid Decomposition in Relation to the Water-Gas-Shift Reaction", Y. Yasaka, K. Yoshida, C. Wakai, N. Matubayasi, and M. Nakahara, J. Phys. Chem. A 110, 11082-11090 (2006)]. [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 been studying the electric conductivities of 1:1 electrolytes in liquid alcohol (methanol and ethanol) along the liquid-vapor coexistence curve up to about 240 °C to disclose the general trends of the density dependence of ionic mobilities at medium and low densities, and to examine the validity of the Hubbard-Onsager (HO) dielectric friction theory which is based on the continuum model. We found that ionic mobilities decrease with decreasing the density in the region of the relative density $\rho_r$ ($=\rho/\rho^0$) < 2.0, and that the HO theory does not work in the region. We also study the Computer simulations: Application of Fokker-Planck-Kramers equation treatment for short-time dynamics of diffusion-controlled reaction in supercritical Lennard-Jones fluids over a wide density range [K. Ibuki and M. Ueno, J. Chem. Phys., 124, 134506 1-11 (2006)], and Analysis of short-time transient dynamics of a diffusion-controlled reaction in a hard-sphere fluid based on Fokker-Planck-Kramers equation [K. Ibuki and M. Ueno, Bull. Chem. Soc. Jpn., 79, 1509-1518 (2006)]. In collaboration with Dr. M. Kanakubo, AIST, Sendai, the effect of pressure on transport properties (self-diffusion coefficients and electrical conductivities) of the ionic liquid 1-Butyl-3-methylimidazolium Hexafluorophosphate has been investigated [M. Kanakubo, K. R. Harris, N. Tsuchihashi, K. Ibuki, and M. Ueno, *J. Phys. Chem.* B, **111**, 2062-2069 (2007)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At the Department of Applied Chemistry, Ritsumeikan University, Shiga, Prof. S. SAWAMURA studies the solubility of NaCl and amino acids in water and that of fullerene $C_{60}$ in toluene under high pressure up to 400 MPa [S. Sawamura, N. Fujita, Carbon, 45, 965-970 (2007); S. Sawamura, N. Egoshi, Y. Setoguchi, H. Matsuo, Fluid Phase Equilibria, 254, 158-162 (2007); S. Sawamura, Pure and Applied Chemistry, 79, 861-874 (2007).] and found a high-pressure crystal of leucine as a residue of saturated mixture. [M. Yamashita, S. Inomata, K. Ishikawa, T. Kashiwagi, H. Matsuo, S. Sawamura, and M. Kato, Acta Cryst. E63, o2762-o2764 (2007).] [contact: Prof. S. Sawamura; E-mail: sawamura@se.ritsumei.ac.jp]

**I**nternational **A**ssociation **f**or **t**he **P**roperties **o**f **W**ater **a**nd **S**team

*Russian National Committee*

# Report of Russian National Committee (2007)

## *List of Publications*

1. Voronov V.N., Gotovcev P.M., Smetanin D.S. Building of Water Chemistry Mode Diagnostic Method Complex on the Base of Experemential Plant Monitoring System. // Thermal Engineering, vol. 7,pp. 2-6
2. Petrova T.I., Kashinsky V.I., Verkhovsky A.E., Nikolaev P.A., Repin D.A., Chernichov E.V. ,Bogdanov S.L. The Study of Influence Phosphate Concentration in Drum Water on Conductivity and pH.// Thermal Engineering, vol. 7,pp. 6-10
3. Boglovsky A.V., Chernozubov V.B., Chernih N.E., Gorbunov A.V., Birdin R.H. The Organization of Water Chemistry Mode of Thermal Water Purification Plant// Thermal Engineering, vol. 7,pp. 15-20
4. Smetanin D.S. Optimization Chemistry Monitoring System by Using Technology Algorithm.// Thermal Engineering, vol. 7,pp. 20-25
5. Egochina O.V., Voronov V.N., Nazarenko P.N. The Development of Automatic Control System for Hydrazine Dosation.// Thermal Engineering, vol. 7,pp. 25-28
6. Alexandrov A.A. Orlov K.A. The Thermodynamic Properties of Humid Air under High Temperature and Pressure// Thermal Engineering, vol. 7,pp. 36-40
7. Evsutin A.V., Boglovsky A.V. The Application of Alluminium Oxichloride for Coagulation Water with High Organic Impurities Concentration and Lower Alcalinity.// Thermal Engineering, vol. 7,pp. 67-71
8. Nikolaev P.A. The Influence of Liquid Film Contamination in the Turbin Blade on the Metall Corrosion// Energosberezhenie I Vodopodgotovka, 2007, № 1, pp. 67-68
9. Matsko T.V. The Application of Film-forming Combinations for Water Correction Treatment in Heat Supply Systems. //Vestnik MEI, 2007, № 1, pp. 29-31
10. Alexandrov A.A., Ochkov V.F., Orlov K.A, Ochkov A.V. Thermopysical properties of water and steam: information in Internet// Industrial energetics, 2007, No 2, P. 29-35

# U.S. National Committee to IAPWS
# 2007 Report on Activities of Potential Interest to IAPWS

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

The Energy Institutes' Electrochemical Laboratory at Penn State University continues to work in fundamental and applied areas on a variety of electrochemical and materials science studies related to traditional and renewable energy generation systems. We lead interdisciplinary studies on electrochemistry of high-temperature aqueous systems in a number of scientific areas including corrosion and protective coatings, proton exchange membrane and solid oxide fuel cells, surface electrochemistry and chemistry, etc. The main research directions and key publications in 2006-2007 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*, 2006, **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*", Eds. A.J. Bard and M. Stratmann, Vol. 5. Electrochemical Engendering, Eds. D.D. Macdonald and P. Schmuki, 2006, Wiley-VCH, p. 725-747.

**(3) High-Temperature Surface Chemistry**

Machesky M.L., Wesolowski D.J., Palmer D.A., Ridley M.K., Benezeth P., Lvov S.N., and Fedkin M.V., Ion Adsorption into the Hydrothermal Regime: Experimental and Modeling Approaches. Chapter 12, in "Surface Complexation Modeling" (J. Lutzenkirchen, Ed.), 2006, Elsevier, Amsterdam, pp. 324-358.

**(4) High-Temperature Surface Electrochemistry**

Fedkin, M.V.; Chalkova, E.; Komarneni, S.; Wesolowski, D.J.; Lvov, S.N., "Surface Electrochemistry of Composite Materials for High-Temeprature PEM Fuel Cells," ECS Trans. 2006, **1**, 215-225.

**(5) High-Temperature Proton Exchange Membrane Fuel Cells**

Chalkova, E.; Rybka, G.; Fedkin, M.V.; Wesolowski, D.J.; Roelofs, M.; Lvov, S.N., "Nafion/$TiO_2$ Composite Membranes for PEM Fuel Cells Operating at Elevated Temperature and Reduced Relative Humidity," ECS Trans., 2006, **3,** 73-82.

Chung M., Komarneni S., Chalkova E., Lvov S.N. Proton Conductive Composite Materials with Co-continuous Phases Using Silane Functionalized and Crosslinkable PVDF Polymers, 2006, ECS Trans. **3**, 83-90.

Chalkova, E., Fedkin, M.V., Komarneni, S., and Lvov, S.N., Nafion/Zirconium Phosphate Composite Membranes for PEMFC Operating at up to 120°C and down to 13% RH, J. Electrochem. Soc., **154**, B288-B295.

Gong Y., Yeboah Y.D., Lvov S.N., Balashov V., and Wang Z., Fe Modified Pt Based Cathodic Electrocatalysts for Oxygen Reduction Reaction with Enhanced Methanol Tolerance, J. Electrochemical Soc., (in press).

**(6) High-Temperature Sold Oxide Fuel Cells**

Zhou Z.F., Kumar R., Thakur S.T., Rudnick L.R., Schobert H., and S.N. Lvov, Direct oxidation of waste vegetable oil in solid oxide fuel cells. J. Power Sources, 2007, in press.

**(7) High-Temperature Aqueous Corrosion and Protective Coatings**

Zhou Z.F., Chalkova E., Lvov S.N., Chou P., and Pathania R. Development of a Hydrothermal Deposition Process for Applying Zirconia Coatings on BWR Materials for IGSCC Mitigation. Corrosion Science, **49**, 830-847.

**Communicated from The University of Delaware, Newark, DE:**

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

"Potentials of Mean Force of Sodium Chloride in Supercritical Water as a Function of Density and an Equation for Dissociation Constant from 600 K to 1073K and 0 to 9 g/cm3," by Wenbin Liu, Robert H. Wood, and Douglas J. Doren, in preparation.
"Structure of an accurate *ab initio* Model of the aqueous Na+ ion at high Temperatures," by Haitao Dong, Wenbin Liu, Robert H. Wood, and Douglas J. Doren., in preparation.
"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. *J. Phys. Chem. B*, 2006, 110, 18504-18514.
"Dissociation constants and speciation in aqueous $Li_2SO_4$ and $K_2SO_4$ from measurement of electrical conductance to 673 K and 29 MPa," by Andrei V. Sharygin, Brian K. Grafton, Caibin Xiao, Robert H. Wood, and Victor N. Balashov, *Geochim. Cosmochim. Acta* 2006, 70, 5169-5182.

**Communicated from the National Institute of Standards and Technology, Boulder, CO:**
A collaboration is continuing with Prof. Richard Wheatley at the University of Nottingham, developing intermolecular pair potentials for aqueous systems for the quantitative calculation of second virial coefficients. Results for the water-nitrogen and water-oxygen binaries have been published in the past year. These results, along with previous results for water-argon, have allowed a purely predictive calculation of the second virial coefficients for water with "air," which is consistent (with similar uncertainties) with precise data from the humidity community but covers a much larger temperature range. This result should be useful for humidity standards, atmospheric applications, and the energy industry. The next system to be covered in this manner is water with carbon monoxide, which is important for synthesis gases in advanced power cycles.
References: Tulegenov, A.S., Wheatley, R.J., Hodges, M.P., and Harvey, A.H., 2007. "Intermolecular potential and second virial coefficient of the water–nitrogen complex," *J. Chem. Phys*., 126, 094305; Wheatley, R.J., and Harvey, A.H., 2007. "The water-oxygen dimer: first-principles calculation of an extrapolated potential energy surface and second virial coefficients," *J. Chem. Phys*., 127, 074303; Harvey, A.H., and Huang, P.H., 2007. "First-Principles Calculation of the Air-Water Second Virial Coefficient," *Int. J. Thermophys.*, 28, 556.

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.

NIST's Experimental Properties of Fluids group has begun apparatus design for two projects to measure thermophysical properties of aqueous gas-phase mixtures at high temperatures. One apparatus will be a high-temperature (up to 770 K) magnetic-suspension densimeter, which will be used to measure $H_2O$-$N_2$ and $H_2O$-$CO_2$ mixtures of interest for understanding the thermodynamics of combustion gases. An existing high-temperature thermal conductivity apparatus (using the transient hot-wire technique) is being converted to alternating-current operation (needed for polar fluids like water) in order to measure the thermal conductivity of $H_2O$-$N_2$ and $H_2O$-$CO_2$ mixtures at similar conditions (up to 750 K).

**Communicated from Jonas, Inc., Wilmington, DE:**
Jonas, Inc. is working on the following projects related to IAPWS interests:
1. Fusion Reactor ITER/Tokamak: water radiolysis and hydrogen water chemistry, Zn treatment, corrosion and activation of corrosion products (316L, 430ss, CuCrZr, Cu, borated ss)
2. Atmospheric corrosion: influence of cooling tower plumes, seawater for cooling towers, critical relative humidity (salt zone), seashore air, gas turbine compressors, ...
3. Rapid Response Corrosimeter and Surface Conductivity: general corrosion, FAC, steam piping, buried piping
4. On Line Moisture Monitor: % moisture, enthalpy, continuous monitoring
5. Low pressure steam turbine surface chemistry: on-line monitoring of early condensate, moisture drying, deposits, and corrosion.

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|---|---|---|---|
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