THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

MEMBERS ASSOCIATE MEMBERS

Britain and Ireland Argentina and Brazil

Canada Australia
Czech Republic France
Germany Greece
Japan Italy

Russia New Zealand Scandinavia (Denmark, Finland, Norway, Sweden) Switzerland

United States of America

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

Boulder, Colorado 30th September – 5th October 2012

Prepared by: Barry Dooley



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

Boulder, Colorado 30th September – 5th October 2012

Plenary Session. Monday, 1st October 2012. 8:30 am (64 people in attendance)

The President of IAPWS, Daucik, welcomed the Executive Committee (EC) and other IAPWS members to Boulder for the EC and Working Group (WG) Meetings of IAPWS. The President officially opened the 2012 EC Meetings by introducing the National Delegates. Each of the Member and Associate Member countries of IAPWS was in attendance with the exception of Argentina/Brazil, Greece and Italy.

The President indicated to the EC that Dr. Geoff Bignold, Honorary Fellow of IAPWS, had passed away on 4th August 2012 and asked for a moment of silence.

The President asked the delegate of USA to provide some opening comments. Friend welcomed everybody to Boulder and to the 2012 IAPWS meetings. He briefly reviewed some of the events planned for the week and provided some background on the US National Committee which is an ASME entity. He recognized the sponsors for the meetings: EPRI, NIST, GE Energy, Siemens Energy, Nooter/Eriksen and Sentry Equipment.

1. Adoption of Agenda

Provisional agendas had been posted on the IAPWS Website for all IAPWS members by the Executive Secretary. 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. <u>IAPWS Business and Appointment of Committees</u>

2.1 Releases, Advisory Notes, ICRNs and Technical Guidance Documents

The Executive Secretary indicated that seven documents had been circulated to the National Committees during the year since the Plzen meeting for final review prior to being approved before or during the current EC Meeting. The Executive Secretary reminded the EC of these documents:

• IAPWS Guideline: Guideline on a Low Temperature Extension of the IAPWS-95 Formulation for Water Vapor. Distributed 10th April 2012. No objections have been received so the document will be reviewed by the TPWS working group during the week prior to approval at the Friday EC.

- Revised IAPWS Technical Guidance Document: *Instrumentation for Monitoring and Control of Cycle Chemistry for the Steam-Water Circuits of Fossil Fired and Combined Cycle Power Plants*. Distributed 5th June 2012. There was one comment from BIAPWS on the format of the final version. The document will be reviewed by the PCC working group during the week prior to approval at the Friday EC.
- ICRN 20: Sensors for use at Elevated Temperature in the Plant Cycle of the Power Industry. Distributed on 3rd November 2011. No objections were received before 4th March 2012, and thus the ICRN was approved at that time.
- ICRN 27: *Thermodynamic Properties of Humid Gases and CO₂-Rich Mixtures*. Distributed on 29th September 2011. One minor change was made before 1st February 2012, and thus the ICRN was approved at that time.
- ICRN 28: *Thermophysical Properties of Metastable Steam and Homogeneous Nucleation*. Distributed on 7th October 2011. One suggestion was addressed by 10th February 2012, and thus the ICRN was approved at that time.
- IAPWS Release: Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance. Distributed 11th October 2011. No objections were received by 13th January 2011 so the Release was approved at that time
- IAPWS Release: Revised Supplementary Release on Properties of Liquid Water at 0.1 MPa. Distributed 11th October 2011. No objections were received by 13th January 2011 so the Revised Supplementary Release was approved at that time

The respective Working Groups will report to the EC at the Friday meeting on any further changes prior to requesting approval.

2.2 Press Release (to be called Highlights in future).

The President asked Bellows to develop a Press Release on the IAPWS proceedings during the week. Joy was also appointed to the committee. The Clerks of Minutes from each WG were asked to provide input. The Highlights is discussed in Minute 18.3 and is Attachment 10.

2.3 Evaluation Committee on International Collaboration.

The President indicated that two proposals had been received by the Executive Secretary prior to the meeting, and that any further suggestions from WGs should be given to the Executive Secretary by the end of day. The President then reminded the EC that the Committee to review the proposals would consist of the WG Chairmen, with the President and Executive Secretary as ex. officio members. Because one of the proposals caused a conflict of interest for the TPWS Chairman it was suggested that Kretzschmar represent TPWS on the committee. A chairman would be chosen by the Committee. The discussion of this Committee is reported in Minute 15.1.

2.4 IAPWS Awards Committees

2.4.1 Helmholtz Award Committee

The President indicated that there was a Helmholtz Awardee this year. The Executive Secretary then reminded the EC that the Helmholtz Committee for the 2013 award would consist of a member from Germany, Japan, Russia, USA and BIAPWS. The President indicated that Germany would provide the committee chairman. The President asked delegate Kretzschmar to organize the committee and to report back to the EC on Friday with the names of the members of this committee (Minute 16.1).

2.4.2 Honorary Fellow Award Committee

The President requested that Rukes remain on the Committee for a fourth year as the Chairman for 2013 because of the passing of Bignold. The IAPWS President requested that Bellows join the two man committee. The President would be ex. Officio.

2.4.3 Gibbs Award Committee

The President reminded the EC that the next Gibbs Award would be conferred at the 16th ICPWS in 2013 and that the selection process had been initiated in Plzen in 2011. The chairman, Watanabe, was asked to provide an update of the process. The chairman indicated that one of the three nominations made by three IAPWS countries had created a conflict of interest for one of the members of the original committee. Watanabe had requested that this member step down. As this reduced the makeup of the committee the chairman then requested that Petrova from the Russian National Committee join the committee. Watanabe indicated that the committee would meet during the week and report back to the EC on Friday (Minute 16.3).

2.5 IAPWS Statutes and By-Laws

The President requested that the chairman of the committee formed in Plzen provide a status report. Harvey reminded the EC that currently the Statutes can only be changed at a General Meeting by a two-thirds vote of the EC Members present at the meeting in association with each ICPWS. He indicated that the committee (Svoboda and Watanabe) had met electronically during the last year and considered the items raised in Plzen and a few other items that had been raised by the committee. Harvey indicated that further consideration would be given during the week and that a final set of suggestions would be provided at the Friday EC meeting (Minute 18.2).

2.6 International Program Committee for the 16th ICPWS

The President requested Cooper to provide an update on the progress of the 16th ICPWS. Cooper first showed a map of the area around Greenwich where the conference will be held at Greenwich University, which is close to the Greenwich Observatory. The important item for the current IAPWS week in Boulder is a meeting of the International Program Committee (IPC) to decide on the logistics for acquiring abstracts, choosing the papers / presentations, and the timing of the IPC meeting with the Local Organization Committee in London in early 2013 to structure the technical program. The results of this meeting will be provided to the EC at the Friday meeting (Minute14.2).

2.7 Report on BIPM/CIPM and SCOR/IAPSO Interfaces

The President asked the SCSW Chairman, Feistel, to report on this item. Feistel indicated that following the 2011 EC Meetings in Plzen an opportunity arose for a small IAPWS delegation to attend the BIPM meetings in February 2012 to discuss cooperation between the two organizations. This required a special postal ballot to provide the necessary funds for the SCSW Chairman to attend.

The President requested that Harvey include in the revision of the IAPWS Statutes and By Laws facility for IAPWS people in the future to attend similar meetings of major interest to the IAPWS work and working groups (Minute 18.2).

SCSW Chairman Feistel then introduced the opportunity for IAPWS to form a Joint Committee on the Properties of Seawater (JCS) in collaboration with the Scientific Committee on Oceanic Research (SCOR) and the International Association for the Physical Sciences of the Oceans (IAPSO). This will be discussed during the week and a recommendation provided to the EC on Friday (Minute 9).

2.8 Other Business Requiring Extensive Discussions

No other business was raised by the EC.

3. EC Mandate to Working Groups and Membership

The President first requested that Feistel provide a short outline of the new direction within the Sub-Committee on Sea Water and particularly the extension to include the interface between the ocean and the atmosphere. This is reported in the joint TPWS / SCSW Minutes (Attachment 4).

The President then provided the following mandates to the WG Chairmen for action during the week.

3.1 Releases, Guidelines and Certified Research Needs.

The Executive Secretary indicated that four ICRNs had either expired already or will expire in September 2012 and thus needed attention by the WGs during the week: #21 on thermophysical properties associated with ultra-supercritical plants, #23 on dewpoint of flue gases, #24 on thermal conductivity of H_2O at low pressure and high temperatures, and #25 on corrosion mechanisms related to contaminants in steam / water.

3.2 Working Group Directions.

The President emphasized that each WG Chairmen should only report to the EC on Friday about those activities that need approval or discussion by the EC.

4. Preview by the WG Chairmen of the Week's Activities

President Daucik requested each WG Chairman to review briefly the main topics which would be covered in their WGs during the week. The details of the WG meetings are covered in detail in Minutes 7 to 11 (Attachments 4 to 7).

The President closed the opening session of the EC at 9:30am.

Activities During the IAPWS Week in Boulder

The first day activities of the WGs and Executive Committee were followed by the separate and joint WG meetings on Monday, Tuesday and Thursday.

The full IAPWS program for the week is shown in Attachment 2.

The IAPWS Symposium was held on Wednesday, 3rd October 2012. The overall theme was on "The Energy-Water Nexus: Status and Prospectus", and the Symposium Program is shown in Attachment 3.

Executive Committee Meeting. Friday, 5th October 2012

President Daucik opened the continuation of the EC Meeting at 8:30 am. Each of the Member and Associate Member countries of IAPWS was in attendance with the exception of Argentina/Brazil, Greece and Italy. In total there were 28 people assembled for the EC meeting. Daucik 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 from the Monday EC Meeting.

5. <u>Acceptance of Minutes of Previous Meeting</u>

President Daucik asked for comments and changes to the minutes of the EC meeting held in Plzen, Czech Republic in September 2011. No changes were noted, thus the 2011 Minutes were accepted.

6. <u>President's Report</u>

President Daucik opened his report by indicating that another fruitful year of IAPWS history had been written with five documents being published, as well as some revisions of earlier documents, some ICRNs and some new documents. He considered that the process of formation of these documents and workshops is even more fruitful and inspiring which points to the evaluation of new knowledge and new fields of action. The best example of this is the collaboration between the SCSW and international scientific bodies in oceanography and meteorology. Furthermore, the collaboration with Bureau International de Pounds et Measures (BIPM) in the field of seawater gives another interesting perspective.

The President then indicated that:

- PCC is also in the process of extending the field of activity by introducing the Technical Guidance Documents. This year the problems of sampling and quality assurance/control had been dealt with.
- TPWS is working on an extension of the IAPWS-95 formulation into the low temperature regime and even to supercooled water

- PCAS is working on hydration free energy of metal ions and organic species.
- IRS is formulating the future needs of the power industry, especially methods for H₂O properties with high computational speed for property-intensive applications like CFD (computational fluid dynamics), and time-dependent power plant simulations.
- Global economic crises challenge the industry. Reliable data on properties of water and aqueous solutions are critical for optimizing of the power production processes. Thus IAPWS products play an important role for further development of society.
- Climate changes indicate an even more serious problem linked to water resources. Purification and recycling of water are the fields, where IAPWS involvement would improve the possibilities for optimization of the processes.

The President finished his report by indicating that there are a lot of challenges, lots of questions to be answered and lots of problems to be addressed. He thanked all the participants in IAPWS activities for their effort during the past year and encouraged them to continue in this important work. IAPWS is preparing the 16th International Conference on Properties of Water and Steam, and the local organizing committee and international program committee are doing very well and he wanted to encourage all working groups to actively participate in this event with or without papers presenting the fine results of the IAPWS efforts.

7. Report and Recommendations of the Thermophysical Properties of Water and Steam (TPWS) and the Industrial Requirements and Solutions (IRS) Working Groups and the Subcommittee on Seawater (SCSW)

TPWS Chairman Harvey opened this item by indicating that he would report on activities within TPWS, IRS and SCSW during the week. He then highlighted only those activities from the working sessions during the week which needed action by the EC or which he thought were of interest to the EC. He indicated that all of the WG activities had been conducted jointly with the exception of separate meetings for IRS and the Subcommittee on Seawater which are reported in Minutes 8 and 9. Full Minutes and the Agendas for TPWS and SCSW can be found in Attachment 4.

7.1 The WG considered a Guideline on a Low Temperature Extension of the IAPWS-95 Formulation for Water Vapor. This allows the IAPWS-95 thermodynamic formulation to be used for water vapor down to 130 K. This document was approved by the WG. The WG recommends that the EC approves the Guideline.

The EC approved the Guideline Unanimously.

7.2 A Revised Guideline was presented on the Critical Locus of Aqueous Solutions of Sodium Chloride. This is a relatively minor revision of the existing Guideline, reflecting better theoretical understanding. The WGs TPWS and PCAS voted to approve the Revised Guideline and recommend to the EC that it should be sent for Postal Ballot following review by the Editorial Committee.

The EC approved this Process Unanimously.

- 7.3 Chairman Harvey then presented the following informational items to the EC:
 - TPWS approved minor editorial changes to the Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95).
 - TPWS and IRS approved minor editorial changes to the Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS-IF97).
 - A Task Group was appointed to work toward the extension of the seawater thermodynamic formulation to higher temperatures. The Task Group consists of Feistel (chair), Cooper, Harvey, Hiegemann, Hrubý, Kretzschmar and Pawlowicz.
 - A Task Group was appointed to reexamine the behavior of IAPWS-95 when extrapolated into metastable liquid regions. The Task Group consists of Hrubý (chair), Anisimov, Feistel, Hellmuth, Holten and Wagner.
 - As a result of the annual review by the appropriate Task Group, the WG approved a
 minor revision to the Guideline on the Use of Fundamental Physical Constants and
 Basic Constants of Water (consisting of substituting a current reference for an
 obsolete one).
 - A Task Group was appointed to work on a new formulation for the thermodynamic properties of heavy water. The Task Group consists of Harvey (chair), Cooper, Holten, Span and co-opted expert Lemmon of NIST.
 - A Task Group was appointed to examine whether the uncertainty estimates of IAPWS-95 can be improved due to new data that has become available. The Task Group consists of Wagner.
- 7.4 With regard to expiring ICRN-21 (Thermophysical Properties Associated with Ultrasupercritical Coal-fired Steam Generators), TPWS and IRS recommend that the EC allow this ICRN to expire and that the IAPWS contacts prepare a closing statement to be placed on the website.
- 7.5 With regard to expiring ICRN-24 (Thermal Conductivity of H₂O at Low Pressures and High Temperatures), TPWS and IRS recommend that the ICRN be renewed for 3 years after minor modifications to referencing are made to bring the document up to date.

The EC approved this Renewal Unanimously.

- 7.6 TPWS Membership. Chairman Harvey requested that the following new members are approved:
 - M. Fedorov (University of Strathclyde, Scotland, UK)
 - V. Holten (University of Maryland, USA)

The EC approved these Membership Changes Unanimously.

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

IRS Chairman Weber indicated that many of the activities of IRS during the week had been reported in the TPWS report, but the IRS group had one separate meeting during the week. Minutes for IRS and the Agenda can be found in Attachment 5. He covered the following items with the EC.

- 8.1 Industrial Survey. Chairman Weber indicated that a survey questionnaire had been discussed and will be finalized by IRS within the next months. The invitation to the survey will be distributed among IRS members and also will be sent out to the IAPWS National Committees asking for further distribution to companies that are not represented in IAPWS.
- 8.2 Task Group on Advisory Notes. The Chairman informed the EC that the job of the Task Group is to investigate whether the current system of advisory notes is sufficient to ensure that IAPWS formulations are used correctly. Discussion evolved around guidance regarding transport property formulations. Several suggestions were made, including adding an overview table to the IAPWS website and adding transport properties to Advisory Note #2. Discussion will continue within the TG and the final result will be presented in 2013. The Chairman also indicated that Kretzschmar will check if Advisory Note #3 needs an update and will provide such an update in 2013 if required.
- 8.3 With regards to ICRN 23 on Dewpoint of Combustion Gases, Chairman Weber indicated that ICRN 23 had been extended last year because a new publication had become available in 2011. However, background information on the paper could not be obtained so far. So IRS recommends that the ICRN be closed. A formal closing statement will be provided by Okita.

The EC approved this Unanimously.

The chairmen indicated to the EC that the topic remains of interest and activities understanding the background of currently available dew point predictions will continue. If necessary, a new ICRN will be proposed in the future.

8.4 IRS Membership. Chairman Weber requested that the following new member be approved:

R. Pawellek (STEAG Energy Services GmbH, Germany)

The EC approved this Membership Change Unanimously.

9 Report and Recommendations of the Subcommittee on Seawater (SCSW)

The minutes for SCSW are included in the TPWS minutes in Attachment 4.

SCSW Chairman Feistel immediately indicated that he wanted to recommend officer and membership changes to the EC.

9.1. Chairman Feistel recommended to the EC that Vice Chairman Pawlowicz becomes the Chairman of the SCSW and that he becomes the second Vice Chairman.

The EC approved this SCSW Officer Change Unanimously.

Then Chairman Pawlowicz requested that the following new member be approved:

H. Uchida (Research Institute for Global Change, Japan)

The EC approved this Membership Addition Unanimously.

- 9.2 Chairman Pawlowicz provided the following informational items to the EC:
 - Anderko had reported on activities of the Task Group "Transport properties of seawater". A draft guideline for thermal conductivity was not ready for this meeting but should be ready in the next year. To speed process, an evaluation group was appointed in advance (Miyagawa and Blanchetti)
 - IAPWS-2008 refers to 'salinity' but TEOS-10 recommendation developed later formally discourages the use of the word 'salinity' in cases where numerical values are implied or required. In such cases a more precise term associated with a specific definition, such as Absolute Salinity, Reference Salinity, etc. should be used. IAPWS-2008 should include some editorial changes to make this clear. Task group: Feistel, Pawlowicz, McDougall and Friend.
- 9.3 The Chairman next discussed the proposal for a "Joint Committee on the Properties of Seawater" (JCS) with SCOR and IAPSO. He outlined the following terms of reference:
 - 1) To act as a 'point of contact' for issues related to the bulk properties of seawater
 - 2) To maintain and update documents, websites and software of TEOS-10 and other standards.
 - 3) To encourage the uptake of TEOS-10 and other standards by the oceanographic community by acting as a source of advice.
 - 4) To globally coordinate research and the development of standards related to the properties of seawater across different scientific communities.
 - 5) To identify developing needs for standards and encourage research in those areas.
 - 6) To issue reports or other documents on issues relating to the bulk properties of Seawater.
 - 7) To work towards international and interdisciplinary uniformity and consistency of the standards and measurements procedures used in oceanography.

Chairman Pawlowicz then requested approval for the creation of, and participation in JCS.

The EC approved this Unanimously.

He then proposed that the JCS Executive will consist of Pawlowicz (chair) with Feistel and McDougall (vice chairs).

The EC approved this Executive Unanimously.

10. Report and Recommendations of Physical Chemistry of Aqueous Systems Working Group (PCAS)

Chairman Nakahara provided the PCAS Report to the EC. He indicated that a number of very useful joint workshops had been held during the week. Full Minutes can be found in Attachment 6. He covered the following items with the EC:

10.1 PCAS Membership. Chairman Nakahara requested that the following new member be approved:

M. Fedorov (University of Strathclyde, Scotland, UK)

The EC approved this Membership Addition Unanimously.

Chairman Nakahara then addressed the issue of deleting inactive members from the PCAS membership list. For this purpose, three criteria were proposed and accepted by the PCAS WG. An inactive member will be deleted from the list if (1) they have not participated in the activities of PCAS for a long time (substantially longer than the previously used 3-year period of inactivity), (2) their past contributions (such as creation of releases, guidelines or organizational leadership) cannot be reasonably used to justify their retention, or (3) their lack of continued participation is coupled with the associate member status of their home countries. Based on these criteria, the Chairman suggested to the EC that the following seven members are deleted from the PCAS membership list: Covington, Majer, Neumann, Perboni, Regazzoni, Smirnova and You.

The EC approved the Process and these Membership Deletions Unanimously.

Nakahara indicated that they will be welcome to rejoin the group if they choose to do so.

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

Chairman Rziha highlighted those activities that needed action / approval by the EC. A full written report of the PCC WG activities forms Attachment 7. He covered the following items with the EC

11.1 Technical Guidance Documents. Chairman Rziha reminded the EC that four Technical Guidance Documents (TGDs) had been approved between 2008 and 2011. The PCC Task Group had identified a need for a few revisions to the TGD *Instrumentation for Monitoring and Control of Cycle Chemistry in Fossil and Combined Cycle/HRSG Plants*. This document had been revised and circulated to the Task Group, PCC, Editorial Committee and National Committees. Minor changes had been made and the document was reviewed with PCC during the week. Chairmen Rziha requested that the EC approve this document.

The EC approved the Revision of the Technical Guidance Document Unanimously.

Chairman Rziha indicated that a number of new TDGs are in preparation.

- 11.2 ICRN 17 on Amines. The Chairman reported that a major revision of this ICRN is in preparation.
- 11.3 ICRN 19 on Sampling of Corrosion Products. A closing statement is in preparation.
- 11.4 ICRN 25 on Corrosion mechanisms that are related to the presence of contaminants in steam / water circuits, particularly in boiler water was drafted and discussed with PCC during the week. It was approved for finalization through the Editorial Committee prior to sending for a postal ballot.
- 11.5 International Collaboration on Sampling Lines. The Chairman informed the EC that this related to ICRN 19 and had been delayed in 2011 due to the problems in Japan. A final report has been issued and a closing statement for the ICRN will be developed.
- 11.6 PCC Membership. Chairman Rziha recommended to the EC that Thomsen (Denmark) become the second Vice Chairman of PCC.

The EC approved this PCC Officer Change Unanimously.

The Chairman then requested that the following new members be approved:

Anders Fredrikson (Tekniska Verken, Sweden)
Mats Hellman (Hellman Vatten AB, Sweden)
Taro Ichihara (Mitsubishi Heavy Industries, Japan)
Hideo Hirano (CRIEPI, Japan)
Paul McCann (E-on, UK)
David Addison (Thermal Chemistry, New Zealand)
Stephanie Marais (Eskom, South Africa)
Randy Turner (Swan, USA)
David Moed (TU Delft, The Netherlands)
Andy Witney (GE Energy, USA)
Kirk Buecher (Mettler Toledo, USA)

The EC approved these Membership Additions Unanimously.

12. Editorial Committee Report

Editorial Committee Chairman Harvey reported that in the preceding year, the Editorial Committee had reviewed the following documents:

- Revised Release on Thermal Conductivity.
- Revised Supplementary Release on Liquid Water at 0.1 MPa.
- Revised Technical Guidance Document on Instrumentation and Monitoring.
- Guideline on Low Temperature Extension of IAPWS-95 for Water Vapor.
- Revision of Advisory Note 2.

13. Membership and Associates

13.1 Members Defaulting on Dues.

The President asked the Executive Secretary to report on the members that are deficient in paying their dues. All IAPWS Members have paid their 2012 dues.

13.2 Reports on Associate Members

The Executive Secretary requested the delegate from each Associate Member and potential Associate Member to provide a short update.

<u>Australia.</u> Chariman Joy indicated that activities in ANAPWS were moving along nicely with an initial concentration on power plant chemistry. They are seeking other possible involvements in sea water, carbon sequestration and thermodynamics. ANAPWS has 40 members and the Australian Power Industry (API), Aurecon and CS Energy have joined. They are involved in two major conference activities in Australia: Australasian HRSG Users Group (AHUG) and API PowerChem. An Austalian wide steering committee has been formed and a draft of ANAPWS By-Laws has been developed. Discussions are continuing with API to link with ANAPWS. Joy indicated that they are on track to apply for IAPWS Membership at the next ICPWS in 2013.

New Zealand. Chairman Addison provided an update on NZAPWS. One of the main activities is connected with the 750MW of geothermal on the North Island, which represents about 13% of the country's demand. A national committee has been formed and they have held the first one-day Technical Symposium with 30 attendees. This covered power (fossil and geothermal), dairy/milk processing, Universities, Crown Research Institutes, industrial consultants and vendors. NZAPWS will become an incorporated society in New Zealand. They are planning another one-day symposium in 2013 and to apply for full IAPWS Membership at the 16th ICPWS in London.

<u>France.</u> Dorey indicated that after a lapse of about 10 years he is trying to re-activate a French National Committee and will try to get as many French people to the 16th ICPWS in London. All the WG Chairmen were requested to forward names of possible interested people in France that Dorey can contact.

<u>Switzerland.</u> Delegate Hiegermann reported the Swiss National Committee has not had a meeting in the past year and that there are no research programs under way. He indicated that the SNC applies for a prolongation of its status as an associate member with IAPWS, and hopefully it will succeed in its efforts to create a new small member base in the future.

South Africa. Delegate Marais indicates that South Africa is trying to establish a national committee. This has been launched by Eskom, the large national utility that has a large array of power stations. It will initially be from a power cycle chemistry perspective but they want to engage many other fractions of the South African industry. They will try to penetrate the universities, water management and reclamation industries. Marais indicated that they hope to launch a first meeting soon and apply for Associate Membership at the next ICPWS in London.

14. Executive Secretary's Report

14.1 Financial, Auditors and IAPWS Dues

The Executive Secretary reported that IAPWS remained on a sound financial footing with currently over \$93,000 in the US bank account. The status as at 12th September 2012 in the bank account had been provided to each National Delegate present at the EC meeting.

The Executive Secretary next reported that the 2011 financial statements had been forwarded to the IAPWS Auditors in January 2012. Both VDI in Germany and Professor Savarik in Czech Republic had reviewed and approved 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 remains unchanged for 2013.

The EC Unanimously Agreed to this Proposal.

The Executive Secretary also provided a rough estimate of the income and known planned expenditures for 2012 / 2013.

14.2 Time and Place of the 2013, 2014 and 2015 Meetings

<u>2013 IAPWS Meetings</u>. The Executive Secretary indicated that the 2013 IAPWS meetings will be held during the 16th ICPWS in London in September 2013. The President then requested Cooper as Chairman of the ICPWS International Program Committee to provide an update of the activities of the committee during the week.

Cooper indicated that the 16th ICPWS will be held in England and is being arranged by BIAPWS. The Institution of Mechanical Engineers (IMechE) will act as co-hosts and as conference administrators. Cooper confirmed that dates for the conference are Sunday September 1st to Thursday September 5th 2013, and that it will be held at Greenwich University in London.

When asked by the Executive Secretary about the Financial Statement for the 16th ICPWS, Cooper reported that this had not yet been developed. The BIAPWS delegate, McCann, confirmed this, but also indicated that BIAPWS and the Local Organizing Committee (LOC) will meet twice in the next month and that this item will be addressed. As the financial statement and the IAPWS Donation to the ICPWS are very important items within the financial situation of IAPWS, a motion was developed that BIAPWS should provide both to the Executive Secretary as soon as possible (within two months).

The EC Approved this Unanimously.

Cooper, as Chairman of the International Program Committee (IPC), next reported that the IPC had met during the week to develop the key dates for: a) submission of abstracts (11th January 2013); b) IPC meeting at Greenwich with the LOC (31st January / 1st February 2013); and c) acceptance of presentations (15th February 2013). The IPC also agreed that the final submissions for the conference can be formal papers or PowerPoint presentations, and that the format and date of the conference proceedings is a LOC decision. Included within the ICPWS will be a number of workshops on seawater and the environment; there will also be a one day event on power cycle chemistry.

<u>2014 IAPWS Meetings</u>. The Head of the Russian NC, Petrova, indicated that the Russian NC looks forward to welcoming IAPWS and the EC to Moscow. Details will be provided at the 2013 meetings in London.

<u>2015 IAPWS Meetings.</u> The Executive Secretary indicated that SIAPWS has been asked to host the 2015 Annual IAPWS meetings and to report back to the Executive Secretary by the end of 2012. Delegate Hellman indicated that this will be discussed at the next SIAPWS meeting.

15. 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.

15.1 International Collaborative Projects.

The President requested the Chairman of the 2012 International Collaboration Committee (WG and SC Chairs) to report on the findings of that committee during the week. Chairman Weber reported that two collaborative projects had been proposed. The following are overviews of the proposed projects. The details are provided in Attachments 8 and 9:

- An experimental study of viscosity of the binary ammonia and water system at high temperatures and pressures. The IAPWS sponsors are Friend (USA) and Petrova (Russia). The young scientist (Il'giz R. Gabitov or colleague to be named) will be from Kazan National Research Technological University, Russia.
 - It is proposed that IAPWS funding of \$20,000 would cover subsistence for 6-7 months at NIST in Boulder. If approved, a report on the research will be presented by the next annual meeting in London.
- Development of a new Equation of State for Heavy Water.

 The IAPWS sponsors are Harvey (USA) and Span (Germany). The young scientist is Stefan Herrig from Ruhr-Universität Bochum. A total budget of \$7,500 is proposed for this project, which would last for 4 months beginning in early 2013. This would pay for the travel expenses of Herrig to Boulder (IAPWS would be invoiced for \$1,500 or the actual expense, whichever is smaller), and for 4 months of living expenses at \$1,500 per month. If approved, a report on the research will be presented by the next annual meeting in London.

Weber indicated that the Evaluation Committee supported both proposals and that the technical content was of interest to IAPWS. He indicated that normally the committee would recommended to the EC that both are funded, but the committee this year realized that there could be some financial constraint in an ICPWS year, so they ranked the Heavy Water proposal as priority one. This lead to review of the IAPWS Guidelines for Spending of IAPWS Funds (Toronto, September 1999) in relation to the expenditures projected over the next year. The President indicated that there should be discussion on whether the EC thinks this project should be funded.

After much discussion a motion was developed to support the heavy water proposal to the full level proposed (\$7,500).

The EC approved the proposal to fund the project by 5:1 with the delegates from Germany and the US abstaining because of their involvement in the proposal.

16. IAPWS Awards

16.1 IAPWS Helmholtz Award

The President reported that the 2012 Helmholtz Award had been presented to Maxim Fedorov at the IAPWS Symposium on Wednesday.

Daucik then asked the German Delegate, Kretzschmar, for the names of the 2013 Helmholtz Award Committee. The 2013 Helmholtz Committee will consist of: Chairman Kretzschmar (Germany), Yasuoka (Japan), McCann (BIAPWS), Orlov (Russia), and Friend (USA).

Nominations will be due to the Executive Secretary by 31st January 2013.

The previous Helmholtz Committee Chairman, Hruby, wished to encourage national committees and WG Chairmen to generate more candidates in future related to IAPWS activities.

16.2 IAPWS Honorary Fellowships

The President reported that Kretzschmar (Germany) and Friend (USA) had been elected Honorary IAPWS Fellows, following the established procedures and after unanimous approval through the postal ballot conducted by the Executive Secretary. The Fellowship Awards had been presented at the IAPWS Dinner on Thursday evening by the IAPWS President. He reminded the EC of the Awards Committee for 2013 with Rukes as Chairman and Bellows as member with the IAPWS President as ex.-officio member.

Nominations are due to the Executive Secretary by 31st January 2013.

16.3 Gibbs Award

Following the final arrangements for the Gibbs Award Committee on Monday (Minute 2.4.3) the President requested Chairman Watanabe to report on the selection process during the week. Watanabe indicated that after two meetings the committee had ranked

the three nominees and decided to make a recommendation to the EC that Digby MacDonald is nominated for the 2013 Gibbs Award.

The EC Approved this Unanimously.

Chairman Watanabe further suggested that the President informs MacDonald of the nomination and that IAPWS will pay the associated expenses for travel to London. If the suggested nominee cannot attend, then Watanabe indicated that the committee had selected a runner-up.

Chairman Watanabe also had a few suggestions for future Gibbs Award nominations because his committee felt there was insufficient information provided for this most prestigious IAPWS Award. The nomination should include a single page statement providing: a) the contributions to the progress of science and technology, b) contributions to IAPWS activities, and c) a complete CV.

17. Election of IAPWS Officers for 2013 and 2014

The Executive Secretary indiated that the President would step down at the end of 2012 and that Vice President Petrova will assume the position of IAPWS President on January 1, 2013. According to the Statutes, the election of the next Vice President should be made at the end of the EC meeting in even years. The President and Executive Secretary had checked the recent history, and noted that it is 12 years since Canada has held the IAPWS Presidency and proposed that the Canadian National Committee should be asked to nominate one of their committee members for the position. The Executive Secretary asked the EC if there were any other suggestions. None were suggested, so he then requested the EC to approve this selection.

The EC Unanimously Approved this Selection.

Action: The Canadian National Committee should inform the Executive Secretary of their nomination for Vice President after the next meeting of their committee, and before the end of November 2012.

The Executive Secretary thanked the President for his leadership over the last two years, and indicated that his enthusiasm will continue under President Petrova. The EC applauded Daucik.

18. New Business

18.1 EC Preparations for the 16th ICPWS

The President asked BIAPWS about arrangements for the EC and General Meeting (GM) within the 16th ICPWS Week. IPC Chairman Cooper indicated that space would be provided on Sunday 1st and Friday 6th September 2013 for the EC Meetings and that the GM will be arranged in a large enough room during the week.

18.2 IAPWS Statutes and By-Laws

The President requested the Chairman of this Committee to report to the EC on activities during the week following initial brief discussion at the EC on Monday (Minute 2.5). Chairman Harvey reported on the following items:

- Changes to Major Activities and Products of IAPWS. Additions will be made in the Statutes and By-Laws to include up-to-date products and activities. This was originally in 2011 directed towards the PCC Technical Guidance Documents, but discussion by the EC required a little broader coverage (activities with seawater for instance).
- Finances. The requirement for IAPWS to hold a Swiss Bank account disappeared in 2009 when the Swiss banking laws changed. Changes to the Statutes and By-Laws will be made to indicate that the Swiss Franc remains the currency of IAPWS, but that IAPWS business will be conducted in a currency of convenience for the Executive Secretary with approval from the EC. IAPWS Dues will be in the currency of convenience converted from Swiss Francs at the exchange rate on 1st Janaury of that year.
- <u>Associate Members</u>. A clear distinction will be made in the Statutes and By-Laws between new and old Associate Members of IAPWS.
- <u>ICRNs</u>. The time period for existence of ICRNs will be increased to five years with flexibility for a shorter period if a WG or SC requests.
- Acquiring New Members. New writing will be added to the Statutes and By-Laws
 indicating that part of the job description for the President and Executive Secretary is
 to acquire new Members of IAPWS.
- <u>Travel for Officers and WG Chairmen</u>. The consensus of the EC was that there already is coverage in the Statutes and By-Laws for providing support to WG Chairmen and others for making visits to other associations and meetings to represent IAPWS, and to promote further activities of IAPWS. The Executive Secretary can provide funds up to a threshold with approval of the EC.
- Procedure for Changing the Statutes. Currently changing the Statutes can only be accomplished at a General Meeting and this makes it difficult to respond quickly. The initial suggestion from the Committee was to recommend changing the Statutes provisionally at an EC annual meeting with a 2/3 vote of EC members present. This would become final at the second annual EC again by a 2/3 vote. Activity at a GM would then become informational. This then lead to extensive EC discussion which included a 3/4 vote instead of 2/3, provisional versus permanent changes, and absentee EC members. Finally the Executive Secretary requested the following two part motion be considered by the EC. First there will be an advanced circulation to EC members of suggested changes to the Statutes and By-Laws by the Executive Secretary. Secondly at the EC meeting a 3/4 vote of members is required for approval.

The EC Approved this Motion Unanimously.

Harvey indicated that the changes will be drafted, and then the Executive Secretary will circulate the suggested revised Statutes and By-Laws to the EC. If further comments are received there may be two iterations prior to a vote at the EC meeting before the 16th ICPWS in London. The decision will be provided to the GM.

A final request from the EC was that the Statutes committee review the IAPWS Mission Statement to ensure that it reflects the actual current work activities of IAPWS.

18.3 Press Release

The President mentioned that Bellows and Joy had been asked on Monday to develop a Press Release. A "Highlights" had been developed with input provided by each WG and SC. The President asked bellows to circulate it to the WG / SC Chairmen to finalize it. The final version is contained in Attachment 10.

18.4 Other New Business

President Daucik asked the EC if there was any further business. No other business was raised.

18.5 Reports from National Committees.

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:

BIAPWS Attachment 11
Canada Attachment 12
Czech Republic Attachment 13
Germany Attachment 14
Japan Attachment 15
Russia Attachment 16
USA Attachment 17

18.6 Participants

Attachment 18 provides a list of participants at the IAPWS EC and WG Meetings and at the Symposium in Boulder, Colorado, October 2012.

18.7 List of Members

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

19. Closing Remarks and Adjournment

The President thanked Friend and his US NC colleagues for hosting the IAPWS Boulder Meetings. He also thanked everybody for participating at this EC meeting. Then he formally closed the 2012 EC meeting at 12:30pm.

AGENDA for the EXECUTIVE COMMITTEE of IAPWS

Boulder, Colorado. 30th September – 5th October 2012

Monday, 1st October 2012. Opening Session (8:30 – 9:30am)

Opening Remarks and Welcome by IAPWS President, K. Daucik

- 1. Adoption of Agenda
- 2. IAPWS Business and Appointment of Committees
 - 2.1 Releases, Advisory Note, ICRNs and Technical Guidance Documents
 - 2.2 Press Release
 - 2.3 Evaluation Committee on International Collaboration
 - 2.4 IAPWS Awards Committees for 2013 (Honorary Fellow, Gibbs, Helmholtz)
 - 2.5 Report on Committee for IAPWS Statutes and By-Laws. (2011 Minute 17.2))
 - 2.6 16th ICPWS (business activities during the IAPWS week)
 - 2.7 Report on BIPM/CIPM and SCOR IAPSO Interfaces and Future Support for Similar Meetings
 - 2.8 Other business requiring special/extensive discussions
- 3. EC Mandate to Working Groups and Membership
 - 3.1 Releases, Guidelines and ICRNs
 - 3.2 WG Directions
- 4. Preview of Week's WG Activities by WG Chairmen

Friday, 5th October 2012. Executive Committee Meeting. (8:30am – 1:00pm)

- 5. Acceptance of Minutes of Previous Meeting
- 6. President's Report
- 7. Report and Recommendations of TPWS, IRS and the Sub-Committee on Seawater
- 8. Report and Recommendations of IRS
- 9. Report and Recommendations of the Sub-committee on Seawater
- 10. Report and Recommendations of PCAS
- 11. Report and Recommendations of PCC
- 12. Editorial Committee Report
- 13. Membership and Associates
 - 13.1 Report on Membership. Including Members Defaulting on Dues.
 - 13.2 Report on Associate Members, Australia, New Zealand, France, Switzerland and South Africa
- 14. Executive Secretary's Report
 - 14.1 Financial and Auditors
 - 14.2 Time and Place of 2013/2014/2015 Meetings.
 Includes BIAPWS's Update on the 16th ICPWS in 2013
- 15. Guidelines, Releases, Certified Research Needs, and International Collaborations
 - 15.1 International Collaborations
- 16. IAPWS Awards
 - 16.1 Helmholtz Award Committee
 - 16.2 Honorary Fellowship
 - 16.3 2013 Gibbs Award
- 17. Election of Officers for 2013 and 2014

- 18. New Business
 - EC Preparation for 16th ICPWS IAPWS Statutes and By-Laws 18.1
 - 18.2
 - 18.3 Press Release
 - Other items raised during the IAPWS week 18.4
- 19. Adjournment



Schedule of IAPWS Meetings Boulder, Colorado. 30th September – 5th October 2012

(All meetings will be at the Millennium Harvest House Hotel)

Sunday 30 Sept.	6:00 pm	Informal Get-together and Registration
	(Loca	tion will be at the Millennium Harvest House Hotel)

Monday 1 Oct. 8:30am. Opening Plenary Session - Executive Committee

10:00am TPWS/IRS/SCSW 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/IRS/SCSW Joint Meeting

1:30pm. PCC and PCAS Separate WG Meetings

Tuesday 2 Oct. 8:30am. PCAS Workshop (other WG Members will be welcome)

8:30am PCC Workshop (other WG Members will be welcome)
8:30am. TPWS/IRS/SCSW Joint Working Group Meeting

10:30am. TPWS/IRS/SCSW Joint Meeting. PCC, PCAS Separate Meetings

1:30pm TPWS/IRS/SCSW Joint Meeting.

1:30pm PCC/PCAS Joint WG Meeting and Workshop

3:30pm PCC and PCAS Separate Meetings

Wednes. 3 Oct. 9:00-4:00 **IAPWS Symposium.**

The Energy-Water Nexus: Status and Prospectus

(Location will be at Millennium Harvest House Hotel)

Thursday 4 Oct. 8:30am. IRS, SCSW and PCC Separate WG Meetings

8:30am. TPWS/PCAS Joint WG Meeting

WG Chairmen: A. Harvey and M. Nakahara

1:30pm. Separate meetings of Working Groups

(If needed to prepare for Executive meeting)

6:00 pm. **IAPWS Dinner/Banquet**.

(Red Lion Inn, Boulder)

Friday 5 Oct. 8:30am. Executive Meeting (8:30am - 1:00pm)

(Will include at least one member from each National Delegation)

1:30 – 4:00 pm Technical visit to NIST and NOAA

TPWS - Thermophysical Properties of Water and Steam WG

SCSW - Subcommittee on Seawater

IRS - Industrial Requirements and Solutions WG

PCAS - Physical Chemistry of Aqueous Solutions WG

PCC - Power Cycle Chemistry WG

Barry Dooley 21st September 2012



THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM (IAPWS) SYMPOSIUM

The Energy – Water Nexus: Status and Prospectus October 3, 2012, 9:00 – 16:00

Flagstaff Ballroom, Millennium Harvest House Hotel, Boulder, CO - USA

Co-organized by the American Society of Mechanical Engineers (ASME) Chair – Richard T Jacobsen (Idaho State University) Co-Chair – Michael Tinkleman (ASME)

Schedule 9:00 – 9:10	Welcome and Helmholtz Award ¹ presentation (Karol Daucik, IAPWS President)
9:10 – 10:00	Helmholtz Award Lecture: Prof. Maxim Federov, Strathclyde University, "Molecular theory of liquids: approaching chemical accuracy"
10:00 – 10:20	Coffee break
10:20 – 10:45	ASME Energy – Water Nexus Research Activities Dick Jacobsen, Michael Tinkleman, ASME
10:45 – 11:30	<u>KEYNOTE</u> - Michael Hightower, Sandia National Laboratories The Energy – Water Nexus: Status and Prospectus
11:30 – 12:15	Shahid Chaudhry, California Energy Commission New and Emerging Desalination Technologies
12:15 – 13:30	Lunch
13:30 – 15:30	Afternoon Session
13:30 – 14:00	Larry Schimmoller, CH2M Hill, Denver, Colorado The Use of Reclaimed Municipal Wastewater for Cooling and Process Water at Power Plants
14:00 – 14:30	Pavel Gotovtsev, Moscow Power Engineering Institute Water management at thermal power plants. Reuse of water and zero-liquid discharge at existing and new power plants
14:30 – 15:00	Andrew Howell, Xcel Energy, Henderson, Colorado Parallel Wet-Dry Cooling at a 750-MW Coal-Fired Supercritical Unit
15:00 – 15:30	General discussion and wrap-up
15:30 – 16:00	Coffee break

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¹ The IAPWS Helmholtz Award is given each year to an early-career scientist or engineer working in an area related to the purposes of IAPWS.

Minutes

IAPWS Thermophysical Properties of Water and Steam WG IAPWS Subcommittee on Seawater (SC SW)

Boulder, Colorado, USA, October 1-4, 2012

NOTE: These Minutes include many items that were held jointly with the IRS Working Group and/or the Subcommittee on Seawater (SCSW) and/or the Working Group PCAS. Items are listed according to their order on the TPWS agenda, which is Attachment A. **Bold print** denotes significant actions.

- 1-2. The meeting was opened on Monday morning, October 1 by the TPWS Chair, Allan Harvey. The agenda (Attachment A) was adopted after minor additions (attachment reflects additions). The Chair noted that, in accordance with our procedure, the 2011 Minutes had been circulated and approved with minor corrections shortly after the 2011 meeting. Jan Hrubý was appointed Clerk of Minutes for TPWS. Michael Hiegemann was appointed Clerk for SCSW.
- 3. M. Kunick (speaker) and H.-J. Kretzschmar demonstrated access to a password-protected website for documents and presentations of the TPWS and IRS Working Groups and the SCSW. The site is accessible from the Working Groups page on www.iapws.org.
- 4. A. Harvey described the proposed international collaborations. The first proposal concerns the viscosity of ammonia-water mixtures. The proposed project should be carried out by a young Russian scientist hosted in the US. The proposed length of the stay was 6-7 months and IAPWS funding was proposed as USD 20,000. The second proposal concerns work toward a new thermodynamic formulation of the properties of heavy water. The proposed project would be carried out by a young German scientist hosted in the US. The proposed length of the stay was about 4 months with cost 7500 USD.
- 5. R. Feistel reported on the "Guideline on a Low-Temperature Extension of the IAPWS-95 Formulation for Water Vapor". Addition of a few terms allows extension of the ideal-gas part of the IAPWS-95 down to 50 K. The proposed IAPWS has completed Working Group review, review by the Editorial Committee, and it has been circulated to National Committees. No objections were raised. A. Harvey presented a test report prepared by K. Miyagawa and F. Blangetti. The test report confirmed the validity of the suggested low-temperature extension. Sublimation vapor pressures computed using the low-temperature extension and the Revised Release on the Equation of State 2006 for H₂O Ice Ih agree with sublimation pressures obtained from the Revised Release on the Pressure along the Melting and Sublimation Curves of Ordinary Water Substance within the stated uncertainties. The working Groups TPWS and SCSW voted to approve the Guideline on a Low-Temperature Extension of the IAPWS-95 Formulation for Water Vapor and to recommend its adoption by the EC.
- 6. W. Wagner reported on editorial changes to the IAPWS-95 and IAPWS-IF97 documents. First change concerns clarification of the limit of validity of Eq. (18) of the IF-97 describing thermodynamic properties of metastable steam. **The Working Groups TPWS and IRS voted to approve the editorial change.** The second editorial change concerned a statement that the IAPWS-95 formulation can be used for computing the properties of water vapor also in a temperature range

down to 130 K. The ideal-gas part (even without the Low-Temperature Extension) is valid in this range. W. Wagner demonstrated that the second virial coefficient and the compressibility factor at saturation show physically correct behaviors (although they are purely extrapolations). The magnitude of the deviations from the ideal behavior is so small that the IAPWS-95 formulation can be considered as valid also in this region. **The Working Group TPWS voted to approve the proposed editorial changes.**

- 7. W. Wagner reported on the behavior of the IAPWS-95 formulation in the liquid region of water near the melting line at high pressures. In a recent article, extrapolated behavior of the IAPWS-95 formulation was tested in the range of supercooled water between 200 to 300 K and 0.1 MPa to 400 MPa. It was stated that the behavior of IAPWS-95 in this region is not in accord with recent data by Mishima (2010). However, the supercooled region is not included in the range of validity of IAPWS-95 and, therefore, the IAPWS-95 formulation cannot be blamed of wrong predictions in this region. W.W. further demonstrated that IAPWS-95 agrees with recent data in the vicinity of the melting line within the uncertainties stated in the IAPWS-95 release. Deviations in expansivity and isobaric heat capacity at pressures above 100 MPa will require further analysis.
- R. Feistel stated that with respect to the new data for the supercooled water at elevated pressure it was necessary to reconsider the IAPWS-95 properties in the metastable region of seawater freezing point lowering. A task group was formed. Members are: J. Hrubý (chair), M. Anisimov, R. Feistel, O. Hellmuth, V. Holten and W. Wagner
- 8. Industrial Requirements and Solutions for Steam Property Calculations: this item is reported on in the Minutes of the WG IRS.
- 9. Advisory Note on the Properties of Sea Water for Industrial Use: **This item is reported on in the Minutes of the WG IRS.**
- 10.1-10.3 Recent Measurements of Seawater Properties (R. Feistel, J. Safarov). New data for density of seawater at high pressures and temperatures (up to S_A =55 and T=195°C) is available. In the discussion it was found necessary to establish a new Task Group with two goals: 1. Extension of the existing Gibbs formulation to higher temperatures, salinities and pressures, 2. Defining the formal position of the extended formulation with respect to the TEOS-10 formulation (either by replacing it with an improved formulation, or the addition of a correction in this new part of parameter space. The members are: R. Feistel (chair), J. Cooper, A. Harvey, M. Hiegemann, J. Hrubý. H.-J. Kretzschmar, R. Pawlowicz.
- 11.1 R. Feistel presented a report by P. Spitzer concerning a EURAMET Project on the metrology for oceanic salinity and acidification. One of its main topics is establishing SI traceability of practical salinity based on density standards. Further topics are: SI traceability of pH measurements, extension of measurement ranges, in particular for the speed of sound. Refractive index of seawater is not yet considered mature. It is desirable to have a formulation for the refractive index of seawater in IAPWS.
- 11.2 A. Anderko (speaker) and A. Harvey reported on the activities of the Task Group "Transport Properties of Seawater". A model for multicomponent salt solutions was developed, applied to seawater and compared with experimental data. During the past year the reference pure-water equation was replaced by the new formulation of thermal conductivity of ordinary water. The plan is to prepare a draft IAPWS guideline for thermal conductivity of seawater about by March 2013. An

Evaluation Task Group was established consisting of K. Miyagawa and F. Blangetti (subject to his acceptance). M. Hiegemann made a comment that it was desirable to develop a model for seawater viscosity in the near future.

- 11.3 Rich Pawlowicz reported on high temperature and high salinity electrical conductivity of seawater. The PSS-78 standard can be used at high salinities and temperatures with an error of 1 to 2%. (In the Neptunian range less than 0.006%). In response to questions, he mentioned that he felt it would be premature to make an IAPWS recommendation at this stage, since the results were only supported by numerical modelling.
- 11.4 R. Feistel reported on various definitions of relative humidity: relative vapor mass, mixing ration, relative specific humidity, relative vapor mole fraction, relative fugacity, IUPAC/ASHRAE, pure-vapor, extended/pragmatic. Although the various definitions give similar values, they are all mutually inconsistent. It is still an open question which definition will be adopted by the different communities. There was a debate whether the focus should be on physics (fugacity-based RH) or application-oriented RH definition. Problems may occur in the adoption by certain communities if fugacity-based RH is used. One role for IAPWS may be to provide relations between existing definitions.
- 11.5 R. Feistel (speaker) and A. Harvey reported on the effect of air dissolution in water and seawater. He proposed an extension of the TEOS-10 by adding an extra term to the Gibbs function reflecting the dissolved air contribution.
- 11.6 H. Uchida on Reference Materials for Dissolved Oxygen (DO) and S_A (Absolute Salinity). There is a lack of inter-laboratory comparability in DO data. He reported on systematic differences between absolute salinity values calculated based on the practical salinity using different methods. He reported on the development and manufacturing of a new aluminum bottle for sample distribution. Further he reported on sample preparation. Hydrostatic weighing method is being developed.
- 11.7 R. Pawlowicz (speaker) and R. Feistel reported on the salinity and density of freshwaters. He presented several options for the classification of freshwaters. Typically 8 major ions (plus nitrate and silicic acid) are present in freshwaters. He used numerical modeling for electrical conductivities and densities. He suggested an method whereby the seawater algorithms (TEOS-10) can be adapted for use in freshwaters. Using PSS-78 to remove temperature and pressure dependence of conductivity, scale Sp with respect to the characteristic chemistry of the particular freshwater. After scaling the practical salinity properly, density excess to the pure water density can be estimated using TEOS-10 with an accuracy of 10%.

12. Cooperation with other international bodies

- 12.1 R. Pawlowicz informed on the adoption of TEOS-10 by scientific community: www.teos-10.org: since October 2010 12,000 visits and 1,600 downloads. The formulation was implemented in visualization software, industry and numerical models, numbers of cited reference to key papers were given from both Web of Science and Google Scholar, anecdotal evidence given about TEOS-10 awareness.
- 12.2 R. Pawlowicz made a proposal for a "Joint SCOR/IAPSO/IAPWS Committee on the Properties of Seawater". Proposed the Terms of Reference, the executive (R. Pawlowicz, chair, T. McDougall, vice-chair, R. Feistel, vice-chair), and a preliminary member list. He noted that SCOR

may provide a limited financial support to the Committee. The Working Groups endorsed the proposal and recommend it be approved by the EC.

- 12.3-4 R. Feistel reported about contacts with BIPM. He visited BIPM and discussed in particular the climate aspects of standards for water, seawater, ice and humid air. They also discussed the salinity measurements not being traceable to the SI, lack of proper ocean pH measurements. R. Feistel stated that the key process of terrestrial climate is the sea-ice-air interface exchange. Cooperation of several institutions: BIPM and WMO have a Mutual Recognition Agreement (Geneva 2010), further institutions may include IUPAC, IAPWS, IAPWSO. A Task Group was formed in Pilsen. An IAPWS delegation travelled to Paris to discuss the possibilities of future cooperation. The outcome of the visit: A position paper (in preparation) will describe the aims, tasks and benefits of the intended BIPM/IAPWS cooperation. An IAPWS representative will be officially invited to participate in BIPM Consultative Committees. R.F. attended CCQM (Consultation Committee on the Amount of Substance) and CCT (Consultation Committee on Thermometry) meetings positive response to the cooperation proposal. WG2 (contact thermometry), WG6 (humidity), WG9 (thermophysical quantities). IAPWS sent an Invitation Letter to CCT to the 16ICPWS in 2013. During the workshops, the further procedures will be discussed.
- 12.5 R. Pawlowicz proposed editorial changes in the Release on the IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater, since recommendations on nomenclature for salinity have been developed since this was released. In particular the term "salinity" should be used only in cases when it is not related to a particular numerical value. Otherwise it must be specified, e.g. Absolute Salinity or Practical Salinity according the definitions which are part of TEOS-10. To clarify the meaning, editorial changes will be done in the Release by a Task Group consisting of R. Feistel, R. Pawlowicz, D. Friend and T. McDougall.
- 13. Properties of Supercooled Water, joint with PCAS and SC SW.
- V. Holten (speaker), M. Anisimov, J. Sengers presented a report "Towards a Guideline for the thermodynamic properties of supercooled water". V.H. presented a formulation of thermodynamic properties of supercooled water based on the two-state mixture model of water. The formulation is valid in the region of supercooled water up to pressure of 400 MPa. The formulation included a noncritical background Gibbs function and a mixture part. The proportion of the two states of liquid water – low density and high density – corresponds to the minimum of the Gibbs function. The new formulation was proposed to be matched to the IAPWS-95 near the melting curve, but it would result in jumps in properties, in particular for isobaric heat capacity. A smoother connection is possible at somewhat higher temperatures. The developed equation represents the density data within their uncertainties. For isobaric heat capacity data at atmospheric pressure, the predictions lie between the mutually inconsistent data. V.H. mentioned an unclear uncertainty of the expansivity data by Ter Minassian et al. (1981). Expansivity by Asada et al. (2002) are in accord with Ter Minassian. V.H. suspected that thermodynamic properties (in particular isobaric heat capacity and expansivity) derived by Lin and Trusler from their speed-of-sound data have substantially higher uncertainties than stated by the authors. W. Wagner suggested that the presenters contact Trusler and clarify the uncertainties of their speed of sound measurements and the derived properties. Formation of a Task Group was considered in the discussion. It was found that a Task Group is already established concerting a related topic (item 10). K. Watanabe suggested leaving the clarification of these issues with the Maryland group before proceeding to formulation of an IAPWS Guideline.

- 13.2 Surface tension of supercooled water. J. Kalová reviewed the existing literature data and correlations for the surface tension of supercooled water. R. Mareš reported on the measurements of the surface tension of supercooled water performed at the University of West Bohemia in Pilsen. The measurements were performed using the capillary rise method. The measurements extend from 2°C down to -25°C. The liquid meniscus was exposed to air. V. Vinš (speaker) and J. Hrubý reported on independent measurements from -24 to 37°C performed at the Institute of Thermomechanics AS CR in Prague. The liquid meniscus was exposed to helium. Both the Pilsen and Prague data sets almost coincide with extrapolated IAPWS formulation of surface tension of ordinary water. The existence of an inflection point is not supported by the new data.
- 13.3 Olaf Hellmuth reported on atmospheric ice formation: questions of interest to IAPWS. He applied the classical nucleation theory to heterogeneous nucleation in clouds. At temperatures above 240 K, nucleation of ice is heterogeneous (it occurs about 12-20 K higher than the homogeneous nucleation). Mineral dust or metallic particles (e.g. condensed vapors evaporated from meteorites), serve as heterogeneous nuclei. The rate of heterogeneous nucleation in the supercooled solution depends on many parameters, in particular on the contact angle of the ice nucleus on the heterogeneous particle: "Icephilic" and "Icephobic" substrates. Densities and melting enthalpies and vapor-liquid surface tension are available, problematic estimation of solution/ice, solution/substrate and ice/substrate interface energies. O.H. made a call for collaboration between meteorological community and IAPWS. He suggested establishing a Task Group to work on the interfacial phenomena of aqueous solutions and related subjects; a group of interested people agreed to meet with him later in the week.
- 14. Molecular Simulation and Modeling: this item is reported on in the Minutes of PCAS.
- 15. Reports on Completed IAPWS Collaborative Projects
- 15.1 V. Vinš presented a report on "Development of Thermodynamic Models for Hydrates in Water–Carbon Dioxide Mixtures" resulting from a collaboration between the Czech Republic and Germany.
- 15.2 I. Abdulagatov presented a report on "Experimental Study of the Thermal Conductivity of Ammonia+Water Refrigerant Mixtures at Temperatures from 278 K to 356 K and at Pressures up to 20 MPa resulting from a collaboration between Russia and the US.
- 16. D. Fuentevilla (speaker), J. Sengers and M. Anisimov reported on the new formulation for the critical locus of aqueous solutions. D.F. presented the phase diagram of water-NaCl system. No new data appeared since the acceptance of the original IAPWS Guideline in 2000. Kim and Fisher (2001) developed a theoretical approach. Their theory was revisited and additional terms were obtained. A. Harvey reported test results by the Evaluation Task Group (K. Miyagawa, A. Harvey). The representation of the experimental data is at least as good as by the previous correlation. The new correlation has a sound theoretical basis in contrast to the original one, which was a purely empirical correlation. The Working Group TPWS endorsed the Revised Guideline and recommends that the EC sends it for Postal Ballot after review by the Editorial Committee.
- 17. R. Span (speaker) and A. Harvey reported on the properties of CO₂/H₂O and related systems relevant in particular to the Carbon Capture and Sequestration. International cooperation including TPWS members as well as colleagues outside IAPWS was established. In preparation are measurements of thermodynamic properties (pvT, w), phase equilibria (VLE, LLE, VLSE), transport

properties (viscosity). Accurate property models for CO₂-rich mixtures and phase equilibria including solid phases will be developed. Phase equilibrium algorithms will be improved, the new property models will be tested for various applications. Relevant systems are mixtures of CO₂, N₂, O₂, Ar, CO, H₂O. Considered components are covered by the GERG equation of state, however the main focus of GERG is natural gas modeling. Further components: SO₂, NO₂, H₂S. Finalization of mixture model needs at least another five years. Workshop is planned in Bochum, R.S. invited interested researchers.

- 18. Discussion of 16th ICPWS 2013 in London: No further suggestions were given.
- 19. Reports on Other TPWS, IRS and SC SW Activities
- 19.1 A. Harvey reported on the Guideline on Fundamental Constants. Small revisions were done in 2002, 2005, 2008, reflecting the adoption of universal constants and atomic weights. 2012 revision reflects newly recommended values of the fundamental physical constants by Mohr et al. 2012 (simultaneously in Rev. Mod. Phys. and J. Phys. Chem. Ref. Data, in press). **The working groups TPWS, IRS and SCSW adopted the revision.**
- 19.2 J. Hrubý reported on proper incorporation of systematic experimental uncertainties in thermodynamic models based on regression and realistic uncertainties of predicted values. Systematic uncertainties generate covariances of experimental data. Method of uncertainty estimation using the full covariance matrix and the generalized least squares method were introduced. Their applicability was demonstrated on the saturation pressure equation by Wagner and Saul (1986), which is part of the Revised Supplementary Release on Saturation Properties of Ordinary Water Substance. It was shown that realistic uncertainties of predicted pressures can be obtained when systematic errors are included, whereas considering the uncertainty as purely random leads to unrealistically low uncertainties.
- 19.3 M. Duška (speaker) and J. Hrubý presented some remarks on re-evaluation of thermodynamic data for steam at low pressures. pvT data, Joule-Thomson coefficient and speed of sound were considered for evaluation of the second virial coefficient. At low temperatures, the experimental uncertainties are too large which makes the extrapolation into the metastable steam region unreliable.
- 19.4 J. Hrubý (speaker) and A. Harvey reported on the status of ideal-gas properties for ordinary and heavy water. Present formulations for ordinary water are based on data by Woolley (1980) and for the heavy water on Friedman and Haar (1954). There is a space for improvement. Specroscopist groups of J. Tennyson (London) and A. Csaszar were contacted. Preliminary data for isobaric heat capacity of H₂¹⁶O were provided in the range from 0 to 1199 K. Large differences of the new data from Woolley (1980) below 50 K are due to a different treatment of the ortho and para waters. About above 800 K, deviation is increasing, but it remains within stated uncertainty of the IAPWS-95 formulation. The spectroscopist groups were asked to provide data at least up to 6000 K and also data for other isotopologues forming the ordinary water and heavy water isotopic mixtures.
- 19.5 A. Harvey (speaker) and E. Lemmon reported on the status of D₂O properties. Current (1984/2005) IAPWS D₂O release is based on IPTS-68 (adjusted in 2005), equation has 50 terms (new fit probably down to 15 or 20 terms), extrapolation to high temperature shows an unphysical behavior, incorrect behavior of cp near the critical point. New data are available. Collaboration project between Ruhr Universität Bochum and NIST was suggested. In the discussion it was suggested that the region of supercooled heavy water should be described in accord with the latest knowledge. A task group dealing with thermophysical properties of D₂O was established: A. Harvey (chair), J. Cooper, V. Holten, E. Lemmon [co-opted expert], R. Span.

- 19.6 A. Harvey asked whether any changes of IAPWS Statutes and By-Laws were suggested specific for these Working Groups. No suggestions were given.
- 19.7 V. Ochkov (speaker), K. Orlov, and G. Kondakova reported about live calculations linked from IAPWS website. The linked site provided by Russian National Committee enables online computations using IAPWS formulations. A useful feature for program developers is that intermediate computation results are shown besides the final results. In a short discussion it was reminded that IAPWS by decision of the EC does not provide software. However, it is desirable to have links to web sites allowing online computations and software download.
- 19.8 M. Kunick (speaker) and H.-J. Kretzschmar reported on Steam Tables for Excel®, Mathcad®, MATLAB, smart phones and Pocket Calculators for Education. A link is provided on the IAPWS Website.
- 19.9 Task Group concerning the uncertainties of IAPWS 95: W. Wagner was appointed to consider possible changes in estimates of uncertainties of the IAPWS-95.
- 20. Other Business
- 20.1 Report on International Collaborative Projects
- V. Holten presented a preliminary report (item 13.1.)
- V. Vinš presented his final report (item 15.1) and a short written report was sent to the Executive Secretary.
- I. Abdualgatov presented his final report (item 15.2) and a short written report was sent to the Executive Secretary.
- 20.2 Report on ICRNs

The status of existing ICRNs was reviewed.

ICRN 21 (Properties for ultra supercritical power plants) is expiring and it was recommended that it be closed.

ICRN 24 (High temperature thermal conductivity of water vapor) was recommended to be extended for another 3 years after a minor revision.

During 2012, a new ICRN 28 (Metastable steam and nucleation) was adopted.

- 21. Membership and chairmanship
- 21.1 **Prof. Maxim Fedorov** (University of Strathclyde) and **Dr. Vincent Holten** (University of Maryland) were **adopted as TPWS members unanimously**.
- 22.2 Reiner Feistel stepped down from the chair of the SCSW and will remain a vice-chair. Rich Pawlowicz was elected the new chair. M. Hiegemann remains as another vice-chair.
- 22. Contribution to Press Release

The chair and the clerk of minutes were assigned to prepare the contribution to the Press Release.

23. Preparation of the Formal Motion to the EC

The chair and the clerk of minutes were assigned to prepare the Formal Motion to the EC.

24. Adjournment

The meeting was adjourned at 4:15 p.m. Thursday October 4.

Agenda for the IAPWS Working Group Thermophysical Properties of Water and Steam (TPWS) Boulder, Colorado, USA, 01-05 October 2012

- 1. Opening Remarks; Adoption of Agenda
- 2. Appointment of Clerk of Minutes
- 3. OPAL Web Space for Working Material for WGs TPWS, IRS, and SC SW, joint with WG IRS and SC SW (H.-J. Kretzschmar)
- 4. Potential International Collaborative Projects
- 5. Guideline on a Low-Temperature Extension of the IAPWS-95 Formulation for Water Vapor, joint with SCSW
 - Report (R. Feistel, W. Wagner)
 - Test Report (K. Miyagawa, F. Blangetti)
 - Formal consideration of the Guideline
- 6. Editorial changes to the IAPWS-95 and IAPWS-IF97 documents, joint with WG IRS
 - Report (W. Wagner, I. Weber)
 - Formal consideration of the editorial changes
- 7. Report on behavior of the IAPWS-95 Formulation in the Liquid Region of Water near the Melting Line at High Pressures (W. Wagner) [Monday PM]
- 8. Industrial Requirements and Solutions for Steam Property Calculations, joint with WG IRS [Monday PM]
 - 8.1 Report of the New Industrial Requirements Task Group (I. Weber)
 - 8.2 Report of the Industrial Survey Task Group (A. Singh)
 - 8.3 Report of the Task Group "Advisory Notes" (M. Hiegemann, W. Parry, B. Rukes, P. Murphy)
 - 8.4 Usage of thermal property calculations in power plant simulations and performance monitoring (R. Pawellek, STEAG Energy Services)
 - 8.5 Modernization Efforts in Steam Properties Modeling for Enhanced Flexibility & Scalability (A. Singh)
 - 8.6 Report of Task Group "CFD Steam Property Formulations" (J. Hrubý, H.-J. Kretzschmar, A. Singh)
 - 8.7 Steam Property Calculations for CFD Applications (A. Singh)
 - 8.8 Formulation of thermodynamic properties of steam for CFD computations based on a global function s(u,ρ) (J. Hrubý, M. Duška, J. Pátek)
 - 8.9 Fast and Accurate Calculation of Thermodynamic Properties Using a Spline-based Table Look-up Method (M. Kunick, H.-J. Kretzschmar, and U. Gampe)
- 9. Advisory Note on the Properties of Sea Water for Industrial Use, joint with WGs IRS and SC SW
 - Report of the Task Group (H.-J. Kretzschmar)

- 10. Extension of Range of Formulation for Thermodynamic Properties of Sea Water, joint with WGs IRS and SC SW
 - 10.1 New Seawater Measurements (R. Feistel, J. Safarov)
 - 10.2 Discussion of data situation
 - 10.3 Discussion of steps toward an extended formulation
- 11. Additional Seawater-related Topics (R. Feistel), joint with SC SW and partly with WG IRS
 - 11.1 EURAMET Project Ocean Metrology on seawater salinity, pH and dissolved oxygen (P. Spitzer)
 - 11.2 Task Group Report "Transport Properties" (A. Anderko, A.H. Harvey)
 Report on future Guideline for seawater thermal conductivity
 Appointment of Evaluation Task Group and setting target dates for steps in IAPWS process for 2013 approval
 - 11.3 Electrical Conductivity of Seawater (R. Pawlowicz, R. Feistel)
 - 11.4 On the Definition of Relative Humidity (J. Lovell-Smith, R. Feistel)
 - 11.5 Air saturation of water and seawater effect on properties (A. Harvey, R. Feistel)
 - 11.6 pH of seawater (P. Spitzer)
 - 11.7 Electrical conductivity and density of Lake and River Waters (R. Pawlowicz, R. Feistel)
- 12. Cooperation with other international bodies, joint with SC SW
 - 12.1 Report on TEOS-10 acceptance by user community (T. McDougall?)
 - 12.2 IAPWS/IAPSO/SCOR Joint Committee on Seawater (R. Pawlowicz)
 - 12.3 Cooperation with BIPM (CCQM and CCT) (R. Feistel, D. Friend, P. Spitzer)
 - 12.4 ICPWS workshops for IAPWS-BIPM cooperation at ICPWS (J. Cooper)
 - 12.5 Cooperation with WMO (P. Dexter?)
- 13. Properties of Supercooled Water, joint with PCAS and SC SW [Tuesday PM]
 - 13.1 Towards a Guideline for the thermodynamic properties of supercooled water (V. Holten (speaker), M. Anisimov, J. Sengers)
 - 13.2 Surface tension of supercooled water (J. Kalova, R. Mareš, V. Vinš)
 - 13.3 Atmospheric freezing processes: Questions of interest for IAPWS (O. Hellmuth)
- 14. Molecular Simulation and Modeling, joint with PCAS [Thursday AM]
 - Valeria Molinero (University of Utah), "Structural transformation in supercooled water controls the crystallization rate of ice"
 - Amadeu K. Sum (Colorado School of Mines), "The structuring of water in the nucleation of clathrate hydrates"
 - Kenji Yasuoka (Keio University), "Melting and Freezing point of rigid water models"
- 15. Reports on Completed IAPWS Collaborative Projects, joint with PCAS [Thursday AM]
 - 15.1 Development of Thermodynamic Models for Hydrates in Water–Carbon Dioxide Mixtures (V. Vinš (speaker), J. Hrubý, R. Span)
 - 15.2 Experimental Study of the Thermal Conductivity of Ammonia+Water Refrigerant Mixtures at Temperatures from 278 K to 356 K and at Pressures up to 20 MPa (I. Abdulagatov (speaker), M.L. Huber, F.N. Shamsetdinov)

- 16. Critical locus of aqueous solutions of sodium chloride, joint with PCAS [Tuesday PM]
 - Report (D. Fuentevilla (speaker), J. Sengers, M. Anisimov)
 - Test Report (K. Miyagawa, A. Harvey)
 - Formal consideration of the Guideline
- 17. Properties of CO₂/H₂O and related systems, joint with WG IRS (R. Span, A. Harvey)
- 18. Discussion of 16th ICPWS 2013 in London, joint with WG IRS and SC SW (J. Cooper and WG Chairs)
- 19. Reports on Other TPWS, IRS and SC SW Activities
 - 19.1 Guideline on Fundamental Constants (A. Harvey), joint with WG IRS and SC SW
 - 19.2 Proper incorporation of systematic experimental uncertainties in thermodynamic models based on regression and realistic uncertainties of predicted values (J. Hrubý)
 - 19.3 Remarks on new data and re-evaluation of older data for steam at low pressures (J. Hrubý and M. Duška)
 - 19.4 Status of ideal-gas properties for ordinary and heavy water (A. Harvey, J. Hrubý)
 - 19.5 Status of D₂O Thermodynamic Properties (A. Harvey, E. Lemmon), joint with IRS
 - 19.6 Changes of IAPWS Statutes and By-Laws (A. Harvey)
 - 19.7 Live calculations linked from IAPWS website (V. Ochkov [speaker], K. Orlov, and G. Kondakova)
 - 19.8 Steam Tables for Excel®, Mathcad®, MATLAB, smart phones and Pocket Calculators for Education on the IAPWS Website (H.-J. Kretzschmar, M. Kunick), joint with WG IRS
 - 19.9 Possibility of improving uncertainty estimates of IAPWS-95
- 20. Other Business
 - 20.1 Report on International Collaborative Projects
 - 20.2 Report on ICRNs [Monday or Tuesday]
- 21. Membership
- 22. Contribution to Press Release
- 23. Preparation of the Formal Motion to the EC
- 24. Adjournment

Draft Agenda for the Subcommittee on Seawater (SC SW) Boulder, Colorado, USA, 01-05 October 2012

- 1. Opening Remarks; Adoption of Agenda
- 2. Appointment of Clerk of Minutes
- 3. OPAL Web Space for Working Material for WGs TPWS, IRS, and SC SW, joint with WG TPWS and IRS (H.-J. Kretzschmar)
- 4. Potential International Collaborative Projects
- 5. Guideline on a Low-Temperature Extension of the IAPWS-95 Formulation for Water Vapor, joint with TPWS
 - Report (R. Feistel, W. Wagner)
 - Test Report (K. Miyagawa, F. Blangetti)
 - Formal consideration of the Guideline
- 6. Editorial changes to the IAPWS-95 and IAPWS-IF97 documents, joint with WGs TPWS, IRS
 - Report (W. Wagner, I. Weber)
 - Formal consideration of the editorial changes
- 7. Report on behavior of the IAPWS-95 Formulation in the Liquid Region of Water near the Melting Line at High Pressures (W. Wagner), joint with WG TPWS
- 8. Advisory Note on the Properties of Sea Water for Industrial Use, joint with WGs TPWS, IRS
 - Report of the Task Group (H.-J. Kretzschmar)
- 9. Extension of Range of Formulation for Thermodynamic Properties of Sea Water, joint with WGs IRS and SC SW
 - 9.1 New Seawater Measurements (R. Feistel, J. Safarov)
 - 9.2 Discussion of data situation
 - 9.3 Discussion of steps toward an extended formulation
- 10. Additional Seawater-related Topics, joint with TPWS and partly with WG IRS
 - 10.1 EURAMET Project Ocean Metrology on seawater salinity, pH and dissolved oxygen (P. Spitzer)
 - 10.2 Task Group Report "Transport Properties" (A. Anderko)
 Presentation of draft Guideline for seawater thermal conductivity
 Appointment of Evaluation Task Group and setting target dates for steps in IAPWS process for 2013 approval
 - 10.3 Electrical Conductivity of Seawater (R. Pawlowicz, R. Feistel)
 - 10.4 On the Definition of Relative Humidity (J. Lovell-Smith, R. Feistel)
 - 10.5 Air Saturation of Water and Seawater effect on properties (A. Harvey, R. Feistel)
 - 10.6 pH of Seawater (P. Spitzer)
 - 10.7 Electrical conductivity and density of Lake and River Waters (R. Pawlowicz, R. Feistel)

- 11. Cooperation with other international bodies, joint with TPWS
 - 11.1 Report on TEOS-10 acceptance by user community (T. McDougall/R. Pawlowicz)
 - 11.2 IAPWS/IAPSO/SCOR Joint Committee on Seawater (R. Pawlowicz)
 - 11.3 Cooperation with BIPM (CCQM and CCT) (R. Feistel, D. Friend, P. Spitzer)
 - 11.4 ICPWS workshops for IAPWS-BIPM cooperation at ICPWS (J. Cooper, R. Pawlowicz, P. Spitzer, O. Hellmuth)
 - 11.5 Cooperation with WMO (P. Dexter?)
- 12. Properties of Supercooled Water, joint with PCAS, TPWS [Tuesday PM]
 - 12.1 Towards a Guideline on thermodynamic properties of supercooled water (V. Holton, M. Anisimov, J. Sengers)
 - 12.2 Ice nucleation (J. Kalova, R. Mareš, V. Vinš)
 - 12.3 Atmospheric freezing processes: Questions of interest for IAPWS (O. Hellmuth)
- 13. Critical locus of aqueous solutions of sodium chloride, joint with TPWS, PCAS (D. Fuentevilla, J. Sengers, M. Anisimov) [Tuesday PM]
- 14. Properties of CO₂/H₂O and related systems (R. Span, A. Harvey), joint with TPWS
- 15. Discussion of 16th ICPWS 2013 in London, joint with WG IRS and TPWS (J. Cooper, WG Chairs)
- 16. Reports on Other TPWS, IRS and SC SW Activities, joint with WG IRS and TPWS
 - 16.1 Guideline on Fundamental Constants (A. Harvey)
 - 16.2 Proper incorporation of systematic experimental uncertainties in thermodynamic models based on regression and realistic uncertainties of predicted values (J. Hrubý)
 - 16.3 Remarks on new data and re-evaluation of older data for steam at low pressures (J. Hrubý and M. Duška)
 - 16.4 Status of Ideal-Gas properties for ordinary and heavy water (A. Harvey, J. Hrubý)
 - 16.5 Status of D₂O Thermodynamic Properties (A. Harvey, E. Lemmon)
 - 16.6 Changes of IAPWS Statutes and By-Laws (A. Harvey)
 - 16.7 Live calculations linked from IAPWS website (V. Ochkov, K. Orlov, G. Kondakova)
- 17. Other Business
 - Report on International Collaborative Projects
- 18. Membership
- 19. Contribution to Press Release
- 20. Preparation of the Formal Motion to the EC
- 21. Adjournment

Sept. 28, 2012, R. Feistel (Chair), R. Pawlowicz (Vice-Chair), M. Hiegemann (Vice-Chair)

Meeting Notes for the IAPWS Working Group Industrial Requirements and Solutions (IRS) Boulder, Colorado, USA, 01 - 05 October 2012

- 1. Opening Remarks; Adoption of Agenda Agenda was unanimously accepted.
- 2. Appointment of Clerk of Minutes
 - A. Singh was unanimously appointed as the clerk of minutes.
- 3. OPAL Web Space for Working Material for WGs TPWS, IRS, and SC SW, joint with WG TPWS and SC SW (H.-J. Kretzschmar)

 See TPWS meeting notes.
- 4. Potential International Collaborative Project See TPWS meeting notes.
- 6. Editorial changes to the IAPWS-95 and IAPWS-IF97 documents, joint with WG TPWS
 - Report (W. Wagner, I. Weber)
 - Formal consideration of the editorial changes

See TPWS meeting notes

- 8. Industrial Requirements and Solutions for Steam Property Calculations, joint with WG TPWS
 - 8.1 Report of the New Industrial Requirements Task Group (I. Weber)
 - A. Singh reported on some new requirements that covered the needs in areas such as dynamic and transient simulations, plant optimization & control, in-house or proprietary tool usage. The major theme was speed, consistency and robustness of the steam properties.
 - 8.2 Report of the Industrial Survey Task Group (A. Singh)
 - A. Singh presented a proposal for an industrial survey. The proposal was discussed and the following steps were defined:
 - Singh will prepare a draft questionnaire, distribute it among IRS and collect comments
 - Weber will prepare an introduction section with some background information for recipients not familiar with IAPWS.
 - The survey should be limited to 10 questions and clearly state that any further distribution is welcome

- When the final questionnaire is available the survey will be distributed to IRS
 members and the national committees of IAPWS for further distribution to
 companies not involved in IAPWS business, and also to companies in other countries
- 8.3 Report of the Task Group "Advisory Notes" (M. Hiegemann, W. Parry, B. Rukes, P. Murphy)

M. Hiegemann discussed the requirements for the task group and went over current advisory notes (4 in total – details of each advisory notes can be found in the slides presented). It was concluded that these notes are considered necessary, seems ok in language and needs minor editorial changes for the correctness of names, addresses etc.

Advisory note 2 doesn't mention any document related to transport properties and question was posed if this is ok. The completeness of references is essential.

Advisory note 4 is in a subpage of the respective webpage. It was proposed that the content be made part of the note itself instead of providing separately in the webpage.

It was recommended that Advisory note 2 should be updated to include transport properties and also change the title of the note to say thermo physical properties (instead of thermodynamic properties) and also include details for the additional properties in the note. Advisory note 3 should also be updated as necessary.

I. Weber put the question on the general ownership of these documents. After discussion it was decided that the question should be put forth to the EC to get a clear direction or decision on it

Later in the joint TPWS and IRS meeting, M. Hiegemann presented the material again to the joint audience. Extended discussions on advisory note 2 and if transport properties should be included or not as proposed. J. Cooper suggested that it's not needed in this case and A. Harvey extended and agreed that we shouldn't include. M. Hiegemann referred to the book by Wagner and potential conflicts due to differences in standards and a lack of completeness. J. Cooper agreed to the issue, and proposed if a table listing all documents would suffice. J. Sengers & A. Harvey pointed that in some sense we already have a web page listing all this. J. Sengers suggested that this requires some more discussion. A. Harvey agreed. I. Weber suggested continuing the Task Group to look into these suggestions. A. Harvey was added to the task group as a member.

- 8.4 Usage of thermal property calculations in power plant simulations and performance monitoring (R. Pawellek, STEAG Energy Services)
- R. Pawellek from STEAG Energy services gave a demo of their plant modeling tool Ebsilon He demonstrated some complicated cycles such as solar and district heating and transient simulations of a plant. At the moment transient modeling is achieved as a correction to the steady state solution and is available for limited components only. He pointed that Ebsilon's current implementation achieves very good execution speed; however he expressed a need for faster properties and better precision.

- 8.5 Modernization Efforts in Steam Properties Modeling for Enhanced Flexibility & Scalability (A. Singh)
- A. Singh discussed the modularization efforts that are being done as part of ASME steam property work. This includes rewriting or improving the current wrapper ASME routines to better facilitate inclusion in various tools.
- 8.6 Report of Task Group "CFD Steam Property Formulations" (J. Hrubý, H.-J. Kretzschmar, A. Singh)
- J. Hrubý reported on formulation needs for use in CFD applications. Important issues related to CFD simulations were discussed including, speed, super saturated metastable region, artificial boundaries across regions in current formulation, uncertainty compared with other sources of uncertainty, continuity etc.
- 8.7 Steam Property Calculations for CFD Applications (A. Singh)
- A. Singh continued on discussing the needs for CFD applications and demonstrated some typical applications especially in the metastable region, simulation issues arising out of boundary definitions, comparison with experimental data and simulations based on equilibrium and multi-phase 3D CFD.
- 8.8 Formulation of thermodynamic properties of steam for CFD computations based on a global function $s(u, \Box)$ (J. Hrubý, M. Duška, J. Pátek)
- J. Hrubý gave a detailed overview of developments for an equation of state for use with CFD. He also provided uncertainty comparisons with IAPWS-IF97 & IAPWS95. Questions about comparison of speed/computing time w.r.t. IAPWS-IF97
- 8.9 Fast and Accurate Calculation of Thermodynamic Properties Using a Spline-based Table Look-up Method (M. Kunick, H.-J. Kretzschmar, and U. Gampe)
- M. Kunick described the spline based method, its speed and accuracy comparisons in the validity region and comparison with Tabular Taylor Series Expansion method. He demonstrated the software to generate the spline function tables (FluidSplines). The method overall provides better accuracy and speed. Results of process simulation are not expected to change. It covers wet steam and metastable region and provides numerical consistency.

Following the presentations an extensive discussion on the two approaches for CFD applications ensued and it was decided that the TG will continue to exist and will review available information and development in next year meeting and make a decision. At this point more information is required w.r.t. to benefits and challenges associated with either method.

Additional information on items 8.6 to 8.9:

Later during the week the TG discussed the next steps. If evaluation and testing of the spline interpolation method is successful with no major show stoppers, the TG plans to present a draft guideline on the spline interpolation method for discussion at the 2013 IAPWS meeting.

- 9. Advisory Note on the Properties of Sea Water for Industrial Use, joint with WGs TPWS and SC SW
 - Report of the Task Group (H.-J. Kretzschmar)
 - I. Weber introduced the topic and gave a brief overview and background of the task group covering subjects such as how the task group came into existence, its purpose and it relevance to the subject matter being discussed.
 - H.-J. Kretzschmar presented covering this in more detail that included the motivation for this work, details of proposals and references to Miyagawa's report confirming its usability and correctness of the proposed draft advisory note.

An evaluation TG was recommended to be formed and was unanimously agreed upon by the working groups involved. The evaluation task group would consist of the following members:

I. Weber, A. Singh (Chair), K. Orlov, F. Blangetti

A schedule was also agreed upon as follows:

Dec. 31, 2012 Advisory Note drafted & sent to Evaluation TG

Feb. 28, 2013 Completion of evaluation by Evaluation TG

March 15, 2013 Distribution of Advisory Note and evaluation report to WG

April 15, 2013 Deadline for input from WG members

May 15, 2013 Finalized draft to Editorial Committee

June 15, 2013 Approval by Editorial Committee

Refer to H.-J. Kretzschmar slides available at Opal Webspace (for access details refer to bullet 3).

10. Extension of Range of Formulation for Thermodynamic Properties of Sea Water, joint with WGs TPWS and SC SW

See TPWS notes

- 11. Additional Seawater-related Topics (R. Feistel), joint with SC SW and WG TPWS See SC SW notes
- 17. Properties of CO2/H2O and related systems, joint with WG TPWS (R. Span, A. Harvey)

See TPWS notes

18. Discussion of 16th ICPWS 2013 in London, joint with WG TPWS and SC SW (J. Cooper and WG Chairs)

See TPWS notes

- 19. Reports on Other TPWS, IRS and SC SW Activities
 - 19.1 Guideline on Fundamental Constants (A. Harvey), joint with WG TPWS and SC SW

See TPWS Notes.

19.2 Proper incorporation of systematic experimental uncertainties in thermodynamic models based on regression and realistic uncertainties of predicted values (J. Hrubý)

See TPWS Notes.

19.3 Remarks on new data and re-evaluation of older data for steam at low pressures (J. Hrubý and M. Duška)

See TPWS Notes.

19.4 Status of ideal-gas properties for ordinary and heavy water (A. Harvey, J. Hrubý) See TPWS Notes.

19.5 Status of D2O Thermodynamic Properties (A. Harvey, E. Lemmon), joint with WG TPWS

See TPWS Notes

19.6 Changes of IAPWS Statutes and By-Laws (A. Harvey)

See TPWS Notes

19.7 Live calculations linked from IAPWS website (V. Ochkov [speaker], K. Orlov, and G. Kondakova)

See TPWS Notes

19.8 Steam Tables for Excel®, Mathcad®, MATLAB, smart phones and Pocket Calculators for Education on the IAPWS Website (H.-J. Kretzschmar, M. Kunick), joint with WG TPWS

See TPWS Notes

20. Other Business

20.1 Report on International Collaborative Projects

20.2 Report on ICRNs

ICRN 23 – I. Weber gave an overview, background on the ICRN and presented a progress report on behalf of N. Okita: No additional information on the iranian paper that came out in 2011 could be obtained so far. Therfore it was suggested to close the ICRN. The WG agreed to this, N. Okita will be asked to provide an official closing statement.

21. Membership

H.-J. Kretzschmar nominated R. Pawellek as a new member of IRS WG. R. Pawellek was unanimously accepted as a member of IRS.

- 22. Contribution to Press Release
 - I. Weber agreed to prepare this IRS WG based on the notes and report to J. Bellows.
- 23. Preparation of the Formal Motion to the EC
 - I. Weber will prepare the formal motion to EC
- 24. Adjournment
 - I. Weber adjourned the IRS session at 05-Oct-2012, 16:20 EST

2012 IAPWS Annual Meeting Boulder, CO, USA September 30 – October 5, 2012

PCAS WG Minutes

Present:

Masaru Nakahara (chair) Andre Anderko (vice chair, clerk of minutes) Jana Ehlerova Maxim Federov Frantisek Marsik Tomas Nemec nakahara@scl.kyoto-u.ac.jp aanderko@olisystems.com jana.ehlerova@tul.cz maxim.federov@strath.ac.uk marsik@it.cas.cz nemec@it.cas.cz

Monday, October 1

- 1. **Opening remarks.** Masaru Nakahara presented the meeting agenda (PCAS Attachment A). Andre Anderko was appointed clerk of minutes.
- 2. **PCAS mission and activities.** Masaru Nakahara summarized the group's organizational policy. PCAS will meet for internal discussions in separate meetings whereas most technical presentations and discussions will be carried out in joint meetings with other working groups. The members have summarized their research interests and current activities. Water and aqueous solution interfacial and hydration phenomena were focused on. Light and heavy metal ions and organics like formic acid as well as simple gases were taken as solutes in terms of free energies, equilibrium constants to seek for likely outputs.
- 3. **Membership.** The group welcomed Maxim Fedorov (Strathclyde University, Glasgow, UK) as a new member of PCAS

Masaru Nakahara addressed the issue of deleting inactive members from the PCAS membership list. For this purpose, three criteria have been proposed and accepted by the group. An inactive member will be deleted from the list if (1) they have not participated in the activities of PCAS for a long time (substantially longer than the previously used 3-year period of inactivity), (2) their past contributions (such as creation of releases, guidelines or organizational leadership) cannot be reasonably used to justify their retention or (3) their lack of continued participation is coupled with the associate member status of their home countries. Based on these criteria, seven inactive members have been identified and they are listed in the Appendix. They will be welcome to rejoin the group if they choose to do it.

4. Progress of the PCAS-sponsored project "Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Solutes and Gases". Jana Ehlerova gave the following update:

Over 150 organic solutes and 11 inorganic gases were studied in this work. Data retrieval from literature sources has been finished and hydration properties (in most cases

recalculated from their original format) were entered into the databases. Data processing has been performed. At this point, a paper is being prepared for the Journal of Physical Chemistry Reference Data, to be submitted in November 2012.

There have been no expenditures of IUPAC or IAPWS funds since the last report.

5. Presentation:

Maxim Fedorov, Ions and Interfaces: Understanding of Interfacial Behavior of Inorganic and Organic Ions by a Combination of Molecular Simulation and Experiments

Tuesday, October 2, morning

6. **Joint PCC/PCAS workshop on water and energy chemistry.** The following presentations were given:

David Addison, Areas of key interest for the New Zealand National Committee

Frantisek Marsik, Enhancement of hydrogen fuel cell efficiency by the water surface tension control

Hiroshi Takano, Characterization of oxide films formed on welded surfaces of carbon steel for boiler tubes

Andre Anderko, Modeling the effects of solution chemistry on the localized corrosion of engineering alloys

David Addison, Geothermal power – in brief

Masaru Nakahara, Conversion of carbon dioxide and hydrogen into formic acid for CCS: in ambient water without catalyst

Tuesday, October 2, afternoon

7. **Joint PCAS/TPWS/IRS/SCSW Workshop.** The following presentations were given:

Vincent Holten, Mikhail Anisimov, Jan Sengers, Towards a guideline for the thermodynamic properties of supercooled water

Jana Kalova, Surface tension of supercooled water

Radim Mares, Measurement of surface tension of supercooled water

Vaclav Vins, Measurement of surface tension of supercooled water

Olaf Hellmuth, Atmospheric ice formation: Questions of interest to IAPWS

Daphne Fuentavilla, Revised guideline on the critical locus of aqueous solutions of sodium chloride

Further, the following brief communications about recent developments were given:

Andre Anderko, Progress in the development of thermal conductivity guideline for seawater

Richard Pawlowicz, Definition of salinity

Rainer Feistel, Cooperation with BIPM (CCQM, CCT)

CCQM – Consultative Committee on the Amount of Substance

CCT – Consultative Committee on Thermometry

A task group will be appointed for the evaluation of the anticipated guideline for the thermal conductivity of seawater. Allan Harvey suggested that Kiyoshi Miyagawa could check the guideline. Hans-Joachim Kretschmar suggested Andrew Blanghetti. Allan Harvey will check their availability. Andre Anderko has stated that his target for preparing the guideline is Q1 2013.

Thursday, October 4, morning

8. Joint PCAS/TPWS/IRS/SCSW Workshop. The following presentations were given:

Amadeu Sum, The structuring of water in the nucleation of clathrate hydrates

Valeria Molinero, Structural transformations in supercooled water

R. Sakamaki, A. Sum, T. Narumi, K. Yasuoka, melting and freezing point of rigid water models

Subsequently, reports were given on three collaborative projects that were performed under the auspices of IAPWS:

Vaclav Vins, Progress in modeling H₂O - CO₂ mixtures with gas hydrate formation (collaboration between the Institute of Thermomechanics, Prague, Czech Republic, and Ruhr University, Bochum, Germany)

Ilmutdin Abdulagatov, E.N. Shamsetdinov, Experimental study of thermal conductivity of ammonia – water refrigerant mixtures from 278 K to 356 K and pressures up to 20 MPa.

Jan Hruby and Allan Harvey, New data for thermodynamic properties of water in the ideal gas state.

The following announcements were made:

Olaf Hellmuth presented plans for establishing a working group on interfacial properties in aqueous solutions, including supercooled solutions. A secondary objective of the group is the study of properties that control deliquescence and efflorescence.

Maxim Fedorov announced a "satellite" International Workshop on Molecular Solvation to be held in Glasgow in August or September 2013. A discussion ensued whether it would be worthwhile to hold this workshop before, after, or in conjunction with the 2013 IAPWS conference in London. This remains to be determined.

Thursday, October 4, afternoon

Closing session of PCAS

- **9. Transition in chairmanship.** It is expected that a transition in chairmanship will take place at next year's IAPWS conference. Masaru Nakahara and Andre Anderko will step down as chair and vice-chair, respectively. Masaru Nakahara has proposed Andre Anderko as the new chairman and Josef Sedlbauer Frantisek For vice-chair. Marsik nominated Jana Ehlerova. Josef Sedlbauer accepted the nomination via e-mail and Jana Ehlerova indicated that she would not be available in the near future.
- **10. Presentations.** The following presentations were given:

Tomas Nemec, Classical nucleation theory – cavitation in binary systems

Andre Anderko, Thermodynamic modeling of actinide solution chemistry

11. Mission and focus areas of PCAS. A discussion was held to specify the topics that are of particular interest to PCAS.

In accordance with the PCAS mission, which states:

- 1) To provide critically evaluated thermodynamic and transport property data for solutes and interfaces in high-temperature high-pressure aqueous solutions of interest to the electric power industry, *developers of green technologies*, and other industrial applications.
- 2) To develop new experimental techniques and modeling methods needed to obtain key thermodynamic and transport property data for high temperature aqueous solutions and interfaces relevant to the IAPWS mission.

The following topics are considered to be at the core of PCAS activities:

- Hydration of inorganic and organic species
- Surface and interfacial tension in electrolyte and nonelectrolyte systems in various regions including supercooled and supercritical conditions

- Reactions of organic molecules in solutions their mechanisms and applications to green technologies
- Speciation and phase equilibria of electrolyte solutions
- Reactions at metal solution interfaces and their relevance to corrosion phenomena
- Nucleation phenomena
- Interfaces of biomolecules with solutions

Adjournment. The meeting adjourned at 3:30 pm.

Appendix. PCAS members whose membership is not continued

Professor Arthur K. Covington

Dr. Vladimir Majer

Dr. Martin Neumann

Dr. G. Perboni

Dr. A. Regazzoni

Professor N.A. Smirnova

Dr. Dominique You



The International Association for the Properties of Water and Steam http://www.iapws.org

Physical Chemistry of Aqueous Systems Working Group (PCAS WG)

Preliminary Schedule

Boulder, USA, 30 September – 5 October, 2012

Sun 30 Sept.		Informal Get-together, Cocktails and Registration
Mon 1 Oct.	08:30 10:00 13:30	Opening Plenary Session - Executive Committee PCAS Meeting PCAS Meeting
Tue 2	08:30	 PCAS & PCC Joint Workshop on "Water and Energy Chemistry" Presentations by PCAS after PCC WG members. 1) Thermodynamical Analysis of the Enhancement of Hydrogen Fuel Cell Efficiency by the Water Surface Tension Control František Maršík, Tomáš Němec, Michal Pavelka 2) Modeling the effects of solution chemistry on the localized corrosion of engineering alloys Andre Anderko 3) Conversion of carbon dioxide and hydrogen into formic acid for CCS: In ambient water without catalyst Masaru Nakahara
	10:30 13:30 15:30	PCAS Joint (TPWS/IRS/SCSW/PCC) Meeting PCAS/TPWS/IRS/SCSW/PCC Joint Meeting and Workshop PCAS/TPWS/IRS/SCSW/PCC Joint Meeting
Wed 3	09:00-17:00	IAPWS Symposium
Thu 4	08:30	PCAS/TPWS Joint Meeting
	11:00	PCAS Meeting "Classical nucleation theory - cavitation of binary systems" by Tomas Nemec "Thermodynamic modeling of actinide solution chemistry" by Andre Anderko
	13:30	PCAS Meeting (Summary, Report for EC) IAPWS Dinner/Banquet
Fri 5	08:30	EC Meeting (8:30-13:00)
	13:30-15:30	Technical Visit

Agenda

- 1. Opening
- 2. Appointment of Clerk for Minutes
- 3. Adoption of Schedule and Agenda
- 4. Membership
- 5. PCAS Missions and Activity Style
- 6. Progress Report and Future Perspective
- 7. Possibility of International Collaboration Project
- 8. Possibility of Release
- 9. Possibility of ICRN
- 10. Others

TPWS Agenda for PCAS and TPWS Joint Meeting

- 13. Properties of Supercooled Water, joint with PCAS and SC SW
 - 13.1 Towards a Guideline for the thermodynamic properties of supercooled water (V. Holten (speaker), M. Anisimov, J. Sengers)
 - 13.2 Surface tension of supercooled water (J. Kalova, R. Mareš, V. Vinš)
 - 13.3 Atmospheric freezing processes: Questions of interest for IAPWS (O. Hellmuth)
- 14. Molecular Simulation and Modeling, joint with PCAS
- 15. Critical locus of aqueous solutions of sodium chloride, joint with PCAS
- Report (D. Fuentevilla (speaker), J. Sengers, M. Anisimov)
- Test Report (K. Miyagawa, A. Harvey)
- Formal consideration of the Guideline

Masaru Nakahara 10 September, 2012

IAPWS Working Group Power Cycle Chemistry (PCC)

Minutes of IAPWS PCC WG Meetings

Boulder, Colorado 30. Sept – 05 Oct 2012

Chairman: Michael Rziha

Members present See PCC Attachment A

1. Agenda

1.1. Amendments / Adoption of Agenda

There were no amendments to the drafted agenda.

1.2. Week program: split up of PCC for joint workshops and task groups.

M. Rziha summarized the schedule.

2. Appointment of Clerk of Minutes

F.U. Leidich agreed to act as Clerk of Minutes.

3. Approval of Minutes of PCC WG in Plzen, Czech Republic, 2011

The minutes were approved without any corrections.

4. Progress Reports on PCC Activities 2011 / 2012

4.1. International Collaboration

D. Lister reported on progress with the collaboration on sampling and the CFD results gained so far with his presentation given during the PCC meeting.

4.2. ICRN

There have been no new proposals handed in to the chairman of the PCC WG in the last year.

ICRN#13 on Surface tension

Closed already, can be looked at on the IAPWS webpage

ICRN#17 on Amines

Draft agreed, expiry date Sept. 13 needs some attention.

J. Bellows will finish the draft and send it to EPRI for their comments. Afterwards it will be sent-out to the PCC group for further comments and then by M. Rziha in post-carriage for approval by EC

Action: J. Bellows

M. Rziha

ICRN#19 on Sampling of corrosion products

Closing statement on the IRCN will be prepared

Action: D. Lister

ICRN #20 on Sensors for use at elevated temperatures

Work is ongoing. Presentation on the current results is in preparation

Action: S. Uchida

D. Lister

ICRN#25 on Corrosion mechanism that are related to the presence of contaminants in steam/water circuits, particularly in boiler-water.

PCC WG agreed to submit the revised draft to EC for approval.

Action: M. Rziha

ICRN#26 on Behaviour of Aluminium in the Steam Water Cycle of Power Plants

has been circulated to National Committees for postal ballot in October 2010.

M. Rziha, G. Joy, F.U. Leidich: work-out final proposal for approval by the PCC WG.

Action: M. Rziha

G. Joy

F.U. Leidich

4.3. PCC Task Groups

IAPWS Guidance documents

B. Dooley reviewed the progress over the last three years. He also highlighted the importance of the IAPWS guidance documents. The existing guidance documents which have been issued so far, all are now in widespread use worldwide.

Future document proposals presented by B. Dooley are:

- Amendments to the document on instrumentation
- Steam purity
- Sampling QA/QC
- Amendment to the document on carry-over
- Amines
- Others?

A discussion followed on how these document proposals shall be treated by PCC TGs.

The following persons volunteered for it in a first step:

K. Thomson, M. Rziha, D. Lister, F. Gabrielli, F.U. Leidich, D. Addison, G. Joy, J. McKinney, P.

Gotovtsev, S.Marais, R. Turner, H. Takaku

Others are cordially invited to join.

Action: K. Thomson

PCC accepted the revised Sampling guidance document for approval by the EC

Action: M. Rziha

- B. Dooley reported on the progress on proofing elevated importance within IAPWS and by operators (users of the guidance documents)
 - The proposed change of the bylaws as per last year's meeting is done
 - IAPWS to notify manufacturers needs to be completed.

 The question arose, how it can be achieved and ensured that this letter reaches the relevant persons in the manufacturers' organisations.

Action: B. Dooley

B. Dooley presented the current status of the steam purity guideline as a starting point for the discussion to follow.

The following topics were highlighted in particular:

• Industrial steam turbines: J. Tavast as TG lead needs support from others to add this to the guideline. The following members committed to contribute: T. Petrova, F.U. Leidich, J. Bellows, F. Gabrielli

Action: J. Tavast

• Geothermal turbines: D. Addison will lead the TG. He will be supported by T. Petrova, F.U. Leidich, H. Ishihara

Action: D. Addison

• Elevated CO2-Levels: M. Rziha will act as TG lead, supported by R. Turner, J. McKinney

Action: M. Rziha

A voting on the philosophy of the steam purity guideline followed ended with the following results:

- One table for all systems independent from treatment philosophy of the feedwater
- No separate tables for the kind of steam generation

4.4. European Standard EN 12952

The status of the activities on this field remains the same as per last year. It remains a challenge to push the national committees within the CEN organisation to vote for the need of a revision of the a.m. document, which is due latest by after-next year. During the last voting, the need for a revision was missed by only one vote.

All national IAPWS organisations should check whether they have contact through members to the national CEN committees. For a number of countries this can be done by the ETC (European technical committee) on power plant chemistry run by VGB. The next meeting of this group is on Oct. 22nd in Hamburg. M. Rziha, F.U. Leidich, and K. Thomson are members in this group and committed to act accordingly

Action: M. Rziha F.U. Leidich K. Thomson

4.5. PCC Public Relations

M. Rziha informed the audience about the growing links to national and international organisations and bodies as well as conferences.

In 2013 there will be a conference on FAC in Nuclear Power Station in Paris. Organizer will be EdF. A link to this conference will be organized by B. Dooley

Action: B. Dooley

M. Rziha expressed the PCC's gratitude to R. Svoboda for publication of information about PCC meeting in Plzen in the PowerPlant Chemistry magazine. He declared his will to write an article about this year's conference also in PPChem. This was gratefully appreciated by the audience.

Action: M. Rziha

Another FAC conference on fossil Power Plants will happen in March 2013 in Washington DC. The link to IAPWS already exist on this conference (see webpage, was action from last year)

To increase recognition and lever profile of IAPWS PCC by manufacturers of power plant equipment, a letter shall be send to all relevant companies. F. Gabrielli and M. Rziha volunteered to draft such a letter.

Action: M. Rziha F. Gabrielli

4.6. Other Action List Items

There were no other items not covered on the agenda.

5. Priority List Review

The priority list was discussed and updated on a point by point basis. The outcome is attached (attachment C).

6. Other Business

nil

7. Changes in Membership, election of Officers

News of the recent death of G. Bignold was greeted with great sadness.

M. Rziha proposed , seconded by B. Dooley, that K. Thomson shall be asked to stand as new vice-chairman.

PCC WG supported the proposal. K. Thomson expressed to be pleased to take over the role.

Action M. Rziha

The following new members of PCC were proposed and unanimously accepted:

New Member	Proposed by:	Seconded by:
Anders Fredrikson	K. Daucik	M. Rziha
Mats Hellman	K. Daucik	M. Rziha
Taro Ichihara	S. Uchida	F.U. Leidich
Hideo Hirano	S. Uchida	F.U. Leidich
Paul McCann	B. Dooley	M. Rziha
David Addison	B. Dooley	M. Rziha
Stephanie Marais	B. Dooley	M. Rziha
Randy Turner	B. Dooley	M. Rziha
David Moed	B. Dooley	M. Rziha
Andrew Witney	B. Dooley	M. Rziha
Kirk Buecher	B. Dooley	M. Rziha

M. Rziha will propose acceptance of these additional PCC members by the executive committee.

Action: M. Rziha

- 8. Preparation of Action List 2010 / 2011, Task Distribution, Next Year's Agenda
- 9. Preparation of PCC WG Report for Executive Meeting

Action: M. Rziha

10. Miscellaneous and Adjournment

PCC website will go live soon. M. Rziha will send the link to all PCC members when done

Action: M. Rziha

Boulder, Colorado, 30 September - 5 Octoberber 2012

Those present at the PCC WG meeting were as follows:

M. Rziha Germany Netherlands D. Moed S. Uchida Japan H. Hirano Japan T. Ichihara Japan K. Buecher USA K. Thomsen Denmark A. Fredrikson Sweden A. Witney USA F.-U. Leidich Germany J. Bellows USA D. Lister Canada W. Cook Canada R. Turner USA

South Africa S. Marais

J. McKinney USA G. Joy Australia B. Dooley USA T. Petrova Russia P. Gotovtsev Russia P. Mc Cann UK M. Hellman Sweden K. Daucik Denmark P. Safaŕik Czech Republic

F. Gabrielli USA

New Zealand D. Addison M. Rziha Germany H. Takaku Japan Switzerland R. German H. Maurer Switzerland

Boulder (CO), USA, 30 Sept – 05. Oct 2012

PCAS / PCC workshop (Tuesday 08:30 - 12:00)

1.	David Addison	Presentation of NZAPWS - Areas of key interest to NZ
2.	Frantisek Marsik	Thermodynamical Analysis of the Enhancement of Hydrogen Fuel Cell Efficiency by the Water Surface Tension Control
3.	Hiroshi Takaku / Lin-Bin Nin	Characteristics of Oxide Films Formed on Welded Surfaces of Carbon Steel for Boiler Tubes
4.	Andre Anderko	Modeling the effects of solution chemistry on the localized corrosion of engineering alloys
5.	David Addison	Chemistry Aspects of Geothermal Power Plants
6.	Masaru Nakahara	Conversion of carbon dioxide and hydrogen into formic acid for CCS: In ambient water without catalyst

PCC workshop (Tuesday 13:30-17:00 and Thursday 08:30-10:00) <u>Update on Power Cycle Chemistry Research and Experience</u>

1.	Frank-Udo Leidich	The New VGB-Standard on Sampling and Instrumentation for Steam Water Cycles
2.	Paul McCann	Update on the Revision of ISO 5667-7 on Sampling of Water and Steam
3.	Derek Lister	Sampling in Steam Water Systems
4.	Derek Lister / Shunsuke Ushida	Improved Sampling Technique: IAPWS International Collaboration
5.	Ken Ogan	A new approach to on-line monitoring of chloride and sulfate
6.	Gary Joy	CS Energy ACC and Solar Boost Experience – Chemical Aspects
7.	Hideo Hirano / Noburo Kawai	Status of Water Conditioning for Once Through Boiler in Japanese Fossil Plants
8.	Shunsuke Ushida	Determination of Wall Thinning Rates and High Risk Zones for Local Wall Thinning due to FAC
9.	Shunsuke Ushida	A Consideration of Design Procedures Related to Water Chemistry of BWR Power Plants

10. Heini Maurer	Influence of Temperature on Electrical Conductivity of Diluted Aqueous Solutions
11. William Cook	Restart chemistry control at the Point Lepreau nuclear generating station after an extended refurbishment outage
12. Karsten Thomson	Sea water contamination of a once-through boiler
13. Taro Ichihara / Takatoshi Satou	Practice of Amine Treatment on Industrial Power Plants in Japan

PCC Minutes, Niagara Falls July 2010 updated at Plzen, September 2011 updated at Boulder, October 2012

PCC Priority List for Further Research

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)?

Status 2011: Joint PCC/PCAS ICRN #21 is on the IAPWS website Status 2012 : no change

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

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

Status 2010: ICRN #20 has been issued in 2006, some activities known in 2009 (Balashov, Petkin, Lvov), re-formulation in 2010 related to the needs from nuclear industry (Uchida), 2011: still on-going
Status 2012: ICRN # 20 is approved until Sept. 2014

3. * 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

Status 2011: Geoff Bignold drafted ICRN #25 which should be finalized in 2011 (Bignold, Cook)
Status 2012: ICRN # 25 : Draft for EC

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

Main scope will be the minimum requirements for sampling specifically for Fe, Cu, Co, Oxygen, etc.

Status 2011: ICRN #19 on sampling has been extended to 2012. International collaboration 2006/7 2010/2012. (Uchida, Lister, Daucik, Svoboda). 4 papers by Piti et al. IAPWS Guidance Document on sampling under consideration

Status 2012: Papers by Lister, Uchida, et al. had been presented focussing on Fe-oxides. Paper is distributed to relevant PCC members for the preparation of the final report. Investigations on other parameters e. g. Oxygen are still of high interest.

5. * 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: K.Daucik)

Status 2011: available information has been compiled, although insufficient for being basis of an IAPWS document, a publication on the existing results will be made (Daucik, 2012)

Status 2012: ongoing until next meeting in London 2013.

6. 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
- development of liquid films on surfaces in saturated steam environments (especially with regard to Flow Accelerated Corrosion)

ICRN #22 is on the IAPWS website;

Status 2012: ongoing

7. 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 and Al Deposition : (Cu essentially a solved problem from a scientific viewpoint)
- mechanism of deposition on a turbine blade is not understood
- discrepancies in temperature influence on deposition (?)

Status 2011: wide range of information available and research ongoing, opportunity for several ICRN

Status 2012: Topic is actually partly covered by ICRN #22 and ICRN #26 Paper by Uchida and Lister et al. had been presented on transport and deposition of Fe-oxides.

8. Radiation chemistry of water

Radiolysis, main importance for nuclear generation

2007 PCAS/PCC presentations have been made

<u>Status 2011: major issue for supercritical water reactors. Workshops held regularly in connection to the bi-annual International Conference on Water Chemistry in Nuclear Reactor Systems</u>

Status 2012: update will presented at the 16th ICPWS in London 2013 – considering moving to watch list.

9. * Behaviour of Aluminium in the steam / water cycle

- Al release under various water treatment regimes
- volatile carry-over and deposition in the turbine
- depsoition on boiler tubes,
- solubility in water and steam
- behaviour in condensate purification
- interaction of Al with boiler chemistry
- specfication values for Al in feedwater, boilerwater, steam
- impact of the use of Al on materials and cycle chemistry of the rest of the cycle

Status 2011: ICRN #26 in processing, final draft is available (Rziha, Svoboda)
Status 2012: additional input to ICRN #26 by Gary Joy. Draft to EC

10. Water cooling of copper in electrical machines

- generator stators
- accelerators

Status 2011: paper at ICPWS 2008; EPRI guideline 2008, CIGRE guidance document to be published (draft document approved), new investigations Palmer/Svoboda considered Status 2012: remains of interest. Update during 16th ICPWS

11. Water use outside the steam / water cycle

- cooling water
- waste water
- external process
- recycling for use as make-up
- etc.

For further consideration for 2012, possibly new IAPWS sub-committee. PCC does not have the resources to take leadership on these items.

Status 2012: ongoing. Positionpaper in preparation (task group: Stephanie Marais, Andy Howell, David Moed, Gary Joy, Pavel, et. Al)

12. Chemistry in geothermal and oil / sand cycles

Behaviour of water constituents, effects on system materials, geochemical and waste water issues, including behaviour of radionuclides in these waters.

Status 2011: ICRN to be considered for 2012 (Leidich, Rziha, Myszczyszyn) Status 2012: ICRN still to be drafted. (Leidich, Rziha, Myszczyszyn, Addison)

13. Chemistry aspects in solar thermal generation

Status 2012: ICRN is under preparation (Gary Joy)

14. Chemistry of Desalination Systems

Status 2012: "White paper" by Stephanie Marais, David Moed, Pavel Gotovtsev, Gary Joy, Andrew Howell, Paul McCann, describing the needs and recommendation is available. ICRN will be prepared until 2013. Elaboration of TGD is proposed and accepted by WG. Task Group for TGD will be set up at annual meeting 2013.

15. Chemistry of Filming Amines

Status 2012: A "white paper" by Stephanie Marais, David Moed, James Bellows and Tamara Petrova, describing the needs is available. It is recommended to create a separate ICRN beside ICRN #17. The draft will be prepared in advance to the annual meeting 2013.

* urgent priority

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, Generation IV reactor plants, ITER)
- 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)

IAPWS Collaborative Grant Proposal

An experimental study of viscosity of the binary ammonia + water system at high temperatures and pressures

IAPWS Sponsors

Dr. Daniel G. Friend

Material Measurement Laboratory NIST MS 838.00 325 Broadway, Boulder, CO 80305, USA Phone (303) 497 5424

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Visiting Young Scientist
(Il'giz R. Gabitov or colleague to be named)
Kazan National Research Technological University,
K. Marx St., 68, Kazan 420015, Tatarstan, Russia Federation

September 22, 2012

This proposal will have four principal outcomes: it will strengthen collaborations between the Department Theoretical Bases of the Thermal Engineering of the Kazan National Research Technological University (KNRTU) and the National Institute of Standards and Technology (NIST) in the US; it will enable a young scientist to travel from the KNRTU to NIST for training in best practices for calibrations, measurements and data evaluation; it will provide the IAPWS community with new measurements of viscosity for the aqueous system ammonia + water in wide ranges of temperature and pressure; and, it will initiate a broad program of measurements and models for the ammonia + water system.

An IAPWS Certified Research Need [1] indicated a need for properties for ammonia + water mixtures at temperatures to 866 K (593 °C) at pressures up to 35 MPa, covering the complete range of composition. In spite of research activity from 1997 to 2002 that was reported in the Closure Statement for this ICRN, viscosity data are still very limited for ammonia + water mixtures.

The primary reasons for the scarcity of data are experimental difficulties related to the fact that this system is corrosive, toxic, potentially flammable, and has a high relative volatility. Special materials, safety procedures, special equipment and knowledge of their proper use are all required. Only a handful of labs, including NIST, have been able to make sufficient investment in training and materials to make such measurements.

The H₂O + NH₃ mixture is receiving an increasing attention due to the potential use of the system as a working fluid in refrigeration and power plant cycles. The binary H₂O + NH₃ mixture has a large technical significance in the fields of absorption refrigeration machines, absorption heat pumps, and heat transformers. To prevent the destruction of environment, natural working fluids such as ammonia and water have been considered as alternative organic refrigerants to replace chlorofluorocarbons (CFC) in some refrigeration applications. Ammoniawater mixture does not affect the atmospheric ozone layer nor do they contribute to the green house effect. Therefore, the significance of this mixture in refrigeration technology is strongly increasing. Refrigerating cycle with H₂O + NH₃ mixtures as working fluids have been shown to reach higher coefficient of performance than traditional working fluids. Thermophysical modeling of a technological processes is requires information on the both transport properties (viscosity and thermal conductivity) of H₂O + NH₃ mixtures. The important properties as viscosity and thermal conductivity required for absorption cycle analysis and in design of heat exchanger. Power cycles with H₂O + NH₃ mixtures as working fluids also have been shown to reach higher thermal efficiencies than the traditional steam turbine (Rankine) cycle with water as the working fluid. The best H₂O + NH₃ cycle produced approximately 40-70 % more power than a single –pressure steam cycle and 20-25 % more power than a dual-pressure steam cycle. In calculating the performance of the power cycles, the accurate transport properties data of the H₂O + NH₃ mixture play an important role. The demand to decrease the consumption of primary energy is lead to optimization of technological processes. To improve the H₂O + NH₃ cycle efficiency and to operate apparatus at high temperatures and pressures, the need for pertinent data in regions beyond those covered by the available data becomes more urgent. For this aim, engineering design of absorption air-conditioning equipment utilizing the H₂O + NH₃ cycle requires accurate transport property data of $H_2O + NH_3$ mixtures over a wide range of T, P, x. However, reported transport property data cover limited range of T, P, x, and contain large

uncertainties and inconsistency. Number of speeches about geothermal power cycle applications has been presented at the latest geothermal conference in Germany, 2010. Thermophysical Properties Division, TRC (M. Frenkel) and Modeling Group (E. Lemmon), was repeatedly requested from various Industrial Companies (Jim Tindill, Sr. Mechanical Engineer Southern Company Services; BR/Claes) for transport properties of ammonia + water mixture.

Accurate viscosity data are also essential to the development of a reference correlation equation. Experimental data for the dynamic viscosity of liquid ammonia + water mixtures are quite sparse. The currently available viscosity data (see Review [2] paper) cover only very limited temperature and concentration ranges. Pagliani & Battelli (1885) [3] made the first known measurements at 0 °C, 5.8 °C, and 13.4 °C. Kanitz (1897) [4] reports measured data at 25 °C, followed by a few other points, also at 25 °C, measured by Blanchard & Pushee (1904, 1912) [5,6]. Pleskov & Igamberdyev (1939) [7] made measurements at 20 °C, but the largest set of experimental data known is that published by Pinevic (1948) [8]. Frank et al. (1996) [9] carried out a few measurements in a limited range of temperatures and concentrations. Very low temperature measurements of the viscosity were reported by Kargel et al., (1991) [10]. A detailed analysis of the reported data is presented in the report [2]. As was mentioned in Ref. [2], the reported viscosity data show remarkable inconsistencies (large scattered data, large uncertainty). No data under pressure were published before for ammonia+water mixtures. A survey of the literature also reveals that most reported data at atmospheric pressure were published long times ago (between 1885 and 1948). Both the Thermophysical Properties Division of NIST and KNRTU have extensive experience and capabilities in accurate viscosity measurements covering wide ranges of temperature, pressure, and concentration and their modeling (Dr. M. Huber). In a previous IAPWS project we have reported CvVTx [11], PVTx [12], thermal-pressure coefficient [13], and thermal conductivity [14] data for the aqueous system (H₂O + ammonia) in the liquid phase and near-critical and supercritical regions. For the reasons mentioned earlier, the labs of KNRTU and NIST are among the few research facilities in the world with capabilities for H₂O + ammonia viscosity measurements at the high temperatures and high pressures.

Under other funding, Prof. Tarzimanov's team in the KNRTU Labs will investigate viscosity in a temperature range from 298 to 363 K and at pressures up to 20 MPa for the concentrations 25, 50, and 75 mass % of ammonia, with an uncertainty in viscosity of less than 2 %. This investigation will provide reliable viscosity data by using a falling-body technique [15-24].

Following the experiments, we plan to bring a younger KNRTU Labs scientist to the Boulder Labs of NIST for 6 months. Ph.D. Student Il'gis R. Gabitov will be our top choice, since his PhD dissertation is on thermophysical properties of aqueous systems. Mr. I. Gabitov will assist Dr. Huber and her team in the Boulder Labs with the following tasks: (1) analysis of the viscosity data for water+ammonia mixture; and, (2) comparison with published measurements and models; (3) develop new viscosity model for the mixture; (4) prepare MS of the paper for publication. As an additional educational component of his visit, we will conduct detailed discussions and comparisons of the experimental viscosity techniques used in the KNRTU Labs with those used in the Boulder Labs, methods for precise gravimetric mixture

preparation, a propagation of uncertainties analysis, round-robin measurement comparisons, and establishing a chain of traceability to national and international standards.

Budget

We propose a total budget of \$20,000 for this project and a period of performance of 6-7 months. This would pay for the travel expenses and visit for Mr. Il'giz Gabitov or other young KNRTU scientist for his work in Boulder with the US-based research team. A project report will be prepared and submitted to IAPWS by the next annual meeting.

Leveraging of the IAPWS Support

The research team has planned a comprehensive research project on the ammonia + water system, involving partnerships with university-based researchers. To leverage the support from IAPWS, we will seek additional support from other agencies. Toward the end of the proposed 6-7 months IAPWS project, one or more proposals will be prepared to support the following tasks: (1) additional measurements of transport properties (a) viscosity data for the ammonia + water system and (b) thermal diffusivity measurements at high temperatures and high pressures; (3) development of new models for viscosity.

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IAPWS Collaborative Grant Proposal, 2012

Development of a new Equation of State for Heavy Water

IAPWS Sponsors

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Mr. Stefan Herrig
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The properties of heavy water (D_2O) are of significant scientific interest, and also of some industrial interest for certain nuclear power cycles. The current IAPWS formulation for the thermodynamic properties of D_2O was adopted in 1984 (with a minor adjustment for temperature scale in 2005 [1]), and is based on work performed in the group of Prof. Phil Hill over 30 years ago [2].

In the past 30 years, a modest amount of additional data has become available. We know of isochoric heat-capacity measurements [3,4], some new measurements of the density of the high-temperature liquid relative to that of ordinary water [5], some reanalyzed vapor density data [6], and some liquid heat-capacity data [7]. The preceding list is not necessarily complete; we have not yet performed a thorough literature search.

At least as important are the advances in the development of equation-of-state (EOS) technology over the past 30 years. Modern computer technology allows simultaneous optimization of EOS parameters to multiple data types, constraint of the EOS to proper extrapolation, smooth behavior of derivatives and better behavior in the critical region (the current IAPWS EOS for D_2O [2] is not recommended near the critical point), and a reduction in the number of adjustable parameters needed. This modern technology has been applied to numerous fluids (some of the advances were already applied to the IAPWS formulation for H_2O), and it should be possible to apply it to D_2O .

The proposed collaborative project combines the experience in EOS fitting of probably the two leading groups in that field; those at NIST and Bochum. Dr. Eric Lemmon of NIST would train the young researcher in advanced techniques for developing equations of state and guide him in applying the techniques to D_2O .

The production of a final EOS and accompanying paper could not be done in the timescale of an IAPWS collaborative project. Therefore, the goal of this project is to do the basic work necessary to get the project started and most of the way to completion. The student

would develop a complete database, be trained by Dr. Lemmon in the techniques of advanced fitting, and produce a preliminary EOS. This preliminary EOS would then be fine-tuned over the rest of 2013 in a collaboration involving the Boulder and Bochum groups, perhaps in conjunction with feedback and evaluation by the IAPWS TPWS Working Group. It is hoped that this would result in a new IAPWS Release that could be adopted in 2014 or 2015.

Budget

We propose a total budget of \$7,500 for this project, which would last for 4 months beginning in early 2013. This would pay for the travel expenses of Mr. Herrig to Boulder (IAPWS would be invoiced for \$1500 or the actual expense, whichever is smaller), and for 4 months of living expenses at \$1500 per month.

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Highlights International Association for the Properties of Water and Steam 2012 Meeting

Continuing a series of conferences started in 1929, 75 scientists and engineers from 13 countries attended the annual meetings of the International Association for the Properties of Water and Steam (IAPWS), September 30-October 5 in Boulder, Colorado, USA. The meeting was hosted by the United States National Committee of IAPWS. The meeting connects academic researchers with engineers who use their information. It provides the researcher with guidance on useful problems and provides the engineers with the latest research. IAPWS has traditionally concentrated on the science underlying the thermodynamics and chemistry in steam power plants, but is broadening into other aspects of power generation and high temperature aqueous systems as well as seawater and ice. Discussions range from puzzling power plant chemistry results to reports on solutions to such problems to practical implications of fundamental theory and molecular modeling of thermodynamic and transport properties.

The IAPWS delegates were joined by several additional people from the United States for a symposium on The Energy-Water Nexus: Status and Prospectus. The symposium opened with the IAPWS Helmholtz award lecture "Molecular Theory of Liquids: Approaching Chemical Accuracy", given by Maxim V. Fedorov of the University of Strathclyde. The Helmholtz Award is given annually to a young scientist for work of interest to IAPWS. The symposium continued with presentations on the Energy-Water Nexus, Desalination Technologies, and new technological developments in water reuse. water management and power plant condenser cooling systems.



Maxim V. Fedorov presents the IAPWS Helmholtz Award Lecture, introducing many in the audience to molecular integral equation theory.

IAPWS produces releases, guidelines, technical guidance documents, and certified research needs (ICRN's). Information may be found at the IAPWS website: www.iapws.org.

Following the success of the new seawater standard TEOS-10, which was created with the assistance of IAPWS, IAPWS has now formally approved participation in a permanent Joint Committee on the Properties of Seawater (JCS), in collaboration with the Scientific Committee on Oceanic Research (SCOR) and the International Association for the Physical Sciences of the Oceans (IAPSO). This new international committee will serve as a permanent source of scientific expertise on the properties of seawater and will develop and maintain international standards related to seawater. An important initial goal is to develop a means of tracing the definition of salinity to the 7 base units in the International System of Units (SI), which is maintained by the International Bureau of Weights and Measures (BIPM). Workshops on this

topic, open to all interested parties, are scheduled to take place at the 16th International Conference on the Properties of Water and Steam (ICPWS).

IAPWS has developed a new Guideline on the Critical Locus of Aqueous Solutions of Sodium Chloride. A new equation for the properties of supercooled water, relevant to atmospheric and biological systems, has also been developed. Correlation of properties of systems important to carbon capture and sequestration is becoming an important interest of IAPWS.

A joint IAPWS/IUPAC project titled "Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes and Gases" is approaching completion. An IAPWS guideline on the thermal conductivity of seawater is in preparation.

The Power Cycle Chemistry Working Group revised new technical guidance document, "Instrumentation for Monitoring and Control of Cycle Chemistry". The working group keeps a priority list for research related to power plant chemistry. It is currently includes the behavior of aluminum in the steam / water cycle and the corrosion mechanisms that are related to the presence of contaminants in steam/water circuits, particularly in boiler-water. This working group includes in its scope the concentrated solutions found in the cooling water that goes through power plant condensers, makeup water and waste streams.

IAPWS will be sending a questionnaire to industrial organizations eliciting needs for steam properties and new priorities. People interested in receiving the questionnaire are encouraged to contact the Executive Secretary of IAPWS.

IAPWS welcomes scientists and engineers with interest in the thermophysical properties of water, steam, and aqueous systems and in the application of such information to industrial uses. The next IAPWS meeting will be held in conjunction with the 16th International Conference on the Properties of Water and Steam, September 1-5, 2013 in Greenwich, England. Further information on meetings and the conference can be found at the IAPWS website, www.iapws.org, as it becomes available. IAPWS documents may also be found on the 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., 2616 Chelsea Drive, Charlotte, North Carolina 28209, USA, e-mail: bdooley@structint.com. People do not need to be citizens or residents of member countries to participate.

BRITISH AND IRISH ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM



A Member of the International Association for the Properties of Water and Steam

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BIAPWS Annual Report 2012

1. Introduction

The British and Irish Association for the Properties of Water and Steam (BIAPWS) is the UK and Ireland national committee of the International Association for the Properties of Water and Steam (IAPWS) and the representative body for Power Plant Chemistry in the UK and Ireland. BIAPWS is a not for profit organisation. This is the annual report of the activities of BIAPWS for the year to April 2012.

2011/12 has been another successful year for BIAPWS. Membership has remained strong, BIAPWS events have been well supported and the BIAPWS symposium and BIAPWS Award have both been successful. Preparations are progressing well for the 16th International Conference on the Properties of Water and Steam (ICPWS), which will be co-hosted by BIAPWS and the Institution of Mechanical Engineers (IMechE) at the University of Greenwich, 1-5 September 2013.

BIAPWS was pleased at the start of 2012 to welcome new holders of the roles of Chair, Vice-Chair and Secretary. BIAPWS would like to thank all the Officers who stepped down from their positions in 2012, however I would like to highlight our appreciation for the invaluable contributions to BIAPWS that Richard Harries has made over the years, as vice chair, chair and more recently secretary. We were also pleased to introduce an updated BIAPWS web-site in 2011 and our thanks go to our 'webmaster', Ken McGrath, for his diligent work towards this. BIAPWS finances remain in good stable condition and it is pleasing that, as a result, membership fees for sponsoring organisations have remained unchanged for the third year running. I would like to thank Eric Huff for his continuing excellent work as our Treasurer in helping to achieve this good state of financial health.

IAPWS request that National Committees provide, with their annual report, a listing of relevant technical publications that have originated from the respective nation/s during the year. The purpose of this request is to allow National Committees to share such lists and thereby widely

disseminate the international body of work being done on topics of interest to IAPWS and to IAPWS members. The list of publications for the UK and Ireland for the 2011/12 period is therefore provided in the Appendix to this report.

If you would like to know more about BIAPWS, feel free to contact one of the BIAPWS Officers listed above, visit our web site www.biapws.org or e-mail contact.us@biapws.co.uk.

2. BIAPWS Membership

BIAPWS membership has remained strong and BIAPWS is currently supported by nineteen industrial sponsors, six ordinary members and seven corresponding members. In 2011/12 BIAPWS was pleased to welcome AES and Watercare International as new industrial sponsors. BIAPWS committee meetings are held three times a year, and attendance at these continues to be very good, typically around twenty. BIAPWS committee meetings are preceded by a couple of technical presentations, which always generate a high level of interest. Industrial member's representatives are able to bring a colleague to the meeting to benefit from and contribute to the discussions.

BIAPWS has a strong membership representation in the area of power plant chemistry. However, other areas that are of relevance to IAPWS, for example the thermophysical properties of water and steam and the physical chemistry of aqueous solutions, are less well represented and BIAPWS remains keen to expand its individual membership in these areas.

I am very pleased to report that in 2012, BIAPWS formally agreed to new Statutes, the changes in which included the creation of a new individual membership category, that of Honorary Member. This category of membership is reserved for those BIAPWS members who have made a significant contribution to the achievements and aims of BIAPWS over an extended period. I am delighted to report that on completion of the changes to the Statutes, the following individuals were duly elected to the position of Honorary Member: Freddie Bakhtar, Malcolm Ball, Geoff Bignold, Jeff Cooper, Richard Harries, Eric Huff and Ken McGrath.

It was with great sadness that BIAPWS was informed of the sudden death, after a short illness, of Geoff Bignold in August 2012. Geoff was a former vice chair and chair of BIAPWS, an IAPWS Honorary Fellow, and was highly regarded internationally for his work and knowledge of power plant chemistry.

3. IAPWS Activities

BIAPWS has continued to support IAPWS through its formal membership and participation in IAPWS activities. A number of BIAPWS committee members are represented on IAPWS working groups, in particular Power Cycle Chemistry (PCC). BIAPWS members of the PCC working group are also supporting the production of a new suite of IAPWS Technical Guidance Documents that are expected to provide a valuable resource to those involved in power cycle chemistry.

IAPWS holds annual meetings and BIAPWS members support these events by participating in the relevant IAPWS working groups. In addition, BIAPWS is represented on the executive committee of IAPWS. Every four or five years IAPWS holds the International Conference on the Properties of Water and Steam (ICPWS) in place of the annual meeting. The next such conference will be the 16th and this will be hosted by BIAPWS and held at the University of Greenwich, 1-5 September 2013. It has been over fifty years since this conference has been held in the UK and BIAPWS is looking forward to a welcome return to London, where the very first such conference was held in 1929. A BIAPWS sub-group is leading the work on ICPWS 16 in coordination with the IMechE, which is co-hosting the event with BIAPWS and has taken on the role of Conference Organiser. We are very grateful to the ICPWS sub-group, comprising Eric Huff, Hugh Lloyd and Jeff Cooper, and to the IMechE, for their work to make this important event a success. For more information on the Conference go to www.icpws16.org/.

For further information on the activities of IAPWS, visit the IAPWS web site, www.iapws.org.

4. BIAPWS Award

The BIAPWS Award is given annually by BIAPWS to qualifying students as a means of promoting awareness of the topics of interest to BIAPWS and their industrial application. In 2011 the BIAPWS award was co-sponsored by EDF Energy Nuclear Generation and the award recipient was David Docherty from Imperial College, London. The Award is given in the form of contributory funding by BIAPWS for a work experience placement for the student. David spent ten weeks with EDF Energy Nuclear Generation in Gloucester working on techniques to access look-up tables for steam / water properties when running computer simulations of transients in advanced gas-cooled reactors (AGRs). David gave excellent presentations on his work, firstly at the BIAPWS committee meeting in January 2012 and then at the BIAPWS Symposium in March 2012.

Many past BIAPWS Award winners have since gone on to full time employment in power generation, demonstrating significant success for the Award in attracting high calibre individuals to the industry.

BIAPWS has also continued to sponsor and judge prizes for energy related projects at a schools science fair in Hinckley, Leicestershire. We are currently looking for new opportunities to support ventures of this nature.

5. BIAPWS Symposium

The 14th BIAPWS Symposium, 'Progress in Environmental and Cycle Chemistry', took place at the Village Hotel, Nottingham, on 28-29 March 2012.

The Symposium consisted of two sessions: the first session on 28 March, 'Power Plant Fundamentals', was targeted at developing chemists and engineers with an interest in chemical operations and described the principles of cycle chemistry and boiler chemical cleaning. The second session on 29 March consisted of more detailed technical presentations on 'Environmental and Water Treatment Issues' and 'Power Plant Chemistry and Corrosion'.

This annual event continues to be very popular, with over eighty delegates attending the first session and over one hundred delegates attending the second session. This demonstrated not only the continued interest in the UK in developments in cycle chemistry and water treatment, but also the interest in more fundamental aspects. A summary report of the event was published in the journal Power Plant Chemistry, see PPChem 2012, 14(5), 298-305.

BIAPWS would like to extend its gratitude to all those who helped to make this event such a success.

6. BSI Representation

In recent years BIAPWS has participated in formal Standards Committees of relevance to its members. As a result BIAPWS is currently represented on three British Standards Committees:

- PVE/2: Water Tube and Shell Boilers. This committee is of relevance to BIAPWS because it is the UK standards committee with responsibility for BS EN 12952-12:2003: Water-tube boilers and auxiliary installations requirements for boiler feedwater and boiler water quality, and BS EN 12953-10:2003 Shell boilers Requirements for feedwater and boiler water quality. BIAPWS has led on behalf of other European power plant chemistry specialists to lobby for these standards to be revised and improved. Whilst the European body responsible for these standards has agreed to their revision, there has not been any significant developments in 2011/12.
- CII/62: Treatment of water for boilers. This committee is of relevance to BIAPWS because it is the UK standards committee with responsibility for BS 2486:1997 Recommendations for treatment of water for steam boilers and water heaters. Currently, this committee is not active
- EH/3/6: Water quality sampling. This committee is of relevance to BIAPWS because it is the UK standards committee with responsibility for BS 6068-6.7:1994 (ISO 5667-7:1993), Guidance on sampling of water and steam in boiler plants. BIAPWS is expecting to take a lead in revising this document in the forthcoming years and is currently looking at the best way to support the committee.

7. Interaction with Professional Organisations

Because of the diverse nature of the interests of IAPWS, the areas of interest to BIAPWS overlap with the areas of interest of a number of professional bodies. As a result, BIAPWS has corresponded over the last year with a number of bodies with the aim of sharing information and closer working. BIAPWS is now represented on the Water Science Forum of the Royal Society of Chemistry and in 2012 Richard Hill joined BIAPWS as a corresponding member, representing the Water Subject Group of the Institution of Chemical Engineers (IChemE), for which Richard is a Committee member. BIAPWS is also interacting with the Power Industries Division of the IMechE with reference to the organisation of ICPWS 16.

8. Closing Remark

In my last BIAPWS report, I would like to express my sincerest gratitude to all those individuals and organisations who contribute, sometimes in personal time, to the workings of BIAPWS and in support of BIAPWS activities. Without these contributions, BIAPWS would not be able to function effectively.

Dr. Andy Rudge Chair (to January 2012), British & Irish Association for the Properties of Water and Steam July 2012

APPENDIX: List of UK and Ireland Originated Reference Papers in areas of interest to IAPWS, plublished between April 2011 and March 2012:

Adelina Henderson and David Brazil, "Failure Analysis of HP Feedwater Line Elbow", PowerPlant Chemistry 2012, 14(2), 76-82

Richard J. Jones, "Generator Cooling Water Systems: Modelling Flammable Mixture Formation in Hydrogen Detraining Tanks", PowerPlant Chemistry 2011, 13 (10), 614-620

Paul McCann and Mark Robson, "Proceedings of the BIAPWS 2011 Workshop and Symposium on Power Plant Chemistry", PowerPlant Chemistry 2011, 13 (5)

Graham P. Quirk, Ian S. Woolsey, and Andy Rudge, "Use of Oxygen Dosing to Prevent Flow-Accelerated Corrosion in Advanced Gas-Cooled Reactors", PowerPlant Chemistry 2011, 13 (4)

Bakhtar, F. and Zamri, M. Y., "On the Performance of a Cascade of Improved Nozzle Blades in Nucleating Steam - Part 3: Theoretical Analysis", Proc. IMechE, Part C, Journal of Mechanical Engineering Science, 2011, 225 (C7), 1649-1671

C. –W. Lin and J. P. M. Trusler "The speed of sound and derived thermodynamic properties of pure water at temperatures between (253 and 473) K and at pressures up to 400 MPa", J. Chem. Phys. 136, 094511 (2012)

IAPWS Canadian National Committee

Annual Report 2012

Executive: David Guzonas (Chair); William Cook (Vice-Chair); Derek Lister (Secretary-Treasurer); Peter Tremaine (Member at Large); Melonie Myszczyszyn (Member at Large); CANDU Owners Group Representative (Steve McGee)

1. Canadian National Committee: Dues for the Canadian National Committee (CNC) of IAPWS are supported by the National Research Council of Canada. This arrangement requires support and participation by a national organization representing industry. In 2004 the CANDU Owners Group took on this role on a trial basis, and in 2007 the CANDU Owners Group accepted this role for a five year term, including travel support for the academic members of the CNC. The CANDU Owners Group has been very supportive and proactive in supporting the CNC, and discussions are underway to renew their support for another five year term.

2. NSERC/NRCan/AECL Generation IV Energy Technologies Program

A major university-based program to study water chemistry in support of the development of the Canadian Supercritical Water-cooled Reactor concept (NSERC/NRCan/AECL Generation IV Energy Technologies Program) concluded Phase I in 2012. Phase II of this program, which will last for four years, started in 2012 and includes seven water chemistry projects that cover two main themes: a) corrosion product transport and deposition, and b) water radiolysis. The goal is to develop chemistry control strategies for the SCWR as well as recommend realistic chemistry conditions for corrosion testing in support of materials selection. The program also funds eight projects examining materials degradation phenomena (e.g., corrosion, stress corrosion cracking, creep) at temperatures up to 850 °C. A kick-off workshop was held in Saskatoon in 2012 June.

Research on high-temperature water chemistry being funded by this program includes:

- P. Tremaine (U. of Guelph): Aqueous chemistry of metals and fission product under SCWR conditions.
- C. Pye (St. Mary's University): Ab initio calculations on ionic hydration and complexation.
- W. Cook (U. of New Brunswick): Corrosion product transport and deposition under SCWR conditions.
- **I. Svishchev (Trent University):** Water chemistry, pH control and particle formation process in an SCWR.
- **A. Anderson (St. Francis Xavier University):** Time-resolved investigations of metal oxide-water systems under conditions of extreme temperature, pressure and radiation.
- **P. Percival (Simon Fraser University), K. Ghandi (Mount Allison University**): Reaction kinetics in SCW probed using muonium.
- **J.-P. Jay-Gerin (U. of Sherbrooke):** Computational modelling of water radiolysis in high temperature water (including SCW).
- **C. Wren (U. of Western Ontario):** Water radiolysis effects on materials degradation in high temperature water (including SCW).

The chemistry program is co-ordinated by D. Guzonas (AECL).

3. Activities at the University of New Brunswick (UNB)

D. H. Lister

International Collaboration on "Improved Sample Technique"

The joint activity with Japan on sampling steam/water systems continued, despite the tragedy in Japan in early 2011 and the withdrawal of the University of Tokyo from the project. UNB took over the CFD simulation of the heat exchanger and sample line attached to their laboratory autoclave, and Dr. Uchida (JAEA) developed the mathematical model to describe the hold-up of corrosion products seen in the UNB experiments. Following the recommendations made at the 2011 meeting of the PCC Working Group in Plsen, several more experiments on sampling from high-temperature water containing iron corrosion products under different temperatures and pHs were undertaken. The CFD simulation was completed and compared with the measurements, and the mathematical model was developed and helped to explain the observations. Presentations on progress were made at this week's PCC meeting, and a final report has been prepared.

Complementary Sampling Experiments – Sampling from a Two-Phase Steam-Water System

In an experimental program looking at flow-accelerated corrosion (FAC) of carbon steel in two-phase steam-water mixtures, a sample system was installed in the high-temperature loop to draw fluid from the wall of a pipe and from the centre flow. Samples of ammoniated fluid taken at various sampling flow rates indicated the kinetics of distribution of the ammonia between liquid and vapour and allowed estimates to be made of the flow regime and the thickness of the liquid film at the wall – important parameters for understanding FAC. The work was described in presentations at this week's PCC meeting.

General Research on Chemistry and Corrosion in Power System Coolants

Research programs continue on the effects of amine additives on FAC in two-phase systems, on developing an in-plant monitor and modelling capabilities for FAC in fossil and nuclear power systems, on determining the kinetics of corrosion-product dissolution in coolant systems, and on the effects of additives on the fouling of heat exchangers in cooling water systems.

W. Cook

Dr. Cook maintains active research programs related to corrosion and chemistry control in nuclear power reactors and has been very active in the Generation IV International Forum (GIF) through the Canadian National Program. Dr. Cook participated in Phase I of the program and received funding for his Phase II proposal. A major focus is corrosion-product transport and deposition in the core of a SCWR; both experimental techniques and modeling are employed to elucidate material corrosion and the deposition kinetics of the "fall-out" from solution that occurs upon traversing the critical point. The fitting parameters for the R-HKF thermodynamic extrapolation model have been re-examined and applied in the temperature region around the pseudo-critical point. It is believed that electrostatic models such as the R-HKF are applicable in supercritical water (SCW) at moderate temperatures because of the clustering nature of SCW, particularly near a surface, which may allow electric double-layers to persist well beyond the critical transition.

Dr. Cook was on sabbatical leave from UNB, spending four months at Atomic Energy of Canada Limited (AECL) Chalk River Laboratories (CRL) followed by eight months as a technical advisor in the Chemistry Department at the Point Lepreau Nuclear Generation Station; this plant is now being re-started after a prolonged refurbishment outage. During his stay at CRL, he worked closely with Dr. D. Guzonas and the two produced a review article on the link between corrosion and chemistry in a SCWR ("Cycle chemistry and its effect on materials in a supercritical water-cooled reactor: A synthesis of current understanding", Corrosion Science, 2012).

4. Activities at AECL

Recent water chemistry work for the Canadian SCWR concept at AECL has focused on studying the relationship between corrosion in relatively high-density SCW (e.g., above the critical temperature at a pressure of 25 MPa) and in 'superheated steam' (e.g., low density SCW above the critical temperature but below the critical pressure). The important role played by the solubility of the corrosion films formed on alloy surfaces has been demonstrated in a series of corrosion tests at constant temperature and variable SCW density. With Prof. Cook (UNB), a phenomenological model of the change in corrosion mechanism from electrochemical oxidation in high density SCW to gas-phase (chemical) oxidation in low density SCW was developed. The ability of an alloy surface to impose a local structure on the surface that is different than that in the bulk is currently being studied using a combination of neutron scattering and molecular dynamics modeling.

5. Activities at the University of British Columbia

R. Pawlowicz

Activities related to the IAPWS subcommittee on seawater (SCSW):

- 1) Publication of a "history" of TEOS-10. This paper is meant to document the evolution of TEOS-10, and the interactions (both scientific and bureaucratic) between SCOR, IAPSO, IAPWS, and the researchers involved: Pawlowicz, McDougall, Feistel, and Tailleux, An historical perspective on the development of the Thermodynamic Equation of Seawater 2010, Ocean Sci., 8, 161-174, (2012)
- 2) Numerical modelling of electrical conductivity of seawater at high temperatures and salinities, resulting in a publication: Pawlowicz, The electrical conductivity of seawater at high temperatures and salinities, Desalination 300, 32-39 (2012)
- 3) Numerical modelling of electrical conductivity and density of low-salinity lake and river waters, with the aim of adapting TEOS-10 to those kinds of waters. Publication accepted: Pawlowicz and Feistel, Limnological applications of the Thermodynamic Equation of Seawater 2010 (TEOS-10), Limnology and Oceanography: Methods, in press (accepted June 2012)
- 4) Wrote a peer-reviewed pedagogical article on salinity and heat in the ocean: Pawlowicz, "Key Variables: Temperature, Salinity and Density", online in Physical Oceanography Topic Room, Nature Education Knowledge Project (accepted Aug 2012)
- 5) Began translation of some Chinese-language scientific articles on "Chinese Standard Seawater" the oceanographic conductivity reference material used in China, about which little is known in the west (with assistance of Chuning Wang, a new graduate student from China)
- 6) Developed proposal for 'Joint IAPWS/SCOR/IAPSO Committee on the Properties of Seawater', circulated to both SCOR, IAPSO, and the IAPWS SCSW.

REPORT

on IAPWS-related activities: August 2011 - August 2012

submitted by the

Czech National Committee for the Properties of Water and Steam (CZ NC PWS)

to the Executive Committee Meeting of 2012 IAPWS Meeting, Boulder, USA in September 2012

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Participating institutions

The following Czech Institutions have participated in the research of thermophysical properties and chemical processes between August 2011 and August 2012:

Institute of Thermomechanics AS CR, v. v. i., ("IT ASCR"), Department of Thermodynamics, Dolejškova 1402/5, CZ-182 00 Praha 8

Czech Technical University in Prague ("CTU"), Faculty of Mechanical Engineering, Department of Fluid Mechanics and Thermodynamics, and Department of Power Engineering, Technická 4, CZ-166 07 Praha

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

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

ŠKODA POWER, Plzeň, Inc., A Doosan Company, Tylova 57, CZ-316 00 Plzeň

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

SIGMA Research and Development Institute ("SIGMA"), Jana Sigmunda 79, CZ-783 50 Lutín















Funding

The activities described below were sponsored by the Grant Agency of the Academy of Sciences of the Czech Republic (GAAV ČR), the Czech Science Foundation (GAČR), ŠKODA POWER, Ministry of Education, Youth and Sport of the Czech Republic (MŠMT), and Ministry of Industry and Trade of the Czech Republic (MPO).











Board of CZ NC PWS for 2010-2013:

Dr. J. Hrubý Prof. R. Mareš Dr. T. Němec Prof. P. Šafařík Prof. J. Šedlbauer

List of IAPWS-Related Activities

The Czech Committee in collaboration with the University of West Bohemia organized the 2011 IAPWS Meeting in Plzeň (Pilsen). The Meeting was attended by 24 participants from the Czech Republic and they presented 12 papers [1-12].

Information about new documents adopted and authorized by IAPWS were published on the CZ NC PWS website.

The joint project of IT ASCR and UWB sponsored by the Ministry of Education, Youth and Sports of the Czech Republic provided financial support for international collaboration with IAPWS since 2009. The project support will end on 31/12/2012.

Dr. Hrubý (IT ASCR) and his collaborators studied thermodynamic properties of condensing steam flow, measured density of supercooled water at high pressures, and conducted research into thermodynamic modeling of hydrates of water–carbon dioxide mixtures [1, 8, 13-19].

Prof. Mareš (UWB) and his collaborators studied surface tension of water and other properties of water and steam [3, 20-24].

Prof. Mareš and Dr. Kalová (UWB) in collaboration with Prof. Anisimov (USA) studied thermophysical properties of supercooled water [2, 25-27].

Prof. Maršík (IT ASCR) and his research team studied problems of droplet nucleation in water and the influence of thermophysical properties of water on the efficiency of hydrogen fuel cells [6, 7, 28-30].

Prof. Šedlbauer (TUL) coordinated the IAPWS-IUPAC Joint Project entitled "Establishing recommended data on thermodynamic properties of hydration for selected organic solutes and gases" [4].

The research team at CTU continued to study wet steam energy losses in LP steam turbines (publications are in preparation).

Dr. Sedlář (SIGMA) studied the problems of bubble fission and cavitation instabilities in water turbines and pumps [31-32].

Dr. Jiříček (ICT-IE) and his collaborators studied the problem of renewable power sources and chemical effects in water and steam systems of power plants [33-35].

Dr. Hnědkovský (ICT-IPC) and his collaborators studied the properties of organic solutes in water [36-49].

Prof. Šťastný (ŠKODA POWER) and his co-workers tested and applied a numerical model of steam flow in nozzles and turbine blade cascades with NaCl binary nucleation and condensation [4, 50, 51].

IAPWS Young Scientist Fellowships

In 2011, **Dr. Vinš** completed his IAPWS Young Scientist Fellowship Project (exchange between the Czech Republic and Germany) entitled "Development of Thermodynamic Models for Hydrates in Water – Carbon Dioxide Mixtures" jointly supervised by Dr. Hrubý and Prof. Span. The preliminary results were presented and discussed during the 2011 IAPWS Meeting in Plzeň [8]. The final Project Report will be presented during the 2012 IAPWS Meeting in Boulder. Five papers and presentations were published [15-19].

Dr. Holten is currently completing his IAPWS Young Scientist Fellowship Project (exchange between the Czech Republic and USA) entitled "Towards an IAPWS Guideline for the Thermodynamic Properties of Supercooled Water" jointly supervised by Dr. Hrubý, Prof. Anisimov, and Dr. Sengers. The preliminary results will be presented during the IAPWS Meeting 2012 in Boulder. One journal paper was published [25].

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- 5) Stastny, M. Sejna, M.: Effects of Expansion Rate on Binary Condensation of NaCl and Steam Flowing in a Turbine.

- 6) Marsik, F.: Formulation of Aims of WG PCAS for next Years "Application of Physical Properties of Water in technology of Classical and Hydrogen Power Engineering". (A discussion contribution).
- 7) Marsik, F.: Closing Document of the ICRN #10 "pH Measurements and Potentiometric Studies of Supercritical Aqueous Solutions". (Discusion, preparation and formulation of a final statement).
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- 9) Nezbeda, I.: From Ice to Steam and Aqueous Solutions with a Non-Speculative Molecular Model. (A contribution at the 2011 IAPWS Meeting Symposium).
- 10) Prchlik, L.: Large Steam Turbines for Elevated Steam Parameters and Implications for Construction Material Used. (A contribution at the 2011 IAPWS Meeting Symposium).
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- 12) Kysela, J.: Experimental Water Chemistry Research for Boiling and Supersritical Water Cooled Reactor. (A contribution at the 2011 IAPWS Meeting Symposium).
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German National Committee to IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam Report "Research in Progress 2012"

Baltic Sea Research Institute, Warnemuende Dr. Rainer Feistel

Book Publication

Feistel, R., Ebeling, W. (2011): Physics of Self-Organization and Evolution. Wiley-VCH, Weinheim, 517 pp.

Articles

Pawlowicz, R., McDougall, T., Feistel, R., Tailleux, R. (2012):

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New Equations for the Sublimation Pressure and Melting Pressure of H₂O Ice Ih. Journal of Physical and Chemical Reference Data, 40, 043103; doi:10.1063/1.3657937 (11 pages)

Leibniz Institute for Tropospheric Research, Leipzig Dr. Olaf Hellmuth

Recent Publications

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In: C. Bernhofer, J. Schanze and J. Seegert: A Textbook on Integrated Flood Risk Management, Springer-Verlag, Berlin (submitted and accepted in 2011).

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JINR Dubna, 483 pp., ISBN 978-5-9539-0301-8, http://theor.jinr.ru/meetings/2012/nta/

Hellmuth, O., Khvorostyanov, V. I., Curry, J. A., Shchekin, A.K., Schmelzer, J. W. P., Feistel. R., Djikaev, Y., Baidakov V. G. (2012):

Theoretical Aspects of Atmospheric Ice Formation. In: J. W. P. Schmelzer (eds.): Nucleation Theory and Applications. Special Issues.

Review Series on Selected Topics of Atmospheric Sol Formation, Volume 5, JINR Dubna (textbook, in press).

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Prof. Dr. Hans-Joachim Kretzschmar

Projects

- 1. Development of Fast Property Algorithms Based on Spline Interpolation
 - The algorithms for fast spline-interpolation methods was developed and applied to the calculation of thermodynamic properties of water and steam in CFD and non-stationary calculations.
 - An algorithm for generating spline-interpolation data grids with optimized data density for the user requirements 'range of state' and 'accuracy' was developed.
- 2. Stoffwerte für Wasser und Wasserdampf (Steam Tables for Water and Steam), VDI Wärme Atlas 2012

Section D2.1 "Stoffwerte für Wasser und Wasserdampf" (Properties of Water and Steam) of the VDI-Wärme Atlas 2012 (VDI-Heat Atlas), 11th German Edition, is being worked on. The reference for this publication will read: *Wagner, W. and Kretzschmar, H.-J.*, Stoffwerte von Wasser und Wasserdampf, VDI-Wärmeatlas, 11. Auflage, Abschnitt D2.1, pp. 1-15, Springer-Verlag, Berlin. Status: The proofs are being checked.

- 3. Property Libraries for Calculating Heat Cycles
 - The property library LibIF97 for steam and water has been extended to ice properties including sublimation and melting pressures.
 - The property libraries for steam, water, ice, seawater, humid combustion gases, humid air, ammonia/water mixtures and water/lithium bromide mixtures have been connected to LabVIEW.
 - An Online Property Calculator for calculating thermodynamic and transport properties for steam, water and other working fluids in power engineering was installed on the website www.thermodynamics-zittau.com.
 - A steam tables App for iPhone, iPad, and iPod touch has been developed.
 - A student version of the steam tables program FluidLAB for MATLAB was prepared and its link installed on the IAPWS Website www.iapws.org under "Education".

Recent Publications

Kretzschmar, H.-J., Kraft, I.:

Kleine Formelsammlung Technische Thermodynamik, 4. Auflage.

Carl Hanser Verlag, München (2011)

Kretzschmar, H.-J.:

Bereitstellung von thermodynamischen Stoffdaten für Arbeitsfluide der Energietechnik.

In: Aktuelle Beiträge zur Technischen Thermodynamik, Energietechnik und

Fernwärmeversorgung,

Verlag AGFW, Frankfurt am Main (2011)

Herrmann, S.; Kretzschmar, H.-J.; Gattley, D. P.:

Berechnung der thermodynamischen Eigenschaften von feuchter Luft.

KI - Kälte Luft Klimatechnik, 48 (2012) S. 22-28

Kunick, M; Kretzschmar, H.-J.; Gampe, U.:

Schnelle und flexible Berechnung thermodynamischer Stoffwerte mit Spline-Interpolation für die Modellierung instationärer Energieumwandlungsprozesse.

In: W. Honekamp, P. Schindler, Tagungsband der 13. Nachwuchswissenschaftlerkonferenz mitteldeutscher Fachhochschulen Görlitz, S.209-214, Re Di Roma-Verlag, Remscheid (2012), ISBN 978-3-86870-436-5

Kretzschmar, H.-J., Stöcker, I.:

Mollier h,s-Diagramm von Wasserdampf (*Mollier h-s* Diagram for Steam). Siemens Energy, Erlangen (2012)

Ruhr University Bochum, Faculty of Mechanical Engineering, Department of Thermodynamics Prof. Dr. Roland Span

Projects

The group chaired by Prof. Span has actively been involved in a number of research projects related to CO₂-rich mixtures as they are typical for power generation with carbon capture and storage (CCS). On its 2011 meeting IAPWS has encouraged this kind of work under ICRN 27, *Thermodynamic Properties of Humid Gases and CO₂-Rich Mixtures*. The work of Prof. Span primarily addresses the

- improvement of the experimental data base available for CCS-relevant mixtures. As part of this activity co-operations with colleagues at the University of Valladolit and at SINTEF in Trondheim were established.
- improvement of accurate models available for CCS-relevant mixtures. Main foci of this work have been the development of improved mixing models and a consistent description of complex phase equilibria, including the formation of hydrates and other solid phases. This work is linked to close co-operations with the group of Dr. J. Hruby at the Czech Academy of Sciences (Hruby and Vins, see separate report presented by Dr. Vins) and with Dr. E. W. Lemmon at NIST in Boulder.
- application of accurate property models in process simulation. The relevance of the accuracy
 of property models could be shown both for the processes of the LNG product-chain and for
 CCS-applications.

Many aspects of the work on CCS-relevant mixtures are closely related to work on properties of natural gases, particularly in conjunction with LNG processing. However, this work is not considered within the scope of IAPWS.

Journal Articles and Proceedings

F. Dauber, J. Gernert, R. Span and P. Schley:

On the Use of Highly Accurate Thermodynamic Property Models in Process Simulation.

Proceedings International Gas Union Research Conference - IGRC, Seoul (2011).

R. Span:

Kraftwerkstechnik mit CO₂-Rückhaltung – Anforderungen an Stoffdatenmodelle.

In: Nordrhein-Westfälische Akademie der Wissenschaften und Künste, Ferdinand Schöningh Verlag, Paderborn, ISBN 978-3-506-77367-8 (2011).

M. E Mondéjar, M. C. Martín, R. Span and C. R. Chamorro:

New (p,ρ,T) data for carbon dioxide - nitrogen mixtures from 250 K to 400 K at pressures up to 20 MPa.

J. Chem. Thermodynamics 43, 1950–1953 (2011).

M. E Mondéjar, M. C. Martín, R. Span and C. R. Chamorro:

 (p,ρ,T) behavior of two mixtures of carbon monoxide with nitrogen in the temperature range from 250 K to 400 K and pressures up to 20 MPa.

J. Chem. Eng. Data 56, 3933–3939 (2011).

V. Vins, A. Jäger, J. Hrubý and R. Span:

Phase equilibria of carbon dioxide and methane gas-hydrates predicted with the modified analytical S-L-V equation of state.

Proc. Experimental Fluid Mechanics, Czech Republic (2011).

M. E. Mondéjar, R. M. Villamañán, R. Span, and C. R. Chamorro:

Accurate (p,p,T) data for two new (carbon dioxide+nitrogen) mixtures from (250 to 400)K at pressures up to 20MPa.

J. Chem. Thermodyn. 48, 254–259 (2012)

A. Jäger and R. Span:

Equation of state for solid carbon dioxide based on the Gibbs free enthalpy.

J. Chem. Eng. Data 57, 590-597 (2012)

Ruhr University Bochum, Faculty of Mechanical Engineering, Department of Thermodynamics

Prof. em. Dr. Wolfgang Wagner

Projects

1. Stoffwerte für Wasser und Wasserdampf (Steam Tables for Water and Steam), VDI Wärme Atlas 2012

Section D2.1 "Stoffwerte für Wasser und Wasserdampf" (Properties of Water and Steam) of the VDI-Wärme Atlas 2012 (VDI-Heat Atlas), 11th German Edition, is being worked on. The corresponding steam tables are calculated based on the Industrial Formulation IAPWS-IF97 and the current equations for the transport properties and other properties based on the

- corresponding IAPWS Releases. The reference for this publication will read: *Wagner, W. and Kretzschmar, H.-J.*, Stoffwerte von Wasser und Wasserdampf, VDI-Wärmeatlas, 11. Auflage, Abschnitt D2.1, pp. 1-15, Springer-Verlag, Berlin. Status: The proofs are being checked.
- 2. The behavior of the IAPWS-95 Formulation in the liquid region of water near the melting line at high pressures was investigated. A corresponding report on this matter will be presented on the IAPWS Meeting in Boulder 2012 in the Session of the IAPWS Working Group "Thermophysical Properties of Water and Steam" (TPWS).

Recent Publications

Wagner, W., Riethmann, T., Feistel, R., Harvey, A. H.:
 New equations for the melting pressure and sublimation pressure of H₂O ice Ih.
 J. Phys. Chem. Ref. Data 40 (2011), 043103-1 - 043103-11 (online publication 05.12.2011).

Current Status of Research Activities in Japan

Submitted to the Executive Committee Meeting, IAPWS, Bolder, Colorado, USA, September 2012

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- 42. P. Gotovcev, Khizova E. I. Utilization of thermal power plant waste water. Radioelectronics, electrical and power engineering. Seventeenth International Conference of students and post-graduate students. Proceedings. Vol. 3. Moscow. MPEI, 2011.
- 43. P. Gotovcev, Kartsev A.S., Khizova E. I. Mathematical modeling of Water Chemistry Control Systems at Thermal Power Plants. The 4th IWA ASPIRE Conference and Exhibition. 2-6 October 2011 Tokyo Japan. Abstracts p. 179.
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U.S. National Committee to IAPWS 2012 Report on Activities of Potential Interest to IAPWS

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

In collaboration with researchers in Greece and Germany and at the University of Maryland, a new formulation has been developed for the thermal conductivity of water and steam. The complete correlation, which covers a wider range of conditions than the previous formulation and is consistent with IAPWS-95 and the new IAPWS viscosity correlation, has now been adopted by IAPWS and has been published.

<u>Reference</u>: M.L. Huber, R.A. Perkins, D.G. Friend, J.V. Sengers, M.J. Assael, I.N. Metaxa, K. Miyagawa, R. Hellmann, and E. Vogel, New International Formulation for the Thermal Conductivity of H₂O, *J. Phys. Chem. Ref. Data* **41**, 033102 (2012).

In a collaboration with the Kazan State Technological University (Russia) and the Dagestan Scientific Center of the Russian Academy of Sciences (as part of an IAPWS Collaborative Project), the thermal conductivity of binary ammonia+water mixtures was measured over the temperature range from 278 K to 356 K and at pressures up to 20 MPa using the steady-state hot-wire method. Measurements were made for eight compositions over the entire concentration range. Temperature, pressure, density, and concentration dependences of the thermal conductivity of the mixture were studied. Various types of wide-ranging correlation models for the thermal conductivity of these mixtures were also developed using the measured data.

In NIST's Sensor Science Division (Gaithersburg, MD), a gravimetric apparatus has been constructed for measuring the saturation concentration of water as a function of temperature and pressure in compressed gaseous carbon dioxide (equivalent to a dew-point measurement) at pressures up to 6 MPa and temperatures up to 85 °C. Preliminary results with air (which has been studied previously in other apparatus) validate the reliability of the apparatus, and experiments with CO₂ are currently underway.

In collaboration with NIST's Sensor Science Division, a combined experimental and theoretical study was performed of the effect of atmospheric pressure on the ice point of water, which is used in thermometry. Experiment and theory agreed, confirming results for the sea-level ice point dating to the mid-1900s and for the first time providing a validated method for adjusting the ice point for work at higher elevations.

<u>Reference</u>: A.H. Harvey, M.O. McLinden, and W.L. Tew, Thermodynamic Analysis and Experimental Study of the Effect of Atmospheric Pressure on the Ice Point, *Proceedings of the 9th International Temperature Symposium*, in press (2012).

In NIST's Chemical and Biochemical Reference Data Division (Gaithersburg, MD), the vapor pressure of ice has been measured over the temperature range 173 K to 273 K using cavity ring-down spectroscopy to probe the output of a humidity generator which contains isothermal samples of ice in a nitrogen atmosphere. The measurement is relative to the known triple-point pressure, and is corrected for the enhancement factor. Preliminary analysis indicates good agreement with the new IAPWS formulation for the sublimation pressure.

<u>Reference</u>: K. Bielska, D.K. Havey, G.E. Scace, D. Lisak, and J.T. Hodges, Spectroscopic Measurement of the Vapour Pressure of Ice, *Phil. Trans. Royal Soc. A* **370**, 2509 (2012).

Communicated from the University of Maryland

The research on the thermodynamic behavior of supercooled water was continued, yielding the following publications (supported in part by IAPWS):

- 1. V. Holten, C.E. Bertrand, M.A. Anisimov, and J.V. Sengers, "Thermodynamics of supercooled water, J. Chem. Phys. **136**, 0945507 (2012).
- 2. V. Holten, J. Kalová, M.A. Anisimov, and J.V. Sengers, "Thermodynamics of liquid-liquid criticality in supercooled water in a mean-field approximation", Int. J. Thermophys. **33**, 758-773 (2012).

In addition, a new updated equation was developed for the critical locus of aqueous solutions of NaCl:

3. D.A. Fuentevilla, J.V. Sengers, and M.A. Anisimov, "Critical locus of aqueous solutions of sodium chloride revisited", Int. J. Thermophys. **33**, 943-958 (2012).

A draft of a new guideline on the critical locus of aqueous solutions was prepared for IAPWS.

Communicated from Andre Anderko, OLI Systems

In 2011-2012, the work at OLI Systems was focused on the following projects:

- (1) A previously developed comprehensive model for thermal conductivity of electrolyte solutions has been revised by using the new IAPWS formulation for the thermal conductivity of pure water. The application of this model to seawater has been explored in detail and the results have been published. In the near future, we are planning to create an IAPWS guideline for the thermal conductivity of seawater based on this model.
 - <u>Reference:</u> P. Wang and A. Anderko, "Modeling Thermal Conductivity of Electrolyte Mixtures in Wide Temperature and Pressure Ranges: Seawater and Its Main Components", *Int. J. Thermophysics*, 33 (2012) 235-258.
- (2) In collaboration with the Pacific Northwest National Laboratory, work was continued on modeling the behavior of systems containing carbon dioxide, water, and various salts. This work encompasses the behavior of both water-rich and CO₂-rich phases. Also, implications for mineral reaction equilibria have been explored.
 - <u>Reference</u>: R.D. Springer, Z. Wang, A. Anderko, P. Wang, and A.R. Felmy, "A Thermodynamic Model for Predicting Mineral Reactivity in Supercritical Carbon Dioxide: I. Phase Behavior of Carbon Dioxide Water Chloride Salt Systems Across the H₂O-Rich to the CO₂-Rich Regions", *Chemical Geology*, 322-323 (2012) 151-171.
- (3) A comprehensive model has been developed for predicting the phase equilibria of selected actinides (i.e., U, Pu, and Am) in aqueous systems. This includes the behavior of oxides and hydroxides in wide ranges of temperature, pH, and salinity and the behavior of actinides in concentrated acid solutions.
- (4) An electrochemical model has been developed for predicting general and localized corrosion of the copper-nickel alloy CuNi7030. This work extends our previous work on the corrosion behavior of copper-nickel alloys.
- (5) Work was continued on developing a model for predicting interfacial tension.

List of Participants

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